

Supplement of Biogeosciences, 18, 1719–1747, 2021
<https://doi.org/10.5194/bg-18-1719-2021-supplement>
© Author(s) 2021. This work is distributed under
the Creative Commons Attribution 4.0 License.



Supplement of

Modeling silicate–nitrate–ammonium co-limitation of algal growth and the importance of bacterial remineralization based on an experimental Arctic coastal spring bloom culture study

Tobias R. Vonnahme et al.

Correspondence to: Tobias R. Vonnahme (t.r.vonnahme@gmail.com) and Christoph Voelker (christoph.voelker@awi.de)

The copyright of individual parts of the supplement might differ from the CC BY 4.0 License.

Supplementary material

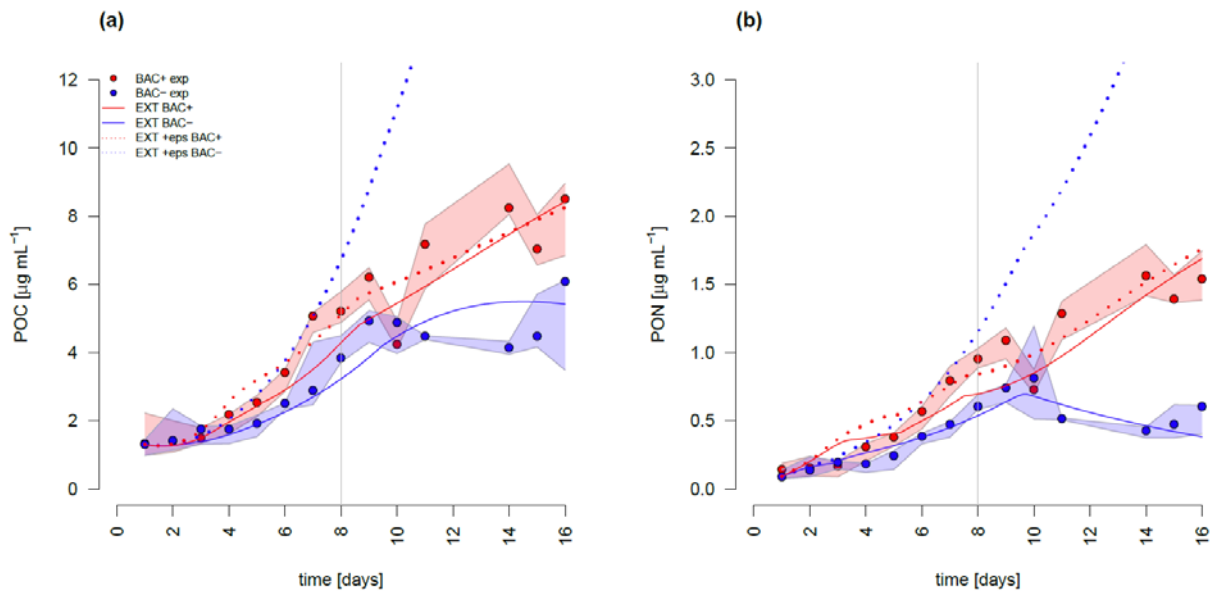


Figure S1. a) POC concentrations of the measured data (circles and polygons) and model (red and blue lines), including the original EXT model run (solid lines) and a model run showing 3% DOC aggregation to EPS as part of the POC pool (dashed line) and reduced inhibition of photosynthesis after Si depletion (S_{iPS} from 0.6 to 0.4). b) PON concentrations of the measured data (circles and polygons) and model (red and blue lines), including the original EXT model run (solid lines) and a model run showing 3% DON aggregation to EPS as part of the PON pool (dashed line) and reduced inhibition of photosynthesis after Si depletion (S_{iPS} from 0.6 to 0.4). The model with EPS coagulation has an overall better fit to BAC+ ($RMSE_{EXT}=2.31$, $RMSE_{EXT+eps}=2.19$), but leads to unrealistic POC and PON fits to BAC-.

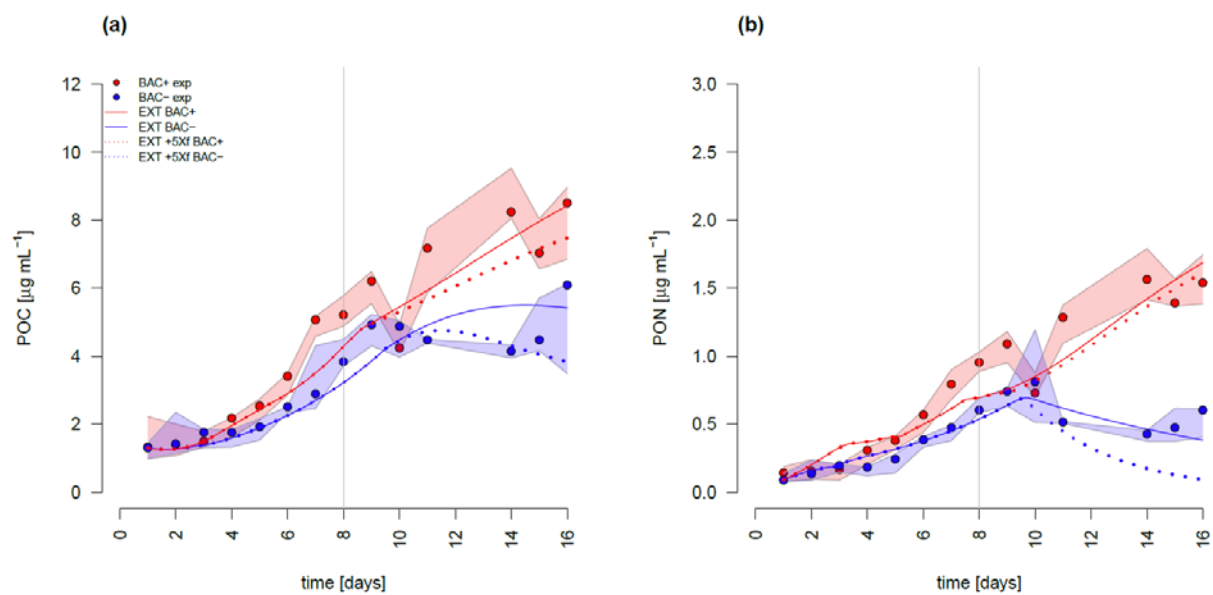


Figure S2. a) POC and b) PON concentrations of the measured data (circles and polygons) and model (red and blue lines), including the original EXT model run (solid lines) and a model run showing a five-fold increased DOM excretion after biofilm formation (dashed line). The difference could be reversed by increasing the S_{IPS} term from 0.6 to 0.8.

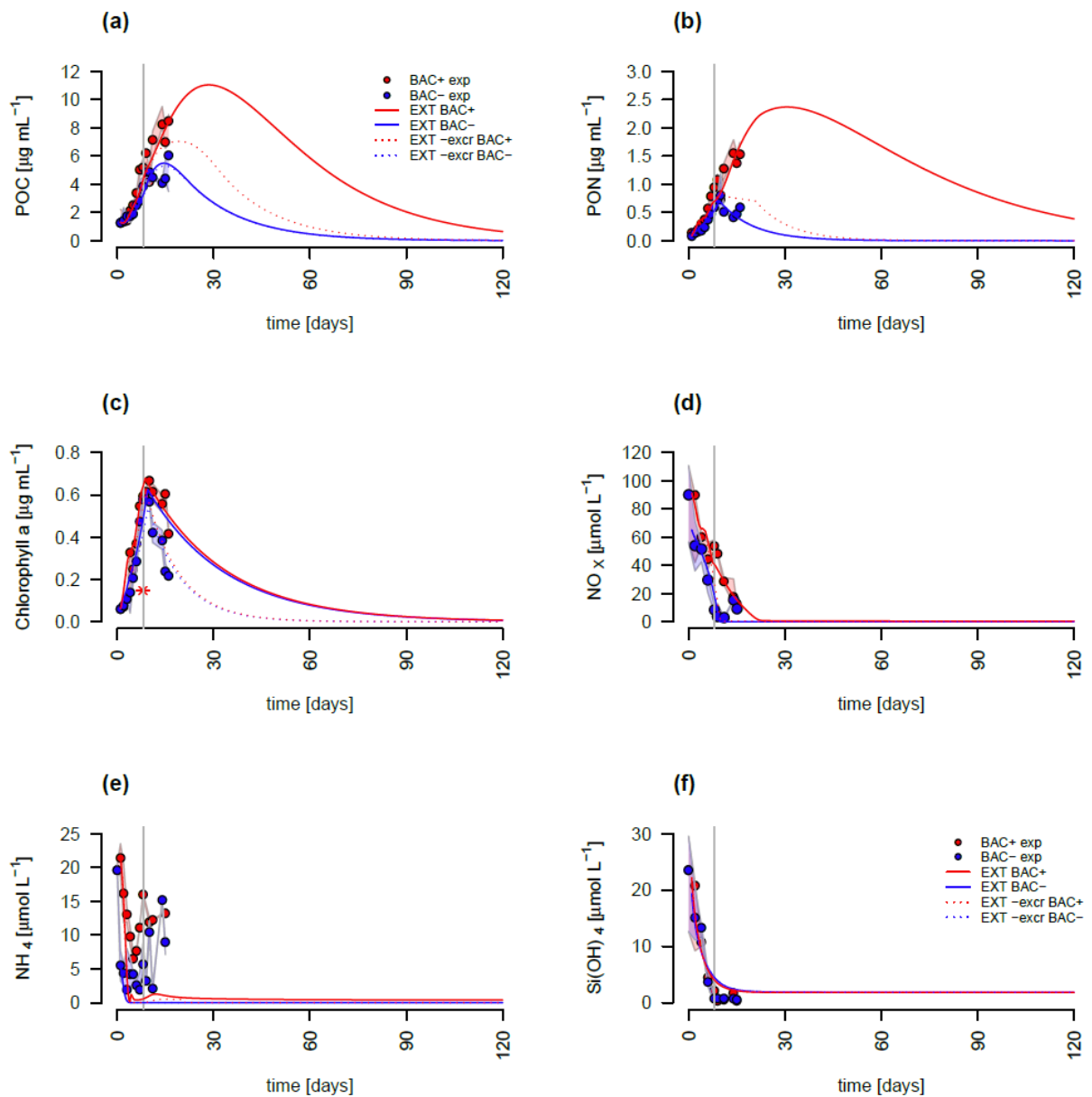


Figure S4. Model fit of the EXT model to the BAC- (blue) and BAC+ (red) experiment. Circles show median values and the colored polygons show the minimum and maximum of the measured data ($n=3$). Solid red and blue lines show the model outputs extended to 120 days of a) POC, b) PON, c) Chl (including outlier at day 8 marked as asterisk), d) NO_x , e) NH_4 , and f) Silicate. The dotted line show the output of EXT without excretion.

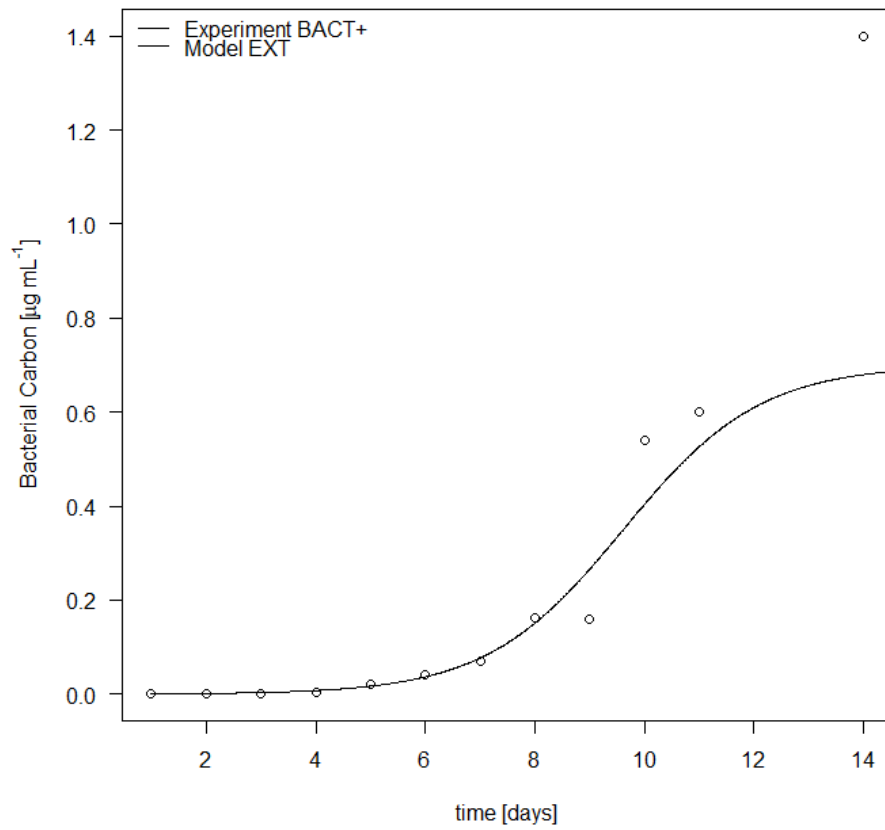


Fig S5. Model fit of the logistic growth curve on bacterial median biomass converted to C data (20 fg Carbon per bacterial cell).

Model tuning protocol (short version)

1. Fitting of the G98 model to the BAC- experiment
 - 1.1. Model programming (R)
 - 1.2. Model solving (ode function, Runge-Kutta method, deSolve package)
 - 1.3. G98 parameter fitting on BAC- experiment
 - 1.3.1. visual tuning (visual comparison with plots)
 - 1.3.2. RMSE tuning (manual minimizing the RMSE Eq C2)
 - 1.3.3. Automated tuning (FME package)
 - 1.3.3.1. Normalize data (POC, PON & Chl x 10, DIN / 10)
 - 1.3.3.2. Sensitivity analysis (SensFun function)
 - 1.3.3.3. Parameter identifiability/ collinearity (Collin function)
 - 1.3.3.4. Parameter selection (identifiable, in doubt higher sensitivity)
 - 1.3.3.5. Automated tuning (RC, Kno3, n, and α Chl, modfit function)
 - 1.3.3.5.1. Global optimum (Pseudorandom search algorithm)
 - 1.3.3.5.2. Local optimum (Nelder Mead algorithm)
 - 1.3.4. Compare automated parameters with initial fit (visual & RMSE)
2. Fitting of the EXT model to the BAC+ experiment
 - 2.1.1. Model programming (R)
 - 2.1.2. Model solving (See 1.2)
 - 2.1.3. EXT parameter fitting to BAC+ experiment (parameters from 1 unchanged)
 - 2.1.3.1. Tuning of Bacterial growth parameters on bacteria (μ bact, bactmax)
 - 2.1.3.2. Tuning of Silicate parameters on silicate (Ksi, Vmax)
 - 2.1.3.3. Tuning of remaining EXT parameters (See 1.3)

Table S1. Model extensions to represent biofilm dynamics. All equations are threshold based after the onset of the biofilm formation.

1)	DOC and DON aggregation as EPS	$\frac{dN_{EPS}}{dt} = don_l x_{eps}$
		$\frac{dC_{EPS}}{dt} = \frac{dN_{EPS}}{dt} \frac{M_N}{M_C} RR$
		$\frac{ddon_l}{dt} = -\frac{dN_{EPS}}{dt}$
2)	Increased DOM excretion	$x_f = x_{f2}$

x_{eps} : fraction of excreted DOC and DON coagulating to EPS, M_C : Molar mass of carbon (12 g mol⁻¹), x_{f2} : DOM excretion after biofilm formation.

Table S2. Replicates for the different parameters per day and treatment (BAC- and BAC+). Replicates used for the model plots are given as n. NH₄ outliers with values over 100 μmol L⁻¹ were removed (cell leakage due to overpressure during filtration) and are given as out. Nut include the other nutrients measured on the nutrient analyzer (Silicate, Nitrate, Nitrite, Phosphate). Particulate organic matter (POM) includes POC, and PON samples.

time	NH ₄		Nut	POM	Chl	Alg	Bac
	n	out	n	n	n	n	n
BAC+							
0	2	0	3	3	3	3	0
1	2	1	0	3	3	3	2
2	2	1	3	3	3	3	3
3	2	1	0	3	3	3	1
4	2	1	3	3	3	3	3
5	3	0	0	3	3	3	3
6	2	0	3	3	3	3	2
7	1	1	0	3	2	2	3
8	2	1	3	3	3	3	2
9	0	0	2	3	3	3	3
10	2	1	0	3	2	2	3
11	1	0	2	3	3	3	3
14	0	0	3	3	2	2	1
15	2	0	2	3	3	3	0
16	0	0	0	3	3	3	0
BAC-							
0	2	0	2	3	3	3	0
1	2	0	0	3	3	3	3
2	3	0	3	3	3	3	3
3	3	0	0	3	3	3	3
4	3	0	3	3	3	3	3
5	3	0	0	3	3	3	3
6	3	0	3	3	3	3	2
7	3	0	0	3	2	2	3
8	3	0	3	3	3	3	3
9	2	0	3	3	3	3	3
10	3	0	0	3	2	2	2
11	3	0	3	3	3	3	2
14	1	0	3	3	2	2	1
15	3	0	3	3	3	3	0
16	2	0	0	3	3	3	0