

## Appendix from C. G. Jäger et al., ‘Physical Determinants of Phytoplankton Production, Algal Stoichiometry, and Vertical Nutrient Fluxes’

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### Technical Details of the Numerical Approach and Additional Results

#### Technical Details of the Numerical Approach and Boundary Conditions

The equations were solved by means of a finite-element method. This type of method provides not only solutions at discrete points, as, for example, finite-difference methods do, but it also provides functions that describe the solution throughout the computational domain. Subsequently, the finite-element method allows for the characterization of the quality of the solution in a strictly mathematical manner everywhere in the domain. Consequently, possible oscillations of the solution in space are reliably detected at run time. Unlike finite-volume methods, which are usually tailored to solve a particular system of equations, the general theory of finite-element methods is restricted neither to a certain system of equations nor even to a certain class of differential equations.

For the spatial discretization, standard second-order Lagrange elements were used, for which the solutions are described by quadratic functions with at least a continuous first derivative. The time discretization was performed with a fully implicit backward-Euler scheme of the first order; that is, every time the unknowns for a certain time step were computed, all dependencies were resolved and, apart from the time derivative, no values of previous time steps had any direct influence on the newly computed solution. Compared with explicit schemes, the use of implicit schemes practically imposed only weak limitation on time step width. We performed the simulations with the finite-element software package COMSOL, version 3.2.

In detail, the model was implemented with two one-dimensional compartments: a water column and a sediment layer. The water column runs from the surface ( $z = 0$ ) to the bottom ( $z = z_{\max}$ ). Within the water column, we calculated algal carbon biomass ( $A$ ), particulate nutrients bound in algae ( $R_b$ ), dissolved mineral nutrients ( $R_d$ ), and light intensity ( $I$ ).  $A$ ,  $R_b$ , and  $R_d$  were calculated with equations (1)–(3). Using equation (4) to compute light intensity requires that algal biomass already be known. Because algal biomass is, in turn, dependent on light intensity, either an iteration between equation (4) and equations (1)–(3) is necessary or values of  $I$  for the previous time step must be used in an explicit manner to solve equations (1)–(3). To avoid this problem, we calculated light intensity as

$$0 = -(kA + k_{bg})I + \frac{\partial I}{\partial z}. \quad (\text{A1})$$

This formulation, which is alternative but equivalent to equation (4), links the computation of  $I$  to the remaining system of equations and can be easily implemented in COMSOL. The boundary condition was assumed to be a fixed light intensity at the surface ( $I_0$ ).

The pool of sedimented nutrients was calculated within the sediment layer only. The pool of sedimented nutrients has no extension in the  $Z$ -direction in the model. We modeled it, however, as a (fictitious) sediment compartment that must have a finite extension in the  $Z$ -direction in order to be linked to the computation of the equations in the water column compartment. To do so, the ordinary differential equation (eq. [5]) describing the rate of change of nutrients per area  $R_s$  was transformed into a partial differential equation that calculates the concentration of nutrients  $R_{s\ conc}$  in the sediment compartment as

$$\frac{\partial R_{s\ conc}}{\partial t} = d_s \frac{\partial^2 R_{s\ conc}}{\partial z^2}. \quad (\text{A2})$$

The thickness of the sediment compartment was arbitrarily chosen to be 1 m, technically simplifying the conversion of the pool of nutrients, where the concentration of nutrients in the sediment  $R_{s\ conc}$  (in mg P m<sup>-3</sup>) is equal to the areal pool of sedimented nutrients  $R_s$  (in mg P m<sup>-2</sup>). This approach does not influence the results as long as there are no vertical gradients within this compartment. This was guaranteed by assuming (hypothetical) fast mixing inside the sediment compartment with a turbulent-diffusion coefficient  $d_s$  of 1,000 m<sup>2</sup> day<sup>-1</sup>. Changes of  $R_{s\ conc}$  were implemented by boundary fluxes over the sediment-water interface, with an influx of sedimented particulate nutrients and an outflux of remineralized nutrients (i.e.,  $vR_b(z_{max}) - rR_{s\ conc}$ ; table A1).

The use of equation (A2) has two advantages. First, it was not necessary to use dissolved and particulate nutrients of previous time steps in an explicit manner (see the calculation of the light intensity). Second, the mass balance of total nutrients (integrated dissolved nutrients + integrated particulate nutrients) could be used to check for potential computational errors. Additional analyses confirmed that these calculations indeed gave close to identical results when compared with calculations where the pool of sedimented nutrients was calculated with an algebraic equation using the mass balance. The results were also very similar to the results of an ordinary differential equation system modeling the special case of a completely mixed water column (see Diehl et al. 2005).

**Table A1**

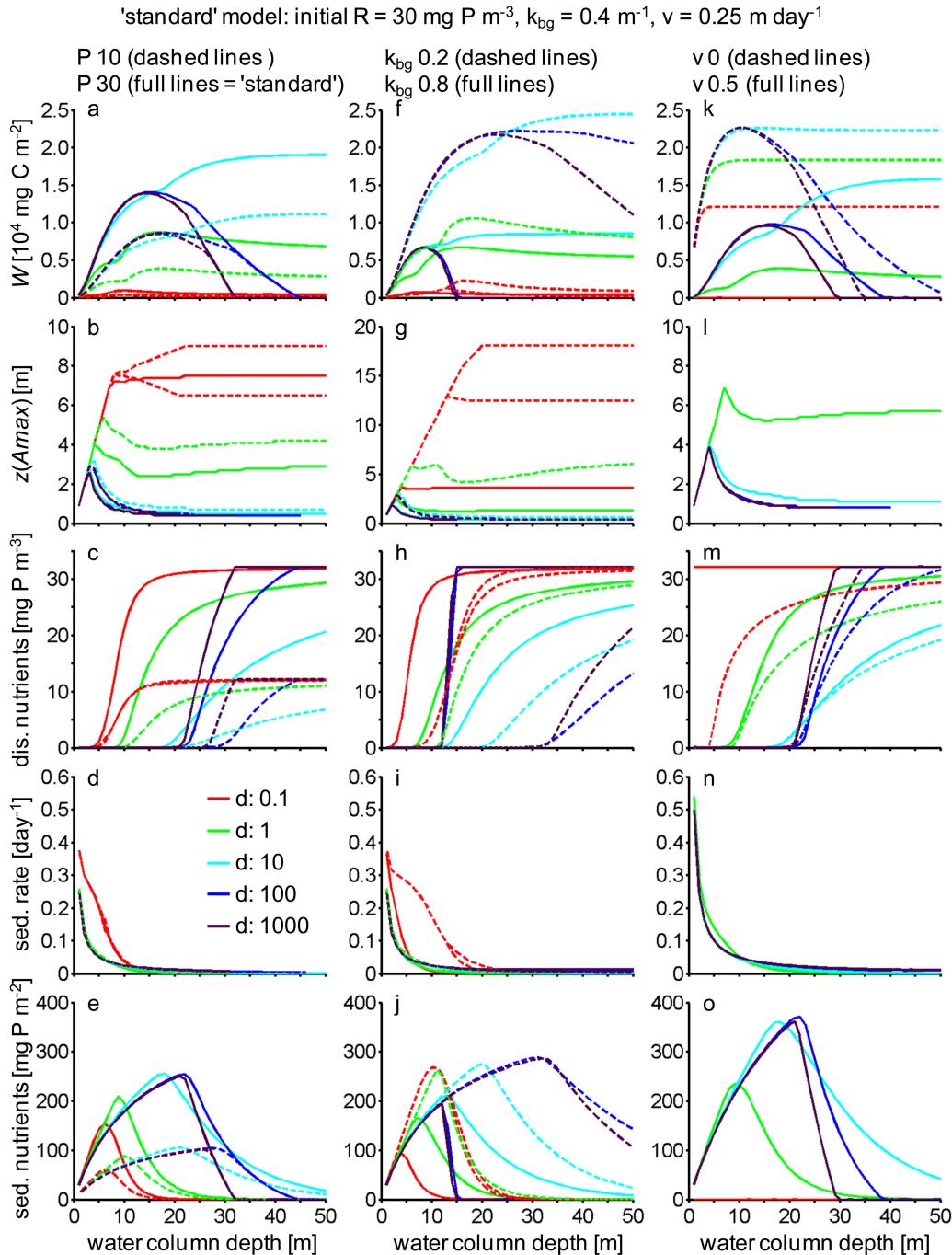
Boundary conditions for algal biomass ( $A$ ), particulate nutrients ( $R_b$ ), dissolved nutrients ( $R_d$ ), light intensity ( $I$ ), and the concentration of sedimented nutrients ( $R_{s\ conc}$ ) at the water surface, at the interface between the water column and the sediment, and at the bottom of the sediment layer

State variable	Layer		
	Water surface	Sediment	Bottom of sediment
$A$	$vA - d(\partial A / \partial z) = 0$		$\partial R_d / \partial z = 0$
$R_b$	$vR_b - d(\partial R_b / \partial z) = 0$		$\partial R_b / \partial z = 0$
$R_d$		$rR_s - d(\partial R_d / \partial z) = 0; a(R_h - R_d) - d(\partial R_d / \partial z) = 0^a$	
$I$	$I = I_0$		
$R_{s\ conc}$		$-vR_b + rR_{s\ conc} - 1,000(\partial R_{s\ conc} / \partial z) = 0$	$\partial R_{s\ conc} / \partial z = 0$

**Note:** For the open model, which has no sediment, boundary conditions at the sediment layer apply to the interface between the water column and a deep water layer. At the water surface, depth  $z = 0$ ; at the interface between the water column and the sediment,  $z = z_{max}$ ; and at the bottom of the sediment layer,  $z = z_{max} + 1$  m.

<sup>a</sup> Boundary condition in the open model.

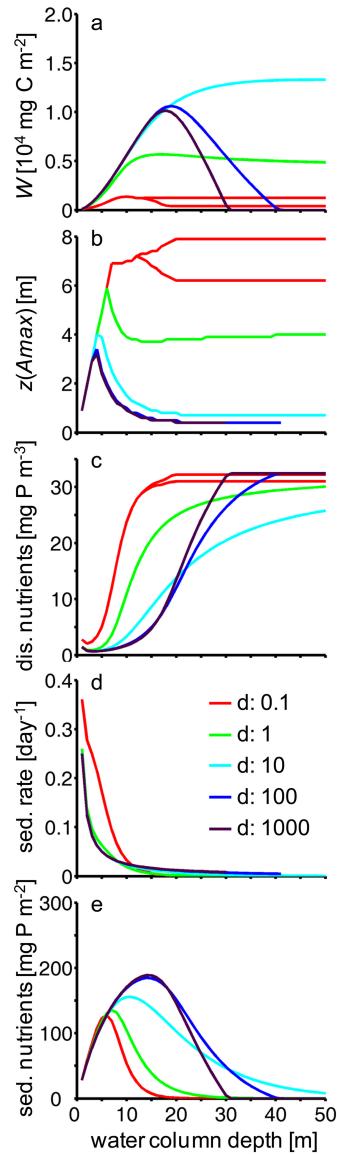
## Standard Model: Influence of Total Nutrient Content, Background Turbidity, and Algal Sinking Velocity on Equilibrium Properties



**Figure A1:** Effects of water column depth and mixing intensity (indicated by the coefficient of turbulent diffusion  $d$ ) on equilibrium values of the standing stock of algal biomass integrated over the water column (a, f, k), the depth at which the vertical algal biomass profile has its maximum (b, g, l), the depth-averaged concentration of dissolved nutrients (c, h, m), the algal sedimentation rate (d, i, n), and the pool of nutrients in the sediment layer (e, j, o). The left column (a–e) is the comparison of different initial dissolved-nutrient

concentrations (*dashed lines*: initial concentration =  $10 \text{ mg P m}^{-3}$ , *solid lines*: initial concentration =  $30 \text{ mg P m}^{-3}$ ; background turbidity  $k_{\text{bg}} = 0.4 \text{ m}^{-1}$  and sinking velocity  $v = 0.25 \text{ m day}^{-1}$  in both cases). The central column (*f-j*) is the comparison of different background turbidities (*dashed lines*:  $k_{\text{bg}} = 0.2 \text{ m}^{-1}$ , *solid lines*:  $k_{\text{bg}} = 0.8 \text{ m}^{-1}$ ; initial dissolved-nutrient concentration  $R_d = 30 \text{ mg P m}^{-3}$  and sinking velocity  $v = 0.25 \text{ m day}^{-1}$  in both cases). The right column (*k-o*) is the comparison of different algal sinking velocities (*dashed lines*:  $v = 0 \text{ m day}^{-1}$ , *solid lines*:  $v = 0.5 \text{ m day}^{-1}$ ; background turbidity  $k_{\text{bg}} = 0.4 \text{ m}^{-1}$ , initial dissolved-nutrient concentration  $R_d = 30 \text{ mg P m}^{-3}$  in both cases). At an algal sinking velocity of  $v = 0$ , the depth at which the vertical algal biomass profile has its maximum is 0 m (i.e., the surface) and the algal sedimentation rate and the pool of nutrients in the sediment are both 0. At an algal sinking velocity of  $v = 0.5 \text{ m day}^{-1}$ , no algal population can persist in the water column at a coefficient of turbulent diffusion  $d = 0.1 \text{ m}^2 \text{ day}^{-1}$ . At a low initial dissolved-nutrient concentration ( $10 \text{ mg P L}^{-1}$  in *a-e*) and at a low background turbidity ( $k_{\text{bg}} = 0.2 \text{ m}^{-1}$  in *f-j*), the system oscillates at a coefficient of turbulent diffusion  $d = 0.1 \text{ m}^2 \text{ day}^{-1}$ ; in these cases, upper and lower bounds are shown by branching lines. Note the different scale in *g*.

## Fixed-Stoichiometry Model: Influence of Water Column Depth and Turbulence on Equilibrium Properties



**Figure A2:** Effects of water column depth and mixing intensity (indicated by the coefficient of turbulent diffusion  $d$ ) on equilibrium values of (a) the standing stock of algal biomass integrated over the water column, (b) the depth at which the vertical algal biomass profile has its maximum, (c) the depth-averaged concentration of dissolved nutrients, (d) the algal sedimentation rate, and (e) the pool of nutrients in the sediment layer in the fixed-stoichiometry model (with  $q_{\text{fix}} = 0.0244$ ). The system oscillates at a coefficient of turbulent diffusion  $d$  of  $0.1 \text{ m}^2 \text{ day}^{-1}$ ; in these cases, upper and lower bounds are shown by branching lines.