Appendix A. Modeling Approach, Parameter, and Rate Updates

This appendix describes updates, including stabilization of sediment fluxes, use of a newer version of the biogeochemical code, and changes to parameterizations. It also contains results of sensitivity tests to changes such as differences in reaeration scheme and bottom friction. Skill statistic formulas used in this appendix are in Appendix D. For definitions of terms, including statistical performance metrics, refer to the glossary in the main report.

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Stabilization of sediment fluxes

Pelletier et al. (2017) describes the Salish Sea Model's (SSM) sediment diagenesis module. The sediment diagenesis module uses a two-layer method developed by Di Toro (2001): a thin aerobic layer at the surface comprised of dynamically calculated variable thickness and a thicker anaerobic layer on the bottom with a thickness equal to the total sediment depth of 10 cm minus the depth of the aerobic layer.

Particulate organic matter (POM) initially decomposes rapidly in the sediments but then slows down as the more labile fraction is consumed (Burdige 2007). To capture this process, the total particulate organic matter deposited to the sediments is fractioned into one of three "G classes" based on overall reactivity (Figure 1 in Di Toro 2001). The three G classes represent a relatively rapidly decomposing labile class (G1), a more refractory form (G2), and a relatively inert form (G3). The fractions assigned to each G class remain the same as those used by Ahmed et al. (2019): 0.5, 0.3, and 0.2 for G1, G2, and G3, respectively. The decomposition of the three G classes of POM occurs in the anaerobic layer. However, since G3 is relatively inert compared to G1 and G2, we expect this fraction to be buried with little, if any, decomposition. Over the long term, we expect sediment concentrations to approach a steady state for G1 and G2.

Based on a peer review comment from Carl Cerco, we visually inspected time series plots for G1 and G2 to confirm that we are providing the model with a stable sediment flux initial condition. We found that the approach used by Ahmed et al. (2019), which consisted of running the model in "cold" start for a year and then followed by rerunning the model in "hot" start mode, did not result in stabilizing the G1 and G2 concentrations so that they approached a steady state. So, we investigated the result of running more iterations after the "cold start" mode to approach a steady state for G1 and G2. We demonstrated that when we run the model ten consecutive times in batch mode after the cold start, feeding each model run with the restart file of the previous run, G1 and G2 approach a steady state. We called each of these iterations a hot start. Including the cold start, we are running each model scenario a total of eleven runs to obtain the output.

The resulting G1 and G2 concentrations in the sediment for all model nodes are shown in box plots in Figure A-1 in terms of g O_2/m^3 after each consecutive run. Note that the modeled G1 medians and outliers beyond the interquartile range change very little or not at all after 6 consecutive iterations. The G2 plot shows asymptotic behavior, with the medians remaining stable around the 7th iteration and the outliers approaching an asymptotic threshold in the last two runs. Carl Cerco (pers. comm, April 2022) deemed it unnecessary to stabilize the G3 component due to its inertness.

We ran all Opt 2 scenarios as described above. Since the water quality input files for the scenario runs were created from a single year concatenated ten times after the initial cold start, we also needed to concatenate the hydrodynamic run. To do so, we repeated the 365-day hydrodynamic netCDF files ten times to provide hydrodynamic fields for the ten-year water quality run.



Figure A-1. Boxplots of predicted labile (G1) and refractory (G2) organic carbon fractions in the sediments for the year 2006.

The y-axis shows the organic carbon fractions in terms of the corresponding oxygen needed for complete oxidation. The x-axis shows the number of consecutive runs or "hot starts."

ICM2 vs ICM4

Ahmed et al. (2019) used FVCOM-ICM2 (ICM2), a model based on CE-QUAL-ICM (Cerco and Cole 1993) that was developed by Pacific Northwest National Laboratory (PNNL) (Kim and Khangaonkar 2012; Bianucci et al. 2018) to operate on the FVCOM framework. Khangaonkar et al. 2021 reported on an updated version called FVCOM-ICM4 (ICM4), which was adapted for use with the SSM framework. The main objective of the ICM4 updates was to incorporate modules available in subsequent ICM code (Cerco and Moore 2001) to predict inorganic suspended solids, turbidity, zooplankton, and submerged aquatic vegetation. While we are not using ICM4 to predict these parameters, we investigated whether any other features in ICM4 might improve dissolved oxygen (DO) predictions. We found two features of ICM4 that could lead to improvements in DO predictions: (1) corrected photosynthetically active radiation (PAR) daily distribution and (2) the capability to use variable bottom friction with FVCOM2.7d. These two updates are described below. Consequently, we are using ICM4 for all Opt2 scenarios.

Corrected PAR daily distribution

Light availability is a key driver for the photosynthetic rate and the total algal biomass produced.

Solar irradiance, or photosynthetically active radiation (PAR), is input to ICM as a daily total in E/m^2 . ICM computes irradiance over time ($E/m^2/d$) as a sine function.

While using the same solar irradiance as input, we noticed differences between the PAR output of ICM2 and ICM4. We found higher PAR values and a different PAR distribution in ICM4 (Figure A2, note the difference in the y-axis scale). Accordingly, we observed differences in LPOC and RPOC between ICM2 and ICM4 output, particularly in inlets, and as a result, ICM4 produces more SOD than ICM2.

A. Nugraha (pers. comm, July 5, 2023) confirmed that ICM4 has a corrected PAR scheme that accurately represents darkness at night by setting PAR equal to zero and allowing for higher PAR values during the day. This scheme ensures that solar radiation, as seen by the model, occurs only during daylight hours. As a result of these changes, ICM4 is performing better for PAR than ICM2. This fix improves overall DO performance.



Figure A-2. Comparison of PAR time series in ICM4 (top) and ICM2 (bottom).

Net heat flux correction factors

We found a limitation during some instances of very cold periods in surface layer temperature model predictions. There are two correction factors in FVCOM that modulate the net heat flux from computationally derived Weather Research Forecast (WRF) model meteorological output. The 'dissipation factor' is applied to reduce the overall net heat fluxes, and then the resulting negative net heat fluxes are 'clipped' at a certain threshold. The value of these correction factors is shown in Table A-1. We found that these correction factors impact water temperatures appropriately during most temperature ranges, except in some instances, during very cold hours at a few specific locations in surface layers. This was an unexpected finding not only in this version of the SSM, but also in Khangaonkar et al. (2018) and in the recently published (Premathilake and Khangaonkar 2022) Salish Sea & Columbia River Operational Forecast System (SSCOFS) version.

We also found that the correction factors referenced above require optimization when using output from other regional meteorological forcings, as was the case for the year 2000 (Y2000) model run. The Y2000 run used meteorological forcings from the model ECHAM instead of WRF. ECHAM is a general circulation model created by modifying global forecast models developed by ECMWF (European Centre for Medium-Range Weather Forecasts).

The table below shows the correction factors used for all four model years.

Year	Meteorology model Dissipation factor		Clip
2000	ECHAM 0.8		-100
2006	MM5	0.65	-150
2008	2008 MM5 0		-150
2014	WRF	0.65	-150

 Table A-1. Correction factors for heat fluxes.

Since these correction factors are not optimized for the coldest temperatures during specific hours in surface layers and at some shallow locations, predicted temperatures are unrealistic (negative) and were discarded from the model output. We noticed that the frequency of these unreasonable temperatures was higher for nodes that exhibited 4m or less water column depth, which can occur at certain shallow nearshore locations during ebb tides. These nodes were masked so that no model output from these locations is used.

The nodes that were not masked had depths greater than 4m during ebb tides, and still had a few hours discarded due to unrealistically low temperatures. These were a very small portion of the total predictions. For instance, for 2014, the total number of grid-cell layer-hours discarded represents 0.00006% of the total grid-cell layer-hours in the unmasked grid cells within the

Washington waters of the Salish Sea. All predicted water quality variables associated with these specific hours were also discarded from the model output.

Distributed bottom friction

FVCOM2.7d allows for spatially varying bed friction inputs. Khangaonkar et al. (2021) employed spatially varying roughness factor (z₀), also referred to as distributed bottom friction, to improve the prediction of water surface elevations on the medium-resolution grid model (consisting of 16,012 nodes) while driving the open boundary with tidal constituents from the Eastern North Pacific (ENPAC) database (Szpilka et al. 2018). This change in hydrodynamics necessitated fine-tuning some biogeochemical parameters (e.g., maximum photosynthetic rates, productivity, and settling rates of organic matter) to ensure overall model performance.

Although Premathilake and Khangaonkar (2022) obtained an average water surface elevation RMSE of 0.185 m using distributed bottom friction (Khangaonkar et al. 2021) and tidal elevation time series, they used a finer SSM grid with a resolution ten-fold greater compared to the medium scale model Khangaonkar et al. (2021) used and that we are using here. Furthermore, the finer scale model was intended to improve hydrodynamic predictions but was beyond this project's scope for water quality calibration.

To optimize water surface elevation with the medium-resolution grid, we tested FVCOM2.7d with tidal forcing at the open boundary as tidal elevation moments based on the ENPAC database (Szpilka et al. 2018), along with and without spatially varying bottom friction. Table A-1 shows that distributed bottom friction performed slightly better, on average, than constant bottom friction. Accordingly, all Opt2 scenarios were run using distributed bottom friction and tidal moments.

Year	Bottom Friction	Seattle	Neah Bay	Tacoma	Port Angeles	Cherry point	Port Townsend	Friday Harbor	Average
2014	constant	0.44	0.45	0.48	0.28	0.54	0.37	0.45	0.43
2014	distributed	0.45	0.46	0.49	0.26	0.48	0.35	0.41	0.41

 Table A-2. Comparison of water surface elevation root mean square error (m) between constant and distributed bottom friction runs.



Figures A-3 and A-4 show scatterplots of predicted and observed tidal elevations at selected NOAA stations with modeled predictions using distributed bottom friction and tidal forcing at the open boundary with tidal moments.

Figure A-3. Scatter plot of model predictions and observations for tidal elevations at selected stations.



Figure A-4. Scatterplots of model predictions and observations of tidal elevations at selected sites.

Improvements to Reaeration Scheme

Ahmed et al. (2019) found that the model is sensitive to the empirical constants in the equation that were used to compute Kr, the reaeration coefficient:

 $Kr = Arear \times Rv \times W_{ms}^{Crear}$

Where:

Kr is in units of cm/h

Arear = empirical constant (0.251) in units of $(cm/hr) (m/s)^{-2}$

Crear = empirical constant (2)

Rv = ratio of the kinematic viscosity of pure water at 20°C to the kinematic viscosity of water at specified temperature and salinity

 W_{ms} = wind speed measured at 10m above surface water in meters per second.

Ahmed et al. (2019) used the above reaeration equation for the entire modeling period with the constants listed above. Khangaonkar and Yun (2023) implemented a new reaeration scheme that uses the equation above during the colder months of the year (mid-September through March) with a value of 0.451 instead of 0.251 for Arear. During the rest of the year, they used the Wanninkhof (2014) reaeration equation, which is like the equation above, with the exception that instead of Rv, the equation uses the term (Schmidt number /660)^{-0.5} with the proportionality constant of 0.251. While Khangaonkar and Yun (2023) used FVCOM4.3, we tested this new reaeration scheme with FVCOM2.7d and ICM4 and obtained improved dissolved oxygen (DO) calibration statistics, as shown below. Definitions for statistical metrics used in the tables below are found in the Glossary, and formulas are found in Appendix D.

Parameter and Run	R	WSS	RMSE	RMSE_C	RE	MAE	Bias	Ν
DO (mg/L) Constant reaeration	0.82	0.87	1.09	0.93	0.12	0.84	-0.56	96152
DO (mg/L) New temporally variable reaeration scheme	0.85	0.91	0.91	0.87	0.09	0.65	-0.27	96152

Table A-2.	Predicted DO statis	tics with constant	and temporally	varying reaeration
scheme.				

Sensitivity Runs and Changes to Parameterizations

Given the adjustments to sediment flux initialization, the use of distributed friction, the updated freshwater input loads (detailed in Appendices B1, B2, and B3), and a new reaeration scheme, we needed to recalibrate the model. We conducted multiple sensitivity runs to ascertain the impact of various parameterizations on the new baseline framework. Below is a listing of the parameters we explored and the basis for any adjustments to the values used in the new baseline parameterization we developed.

Changes to particle settling rates

Particle settling rates are a function of their specific gravity, size, and shape (Sverdrup 1942). ICM employs various parameters to specify particulate settling rates. The settling velocities of particulates in the water column and net settling velocities of particulates at the interface of the water column and the sediment bed are identified in Tables A-3 and A-4. The net settling velocity is the rate of settling and resuspension at the sediment bed surface. We are not using the suspended solids module of ICM, so the model is not sensitive to inert or inorganic suspended solids. However, as Ahmed et al. (2019) reported, the model is sensitive to the organic particulate fractions reaching the sediments.

Water Column Settling Velocities	Definition	Used by Ahmed et al. (2019)	Used in Current Work
WSLAB	Labile particulates (LPOC/LPON/LPOP) settling velocity (m/day)	5	2.5
WSREF	Refractory particulates (RPOC/RPON/RPOP) settling velocity (m/day)	5	2.5
WS1, WS2	Settling velocity for algal groups 1 and 2 (m/day)	0.4, 0.2	0.4, 0.2

Table	A-3.	Water	column	settling	rate	parameters.
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Table A-4. Net settling rate parameters.

Net Settling Velocities	Definition	Used by Ahmed et al. (2019)	Used in Current Work
WSLNET	Net settling velocity of labile particles (G1) to sediments (m/day)	1	1
WSRNET	Net settling velocity of refractory particles (G2) to sediments (m/day)	1	1
WS1NET and WS2NET	Net settling velocities of algal groups 1 and 2 (m/day)	0.2, 0.075	0.2, 0.075

Algal settling rates

Settling rates for diatoms and flagellates are highly variable. EPA (1985) reports a range of 0.02 to 17.1 meters/day (m/d) for diatoms and 0.05 to 8 meters per day for flagellates. In SSM, WS1 is the settling rate for diatoms, and WS2 is the settling rate for dinoflagellates. Khangaonkar et al. (2018) used a value of 0.4 m/d and 0.2 m/d for WS1 and WS2, respectively. However, Bianucci et al. (2018) used higher values of 0.6 m/d and 0.3 m/d for WS1 and WS2, respectively.

Taguchi and Hargrave (1978) observed that, except for winter, algal cell deposition to sediments was about ten times lower than the deposition of organic detritus particles. This approximate relative difference in settling velocity between organic particles in the water column (WSLAB and WSREF) and algal cells (WS1 and WS2) or net organic particles settling into the sediment (WSLNET and WSRNET) and algal cells settling into the sediments (WS1NET and WS2NET) is present in the model calibration Ahmed et al. (2019) employed and was not changed, as shown in Table A-4.

Settling rates for organic detritus

Settling rates for the organic labile (WSLAB) and refractory (WSREF) particulates can significantly affect model performance, but very limited observational data are available to evaluate this parameter. Cerco et al. (2010) used values of 1 m/day for settling rates of both labile and refractory particulate matter, whereas Bianucci et al. (2018) used 10 m/day for both, and Khangaonkar et al. (2018) used 5 m/day. Tests with these values demonstrated the degree of sensitivity. In combination with the updated re-aeration scheme, Khangaonkar and Yun (2023) use 2.0 m/s for WSLAB and WSREF settling rates to achieve a multi-year (2013-2020) continuous run calibration of SSM.

We used SOD predictions to understand the effect of settling rates better. Our approach was to use setting rates that represented SOD more closely. We found that:

Reducing *both* WSLAB and WSREF by a factor of 5 results in SOD rates that are too low.

Reducing water column settling velocities WSLAB and WSREF to 2.5 m/d (by a factor of 2) while keeping net sediment velocity in sediments (WSLNET, WSRNET to 1.0 m/d results in SOD fluxes that generally match observations.

We conducted sensitivity runs to test model performance for varying WSLAB and WSREF. Table A-5 shows the results of those runs.

Sensitivity Run	Variable	R	WSS	RMSE	RMSE_C	RE	MAE	Bias	Ν
Baseline (WSLAB, WSREF = 5 m/day)	DO (mg/L)	0.82	0.87	1.09	0.93	0.12	0.84	-0.56	96152
Decrease in WSLAB, WSREF to 2.5 m/day	DO (mg/L)	0.82	0.88	1.01	0.91	0.11	0.77	-0.44	96152

Table A-5. Sensitivity run comparing lower WSLAB and WSREF to baseline.

Changes to mineralization rates

We sought to improve performance for nitrogen mineralization rates, particularly for NH₄⁺. The final updates to nitrogen mineralization rates are shown in Table A-6.

Mineralization Parameter	Definition	Used by Ahmed et al. (2019)	Used in Current Work
KLDN	Minimum mineralization rate of labile dissolved organic nitrogen (1/day)	0.05	0.075
KLPN	Minimum hydrolysis rate of labile particulate organic nitrogen (1/day)	0.01	0.05
KHNNT	Half saturation concentration of NH4 ⁺ required for nitrification (g N/m ³)	0.5	0.75

 Table A-6. Updates to kinetic mineralization rates.

Dissolved and particulate organic nitrogen mineralization rate

We tested the model's performance for the dissolved and particulate organic nitrogen mineralization rate (KLDN and KLPN). Increases in KLDN and KLPN from 0.05 to 0.1 d⁻¹ and 0.01 to 0.05 d⁻¹ resulted in no improvement to DO performance. However, the NH₄⁺ performance did improve slightly, as shown in Table A-7, when combining changes for KLDN (to 0.075 d⁻¹ and KLPN to 0.05 d⁻¹), with changes to the half-saturation concentration of ammonium ion, as described below. The baseline runs shown in Table A-7 were conducted with the 2014 model, constant bottom friction, and parametrization as reported in Ahmed et al. (2019), except for WSLAB and WSREF set to 2.5 m/d and with the new reaeration scheme described above.

Nitrification

Sensitivity runs demonstrated that the model is sensitive to KHNNT, the half-saturation concentration of ammonium ion required for nitrification. Increasing the half-saturation constant for nitrification from 0.5 to 1 g N/m³ reduced the RMSE of DO slightly (from 0.85 to 0.84), reduced the bias of DO predictions (from 0.12 to 0.08), and improved the NH₄⁺ predictions, particularly the correlation coefficient (R) when coupled with increases in KLDN and KLPN, as shown in Table A-7. The performance for nitrate/nitrite, DO, and chlorophyll remained like the baseline, as shown in Figure A-5. The KHNNT value used in the final model calibration is 0.75 g N/m³, further optimizing NH₄⁺ model performance.

Parameter and Run	R	WSS	RMSE	RMSE_C	RE	MAE	Bias	Ν
NH₄ Baseline (KLDN=0.05 and KLPN = 0.01 d ⁻¹)	0.31	0.53	0.02	0.02	0.6	0.01	0	1595
NH ₄ Increase in KLDN (to 0.075 d ⁻¹)		0.54	0.02	0.02	0.6	0.01	0	1595
$\rm NH_4$ Increase in KLPN (to 0.05 d ⁻¹)	0.34	0.54	0.02	0.02	0.58	0.01	0	1595
NH ₄ Multiple parameter increase (KLDN to 0.075 d ⁻¹ , KLPN to 0.05 d ⁻¹ and KHNNT to 1 g N/m ³)	0.41	0.58	0.03	0.02	0.84	0.02	0.01	1595

Table A-7. Sensitivity in NH₄ concentrations comparing baseline to increased KLDN, KLPN, and KHNNT.



Figure A-5. Comparison of model performance between two runs.

Top row: baseline run (2014, constant bottom friction and parametrization as reported in Ahmed et al. (2019)) with WSLAB and WSREF set to 2.5 m/d and the new reaeration scheme. Bottom row: same baseline run as the top row but with KLDN increased from 0.05 to 0.075 d-1, KLPN from 0.01 to 0.05 d-1, and KHNNT from 0.5 to 1 g N/m³.

Changes to algal rates

Maximum photosynthetic rate

The maximum photosynthetic rate (g C g⁻¹ Chl d⁻¹) can be specified for each algal group. We tried increasing algal growth to match the high chlorophyll concentrations observed primarily in inlets and bays by increasing the maximum photosynthetic rate. Ahmed et al. (2019) used 350 g C g⁻¹ Chl d⁻¹ for both algal groups. Cerco and Noel (2019) used a photosynthetic rate of 450 g C g⁻¹ Chl d⁻¹. We tested matching that higher rate and found a slightly better match during the fall bloom. Consequently, we assigned 450 g C g⁻¹ Chl d⁻¹ to the second algal group.

Initial slope of production (α)

The parameter α (ALPHMN), defined as the initial slope of the photosynthesis vs. irradiance curve, impacts the total productivity and timing of the blooms. A larger α permits greater photosynthesis at low irradiance, thus permitting earlier blooms in the spring and later blooms in the fall. Observations show that blooms in Salish Sea inlets and bays often lasted longer than predicted in Ahmed et al. (2019), and spring blooms showed up earlier at some locations. So, we tested different α values for algal groups 1 and 2 and found a slightly better fit in several inlet stations in spring when α (for algal group 1) is set to 8 and in late summer/fall (for algal group 2) when α is set to 12.

Phosphorus

Observations reveal that, though infrequently, there are a few times and locations in Puget Sound when it appears that production may be phosphorus-limited, but there is no documentation that phosphorus limitation has occurred. We investigated the possibility of calibrating the model for phosphorus. We tested various parameters, including the algal phosphorus-to-carbon ratio (apc), the labile particulate organic phosphorus hydrolysis rate (KLPOP), and the half-saturation for algal phosphorus uptake (KHp). We also reviewed the open-boundary phosphorus concentrations. Unfortunately, the open boundary phosphorus observations are very limited and non-existent for organic phosphorus. We determined that the model cannot be calibrated for phosphorus, given the lack of open boundary data. Figure A-6 shows the model's lack of predictive skill for phosphate in 2014.



Figure A-6. Scatterplot of observed phosphate vs. predictions.

Parameter Type	Variable	Value	Unit	Literature Range	Definition
Algae	ALPHMN1	8	g C g ⁻¹ Chl (E m ⁻²) ⁻¹	_	Initial slope of photosynthesis vs. irradiance curve for algal group 1
Algae	ALPHMN2	12	g C g ⁻¹ Chl (E m ⁻²) ⁻¹	_	Initial slope of photosynthesis vs. irradiance curve for algal group 2
Algae	ANC1	0.175	g N g-1 C	_	Nitrogen-to-carbon ratio for algal group 1
Algae	ANC2	0.175	g N g-1 C	_	Nitrogen-to-carbon ratio for algal group 2
Algae	BM1	0.1	d-1	0.01–0.1	Basal metabolic rate of algal group 1
Algae	BM2	0.1	d ⁻¹	0.01–0.1	Basal metabolic rate of algal group 2
Algae	BPR1	1	d-1	0.05–1.0	Base predation rate of algal group 1
Algae	BPR2	0.5	d-1	0.05–1.0	Base predation rate of algal group 2
Algae	CCHL1	37	g C g ⁻¹ Chl	30–143	Carbon-to-chlorophyll ratio for algal group 1
Algae	CCHL2	50	g C g ⁻¹ Chl	30–143	Carbon-to-chlorophyll ratio for algal group 2
Algae	G1	calculated	d-1	_	Growth rate of algal group 1
Algae	G2	calculated	d-1	—	Growth rate of algal group 2
Algae	PM1	350	g C g ⁻¹ Chl d ⁻¹	200–450	Maximum photosynthetic rate of algal group 1
Algae	KHN1 and KHN2	0.06	g N m-3	0.003– 0.923	Half-saturation concentration for nitrogen uptake for algal groups 1 and 2
Algae	PM2	450	g C g ⁻¹ Chl d ⁻¹	200–450	Maximum photosynthetic rate of algal group 2
Algae	TMP1	12	°C	up to 35	Optimal temperature for growth of algal group 1
Algae	TMP2	18	°C	up to 35	Optimal temperature for growth of algal group 2
Mineralization	AANOX	0.5	—	0-1	Ratio of denitrification to oxic carbon respiration rate
Mineralization	ANDC	0.933	g N g ⁻¹ C	0.933	Mass nitrate-nitrogen reduced per mass diss. organic carbon

 Table A-8. Key parameters and rates used in Salish Sea Model Optimization Phase 2.

Parameter Type	Variable	Value	Unit	Literature Range	Definition
Mineralization	AOCR	2.67	g O ₂ g ⁻¹ C	_	Oxygen-to-carbon mass ratio in production and respiration
Mineralization	AONT	4.33	g O ₂ g ⁻¹ N	_	Oxygen consumed per mass ammonium nitrified
Mineralization	DENIT	calculated	d-1	—	Denitrification rate
Mineralization	KHNDN	0.1	g N m ⁻³	_	Half-saturation conc. of nitrate required for denitrification
Mineralization	KHNNT	0.75	g N m ⁻³	_	Half-saturation conc. of NH4 required for nitrification
Mineralization	KHODOC	0.5	$g O_2 m^{-3}$	_	Half-saturation conc. of DO required for oxic respiration
Mineralization	KHONT	3	$g O_2 m^{-3}$	_	Half-saturation conc. of DO required for nitrification
Mineralization	KLDC	0.025	d-1	0.005– 0.25	Minimum respiration rate of LDOC
Mineralization	KLPC	0.01	d-1	0.005–1.5	Dissolution rate of LPOC
Mineralization	KLDN	0.075	d-1	0.02–2.0	Minimum mineralization rate of LDON
Mineralization	KLPN	0.05	d-1	0.03–0.08	Minimum hydrolysis rate of LPON
Reaeration	Kr	calculated	cm/h	_	Reaeration coefficient, calculated as a function of wind speed
Mineralization	KTNT1	0.0045	°C-2	_	Effect of sub-optimal temperature on nitrification
Mineralization	KTNT2	0.0045	°C-2	_	Effect of super-optimal temperature on nitrification
Mineralization	NT _m	0.4	g N m ⁻³ d ⁻¹	0.01-0.7	Maximum nitrification rate
Mineralization	TMNT	30	°C	25–35	Optimal temperature for nitrification
Settling	SS	0.25	m d⁻¹	_	Fixed solids settling rate
Settling	WS1	0.4	m d⁻¹	0–30	Settling velocity of algal group 1
Settling	WS2	0.2	m d⁻¹	0–30	Settling velocity of algal group 2
Settling	WSLAB	2.5	m d ⁻¹	_	Labile particulate organic solids settling rate
Settling	WSREF	2.5	m d ⁻¹	_	Refractory particulate organic matter settling rate

Parameter Type	Variable	Value	Unit	Literature Range	Definition
Sediment Diagenesis	KPON1	0.018	d-1	_	Decay rate of PON1 in sediments
Sediment Diagenesis	KPON2	0.0018	d-1	_	Decay rate of PON2 in sediments
Sediment Diagenesis	KPON3	0	d-1	_	Decay rate of PON3 in sediments
Sediment Diagenesis	FRNALG1 (1:3)	0.65, 0.25, 0.10	NA	_	Algae 1 split of N for G1, G2, G3 in sediments
Sediment Diagenesis	FRNALG2 (1:3)	0.65, 0.25, 0.10	NA	_	Algae 2 split of N for G1, G2, G3 in sediments
Sediment Diagenesis	FRCALG1	0.65, 0.2, 0.15	NA	_	Algae 1 split of C for G1, G2, G3 in sediments
Sediment Diagenesis	FRCALG2	0.65, 0.2, 0.15	NA	_	Algae 2 split of C for G1, G2, G3 in sediments
Sediment Diagenesis	KPOC1	0.035	d-1	_	Reaction rate constant for G1 class of POC in sediments
Sediment Diagenesis	KPOC2	0.0018	d ⁻¹	_	Reaction rate constant for G2 class of POC in sediments
Sediment Diagenesis	КРОСЗ	0	d-1	_	Reaction rate constant for G3 class of POC in sediments
Sediment Diagenesis	WSLNET	1	m/d	_	Net settling rate of labile POM in bottom layer of water column
Sediment Diagenesis	WSRNET	1	m/d	_	Net settling rate of refractory POM in bottom layer of water column
Sediment Diagenesis	WS1NET	0.2	m/d	_	Net settling rate of algae 1 in bottom layer of water column
Sediment Diagenesis	WS2NET	0.075	m/d	_	Net settling rate of algae 2 in bottom layer of water column
Sediment Diagenesis	VSED	0.2502	cm/yr	_	Sedimentation rate
Sediment Diagenesis	VPMIX	0. 00018	m²/d	_	Particle mixing rate between layer 1 and 2
Sediment Diagenesis	VDMIX	0. 0075	m²/d	_	Diffusion rate across sediment/water interface

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