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Modeling cyanobacteria life cycle dynamics and historical nitrogen fixation in the Baltic Proper

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Table S1

A list of the cyanobacteria life cycle model variables. Note the different units of pelagic and benthic variables.

State variables*	Description	Units
HET	Vegetative cells with heterocysts, cyanobacteria N-fixing stage.	mmol N m^{-3}
AKIW	Akinetes, cyanobacteria resting stage in the water column	mmol N m^{-3}
REC	Recruiting cells with gas vesicles, cyanobacteria non-N-fixing stage	mmol N m^{-3}
AKIB	Akinetes, cyanobacteria resting stage in the sediment	mmol N m^{-2}
NO3	Nitrate	mmol NO3-N m^{-3}
PO4	Phosphate	mmol PO4-P m^{-3}
DETP	Phosphorus detritus (dead organic matter)	mmol DET-P m^{-3}
TEM	Temperature	°C
SAL	Salinity	g kg^{-1}
IZ	Photosynthetically active radiation (at depth Z)	W m^{-2}
τ	Bottom shear stress	N m^{-2}
AREA	Horizontal area of a grid cell	m^2
VOLUME	Volume of a grid cell	m^3

**) Only variables relevant for the present description of the cyanobacteria life cycle model are shown in this Appendix. See Eilola at el. (2009) and Almroth-Rosell et al. (2011) for a comprehensive list of biogeochemical variables in SCOBI and Hense and Beckmann (2006; 2010) for a more detailed description of the cyanobacteria life cycle components.*

Table S2

The source terms describing the change in time for each variable of the life cycle model equations are described and valid for each discrete depth layer in the model. Mass conservation checks may constrain the numerical solutions in SCOBI. The uptake of nutrients as well as the mass content of carbon, nitrogen and phosphorus in the live and dead HET, REC, AKIW and AKIB follows the standard Redfield ratio molecular stoichiometry of phytoplankton C:N:P=106:16:1.

Mathematical formulation

$$S_{HET} = GROWTH_{HET} + REC2HET + RISEI_{HET} - RISEO_{HET} - HET2AKIW - MORT_{HET}$$

$$S_{REC} = GROWTH_{REC} + AKIW2REC + BOT \bullet AKIB2REC + RISEI_{REC} - RISEO_{REC} - REC2HET - MO$$

$$S_{AKIW} = HET2AKIW + SINKI_{AKIW} + BOT \bullet RESUSP_{AKIB} - SINKO_{AKIW} - AKIW2REC$$

$$S_{AKIB} = SINKI_{AKIB} - AKIB2REC - BUR_{AKIB} - RESUSP_{AKIB}$$

The ratio $BOT = \frac{BOTTOMAREA}{VOLUME}$ *between sediment area and the volume of water in the overlying cell is used for the transfer of mass fluxes from the sediment to the water column.*

Table S3

Mathematical formulation of sources and sinks

$$GROWTH_{HET} = DIP_{GROWTH_{HET}} + DETP_{GROWTH_{HET}} \quad (1)$$

$$DIP_{GROWTH_{HET}} = DIPLIM_{HET} \bullet GR_{HET} \bullet HET \quad (2)$$

$$DETP_{GROWTH_{HET}} = DETPLIM_{HET} \bullet \left(1 - DIPLIM_{HET}\right) \bullet GR_{HET} \bullet HET \quad (3)$$ Table

$$DIPLIM_{HET} = \frac{PO4}{KDIP+PO4} \quad (4)$$

$$DETPLIM_{HET} = \frac{DETP}{KDOP+DETP} \quad (5)$$

$$GR_{HET} = SLIM_{HET} \bullet TLIM_{HET} \bullet LTLIM_{HET} \bullet GRMAX_{HET} \quad (6)$$

$$SLIM_{HET} = 1.0 if (3 < SAl \leq 10); else = 0.0 \quad (7)$$

$$TLIM_{HET} = \frac{1}{45.0} + exp\left\{-\left(\frac{(TEM-27.5)}{(4.0-sign\{9,TEM-27.5\})}\right)^{4}\right\}, \quad (8)^{*}$$

where *sign*{9,TEM-27.5}=9 if TEM⩾27.5; else *sign*{9,TEM-27.5}=-9

$$LTLIM_{HET} = \frac{PI_{SLOPE} \bullet IZ}{\sqrt{\left(GRMAX_{HET} \bullet TLIM_{HET}\right)^{2} + \left(PI_{SLOPE} \bullet IZ\right)^{2}}} \quad (9)^{**}$$

$$GRMAX_{HET} = 2.78 \times 10^{-6}$$

$$PI_{SLOPE} = 4.63 \times 10^{-7}$$

$$REC2HET = 1.16 \times 10^{-5} \bullet REC \; if \; GROWTH_{REC} < GROWTH_{HET}; else = 0.0 \quad (10)$$

$$HET2AKIW = 4.63 \times 10^{-5} \bullet TLIM_{HET} \bullet HET \; if \; IZ > 0.0 \quad (11)$$

$$and \; GROWTH_{HET} < GCRIT_{HET}; else = 0$$

$$GCRIT_{HET} = 3.5 \bullet GROWTH_{REC} \quad (12)$$

$$MORT_{HET} = 1.16 \times 10^{-7} \bullet HET \quad (13)$$

$$RISEI_{HET} = WR_{HET} \bullet HET_{BELOW} \quad (14)$$

$$RISEO_{HET} = WR_{HET} \bullet HET \quad (15)$$

$$WR_{HET} = 1.16 \times 10^{-6}$$

$$GROWTH_{REC} = min\left(NGROWTH_{REC}, PGROWTH_{REC}\right) \quad (16)$$

$$NGROWTH_{REC} = NLIM_{REC} \bullet GR_{REC} \bullet REC \quad (17)$$

$$PGROWTH_{REC} = DIP_{GROWTH_{REC}} + DETP_{GROWTH_{REC}} \quad (18)$$

$$DIP_{GROWTH_{REC}} = DIPLIM_{REC} \bullet GR_{REC} \bullet REC \quad (19)$$

$$DETP_{GROWTH_{REC}} = DETPLIM_{REC} \bullet \left(1 - DIPLIM_{REC}\right) \bullet GR_{REC} \bullet REC \quad (20)$$

$$NLIM_{REC} = \frac{NO3}{0.3+NO3} \quad (21)$$

$$DIPLIM_{REC} = \frac{PO4}{KDIP+PO4} \quad (22)$$

$$DETPLIM_{REC} = \frac{DETP}{KDOP+DETP} \quad (23)$$

$$GR_{REC} = SLIM_{REC} \bullet TLIM_{REC} \bullet LTLIM_{REC} \bullet GRMAX_{REC} \quad (24)$$

$$SLIM_{REC} = SLIM_{HET} \quad (25)$$

$$TLIM_{REC} = TLIM_{HET} \quad (26)$$

$$LTLIM_{REC} = \frac{PI_{SLOPE} \bullet IZ}{\sqrt{\left(GRMAX_{REC} \bullet TLIM_{REC}\right)^2 + \left(PI_{SLOPE} \bullet IZ\right)^2}} \quad (27)^{**}$$

$$GRMAX_{REC} = 8.33 \times 10^{-6}$$

$$AKIW2REC = 1.16 \times 10^{-5} \bullet SLIM_{REC} \bullet GERMINATE_{AKI} \bullet AKIW \quad (28)$$

$$AKIB2REC = 1.16 \times 10^{-5} \bullet SLIM_{REC} \bullet GERMINATE_{AKI} \bullet AKIB \quad (29)$$

$$GERMINATE_{AKI} = 1.0\ during\ April\ 20\ to\ end\ of\ April;\ else = 0.0 \quad (30)$$

$$MORT_{REC} = 1.16 \times 10^{-7} \bullet REC\ if\ O_2 > 0\ mll^{-1};\ else\ 0.1 \bullet REC \quad (31)$$

$$RISEI_{REC} = WR_{REC} \bullet REC_{BELOW} \quad (32)$$

$$RISEO_{REC} = WR_{REC} \bullet REC \quad (33)$$

$$WR_{REC} = 1.97 \times 10^{-5}$$

$$SINKI_{AKIW} = WS_{AKI} \bullet AKIW_{ABOVE} \quad (34)$$

$$SINKO_{AKIW} = WS_{AKI} \bullet AKIW \quad (35)$$

$$WS_{AKI} = 1.16 \times 10^{-4}$$

$$RESUSP_{AKIB} = SEDWS \bullet \frac{\tau - \tau_{critical}}{\tau_{critical}} \bullet AKIB \; if \; \tau > \tau_{critical}; \; else = 0.0 \quad (36)$$

$$SINKI_{AKIB} = WS_{AKI} \bullet AKIW_{ABOVE} \quad (37)$$

$$SEDWS = 1.16 \times 10^{-5}$$

$$\tau_{critical} = 0.1$$

$$BUR_{AKIB} = AKIB \bullet BURRATE^{(1)} \; if \; SLIM_{REC} = 1; elseBUR_{AKIB} = AKIB \bullet 10^{15} \bullet BURRATE^{(1)} \quad (38)$$

[1)] Constant burial rate in different Baltic Sea sub basins (Almroth-Rosell et al., 2015).

*) *Fitted to observational data (Lethimäki et al., 1997)*

**) *From Beckmann and Hense (2004)*

Table S4

Description of variables

Name	Unit	Description
BUR_{AKIB}	mmol N m^{-2} s^{-1}	The permanent immobilization of AKIB in the sediment depends on the sediment burial rates defined in SCOBI. To conserve nutrient mass the immobilized AKIB are transferred to the sediment pools of nitrogen and phosphorus. Very high rate of immobilization is used when the salinity is outside of the preferred salinity range for the recruiting cells.
$DETP_{GROWTH_{HET}}$	mmol N m^{-3} s^{-1}	Growth of HET based on uptake of P from detritus (DET-P)
$DETP_{GROWTH_{REC}}$	mmol N m^{-3} s^{-1}	Growth of REC based on uptake of DETP
$DETPLIM_{HET}$	-	DETP limitation of HET growth
$DETPLIM_{REC}$	-	DETP limitation of REC growth
$DIP_{GROWTH_{HET}}$	mmol N m^{-3} s^{-1}	Growth of HET based on uptake of PO4
$DIP_{GROWTH_{REC}}$	mmol N m^{-3} s^{-1}	Growth of REC based on uptake of PO4
$DIPLIM_{HET}$	-	PO4 limitation of HET growth
$DIPLIM_{REC}$	-	PO4 limitation of REC growth

$GCRIT_{HET}$	mmol N m^{-3} s^{-1}	The critical lowest threshold of HET growth that defines the start of transition from HET to AKIW
$GERMINATE_{AKI}$	-	Limitation of germination to the defined time window in spring
GR_{HET}	s^{-1}	Salinity, temperature and light limited growth rate of HET
$GRMAX_{HET}$	s^{-1}	Maximum growth rate of HET
$GRMAX_{REC}$	s^{-1}	Maximum growth rate of REC
$GROWTH_{HET}$	mmol N m^{-3} s^{-1}	Growth of HET
$GROWTH_{REC}$	mmol N m^{-3} s^{-1}	Growth of REC
GR_{REC}	s^{-1}	Salinity, temperature and light limited growth rate of REC
$LTLIM_{HET}$	-	Light limitation of HET growth
$LTLIM_{REC}$	-	Light limitation of REC growth
$MORT_{HET}$	mmol N m^{-3} s^{-1}	Mortality of HET. Dead HET are transferred to the pools of dead organic matter in the model.
$MORT_{REC}$	mmol N m^{-3} s^{-1}	Mortality of REC. Higher mortality under anoxic conditions. Dead REC are transferred to the pool of dead organic matter in the model.
$NGROWTH_{REC}$	mmol N m^{-3} s^{-1}	Growth of REC based on uptake of nitrogen (NO3)
$NLIM_{REC}$	-	NO3 limitation of REC growth
$PGROWTH_{REC}$	mmol N m^{-3} s^{-1}	Growth of REC based on uptake of phosphorus
PI_{SLOPE}	W m^{-2} s^{-1}	Initial slope of the cyanobacteria PI-curve (photosynthesis-irradiance curve)
$RESUSP_{AKIB}$	mmol N m^{-2} s^{-1}	Uplift by resuspension of AKIB from the sediment to the water column AKIW
$RISEI_{HET}$	mmol N m^{-3} s^{-1}	Uplift of HET from the layer below
$RISEI_{REC}$	mmol N m^{-3} s^{-1}	Uplift of REC from the layer below
$RISEO_{HET}$	mmol N m^{-3} s^{-1}	Uplift of HET to the layer above
$RISEO_{REC}$	mmol N m^{-3} s^{-1}	Uplift of REC to the layer above
$SINKI_{AKIB}$	mmol N m^{-2} s^{-1}	Sinking of AKIW to the sediments from the water above
$SINKI_{AKIW}$	mmol N m^{-3} s^{-1}	Sinking of AKIW from the layer above
$SINKO_{AKIW}$	mmol N m^{-3} s^{-1}	Sinking of AKIW to the layer below

$SLIM_{HET}$	-	Salinity limitation of HET growth
$SLIM_{REC}$	-	Salinity limitation of REC growth
$TLIM_{HET}$	-	Temperature limitation of HET growth
$TLIM_{REC}$	-	Temperature limitation of REC growth
WR_{HET}	m s^{-1}	Upward rising velocity of HET
WR_{HET}	m s^{-1}	Upward rising velocity of REC
WS_{AKI}	m s^{-1}	Sinking velocity of AKIW
$\tau_{critical}$	N m^{-2}	Critical bottom shear stress value for onset of resuspension
$AKIB2REC$	mmol N m^{-2} s^{-1}	Transition of benthic AKIB to REC. Depending on germination and favorable salinity conditions for REC.
$AKIW2REC$	mmol N m^{-3} s^{-1}	Transition of pelagic AKIW to REC. Depending on germination and favorable salinity conditions for REC.
$HET2AKIW$	mmol N m^{-3} s^{-1}	Transition of HET to AKIW
$REC2HET$	mmol N m^{-3} s^{-1}	Transition of recruiting cells to HET
$SEDWS$	s^{-1}	Resuspension rate at the bottom
BOT	m^{-1}	Ratio between grid cell area and grid cell volume used for transfer of mass fluxes across vertical grid cell boundaries in the water column

Table S5

Values of constants in the different phosphorus limitation experiments.

	sPlim	**wPlim**	**noOP**	**noP**
$KDIP$ [mmolP/m3]	0.05	1*10^-6	0.05	--
$KDOP$ [mmolP/m3]	0.1	2*10^-6	--	--
$DIPLIM_{HET/REC}$	Eq. 4/22 Table A.3	Eq. 4/22 Table A.3	Eq. 4/22 Table A.3	1
$DETPLIM_{HET/REC}$	Eq. 5/23 Table A.3	Eq. 5/23 Table A.3	0	0

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