

MyLake C

Technical model documentation and user manual

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1 Introduction

MyLake C (Kiuru et al., 2018) is a one-dimensional process-based model code for the simulation of lake water column temperature and water quality. It derives from the following published versions of MyLake: MyLake v.1.2 (Saloranta and Andersen, 2007), MyLake FOKEMA (Holmberg et al., 2014), and MyLake O (Couture et al, 2015). It includes the simulation of dissolved oxygen (DO) and organic and inorganic carbon cycling in a lake. For the purpose of this manual, the new model components, other developments, and model code revisions are described with respect to MyLake v.1.2. As such, this manual can be considered an extension to the documentation of MyLake v.1.1 by Saloranta and Andersen (2004) and MyLake v.1.2 by Saloranta and Andersen (2005).

The structure of this document is as follows. Section 2 gives a detailed description of the different carbon-related processes and formulas included in MyLake C. Section 3 outlines other updates and code revisions made to MyLake C compared to MyLake v.1.2. Section 4 gives brief instructions for setting up and running a MyLake C application. Section 5 presents further extensions of the MyLake C model code considering the simulation of air-water gas exchange.

The MyLake C model code together with a model application using MyLake C is found at https://github.com/biogeochemistry/MyLake_C. The extended version together with a related application is found at https://github.com/biogeochemistry/MyLake_C/tree/MyLake_C-gtsv.

2 Modeling of lake dissolved oxygen and carbon cycling

The following text on the formulations of the in-lake biochemical inorganic and organic carbon processes implemented in MyLake C is based on Kiuru (2019), and the text on the carbonate system is based on Kiuru et al. (2018).

2.1 New model state variables

In comparison to MyLake v.1.2, dissolved inorganic carbon (DIC) including its three fractions, carbon dioxide CO_2 , bicarbonate HCO_3^- , and carbonate CO_3^{2-} ; (dead) particulate organic carbon (POC); hydrogen ion (H^+); and dissolved oxygen (DO) are added as new state variables. The 12 main model state variables whose vertical profiles are simulated by MyLake C are:

T	Temperature [$^{\circ}\text{C}$]
S	Suspended inorganic particulate matter (or particulate inorganic matter, PIM) [kg m^{-3}]
P_D	Dissolved inorganic phosphorus (phosphate) [mg m^{-3}]
P_{IP}	Phosphorus bound to inorganic particles [mg m^{-3}]
P_{DO}	Dissolved organic phosphorus [mg m^{-3}]
$P_{\text{Chla},1}$	Chlorophyll a (group 1) [mg m^{-3}]
$P_{\text{Chla},2}$	Chlorophyll a (group 2) [mg m^{-3}]
C_{DO}	Dissolved organic carbon [mg m^{-3}]

C_{PO}	Particulate organic carbon [mg m^{-3}]
C_{DI}	Dissolved inorganic carbon [mg m^{-3}]
O_D	Dissolved oxygen [mg m^{-3}]
H^+	Hydrogen ion (10^{-pH}) [mol l^{-1}]

In addition to POC and dissolved organic carbon (DOC), a third form of organic carbon in MyLake C is living particulate organic carbon POC_L . It is represented by the carbon content in phytoplankton by using the conversion factor $\frac{s_P}{y_c}$ [$\text{mg C (mg Chl } a)^{-1}$], where $s_P = 50 \text{ mg C (mg P)}^{-1}$ is the mass ratio of carbon to phosphorus in phytoplankton and y_c [$\text{mg Chl } a (\text{mg P})^{-1}$] is the yield coefficient (the mass ratio of chlorophyll *a* to phosphorus in phytoplankton) in MyLake v.1.2. Thus, the concentration of POC_L in the water column [mg m^{-3}] is given by phytoplankton biomass in carbon units

$$C_{PP} = \frac{s_P}{y_c} P_{Chla}. \quad (1)$$

Dissolved organic matter (DOM), living particulate organic matter (POM_L), and (dead) particulate organic matter (POM) are related to DOC, POC, and POC_L , respectively. The mass fraction of carbon in dry living and dead particulate matter both within the water column and in the sediment is defined to be $s_C = 5 \times 10^5 \text{ mg kg}^{-1}$.

2.2 Process descriptions

2.2.1 Organic carbon

Species of organic carbon

Living particulate organic carbon transforms into POC, which is further fragmented into DOC. POC is divided into autochthonous and allochthonous compound classes (pools). Autochthonous POC (POC_1) is generated by the death of phytoplankton and by the flocculation of allochthonous DOC, whereas allochthonous POC (POC_2) enters the lake through stream inflow. DOC is divided into three pools with different degradabilities. The total DOC concentration is expressed as the sum of the three pools with the concentrations of $C_{DO,i}$:

$$C_{DO} = C_{DO,1} + C_{DO,2} + C_{DO,3}. \quad (2)$$

The labile DOC pool (DOC_1) is generated by the fragmentation of autochthonous POC and by excretion from phytoplankton, and the semilabile (DOC_2) and refractory (DOC_3) pools are generated, in equal proportions, by the fragmentation of allochthonous POC. Semilabile and refractory DOC also enter the lake through inflow with fractions set in the model code. The initial, depth-independent fractions of the POC and DOC pools in the water column are set in the initial data file. The settling speed of POC is set equal to that of chlorophyll *a* (P_{Chla}).

The description of the structure of bottom sediment is somewhat modified from that in MyLake v.1.2. The active sediment layer consists of inorganic (S), living organic (P_{Chla}), and dead organic (C_{PO}) particles sedimenting from the water column. The volume fractions of dry inorganic matter, dry living organic matter (or living sedimentary particulate organic matter $SPOM_L$), and dry dead organic matter (or dead sedimentary particulate organic matter $SPOM$) in the total dry sediment solids are v_{IM} , v_{LPOM} , and v_{DPOM} , respectively. The corresponding forms of sedimentary organic carbon are living sedimentary particulate organic carbon POC_{Lsed} and dead sedimentary particulate organic carbon POC_{sed} .

The initial mass fraction of chlorophyll *a* in SPOM_L is given as a constant parameter $s_{\text{Chl, sed}} = 1.25 \times 10^4 \text{ mg kg}^{-1}$, and it is updated along with the sedimentation of living organic matter. The concentration of Chl *a* in the total sediment solids $[\text{mg Chl } a (\text{m dry sediment})^{-3}]$ is given by

$$P_{\text{Chl, sed}} = s_{\text{Chl, sed}} \rho_{\text{org}} V_{\text{LPOM}}, \quad (3)$$

where $\rho_{\text{org}} = 1000 \text{ kg m}^{-3}$ is the density of organic sediment. Correspondingly, the concentrations of POC_{Lsed} and POC_{sed} $[\text{mg C} (\text{m dry sediment})^{-3}]$ are given by

$$C_{\text{PO, sed}} = s_{\text{C}} \rho_{\text{org}} V_{\text{DPOM}} \quad (4)$$

and

$$C_{\text{LPO, sed}} = s_{\text{C}} \rho_{\text{org}} V_{\text{LPOM}}, \quad (5)$$

respectively.

Organic carbon processes in the water column

The term for the in-lake sources and sinks of water column POC is given as

$$S_{\text{POC}} = d_{\text{Chl}} + F - d_{\text{POC}} + S_{\text{POC, sed}}, \quad (6)$$

where $d_{\text{Chl}} [\text{mg m}^{-3} \text{ d}^{-1}]$ is the conversion of phytoplankton to POC, $F [\text{mg m}^{-3} \text{ d}^{-1}]$ is the loss of allochthonous DOC due to flocculation, $d_{\text{POC}} [\text{mg m}^{-3} \text{ d}^{-1}]$ is the fragmentation of POC to DOC, and $S_{\text{POC, sed}} [\text{mg m}^{-3} \text{ d}^{-1}]$ is the resuspension of POC_{sed} from the bottom sediment. The corresponding term for DOC is

$$S_{\text{DOC}} = d_{\text{POC}} + E - F - d_{\text{DOC}}, \quad (7)$$

where $E [\text{mg m}^{-3} \text{ d}^{-1}]$ is the amount of excretion of labile DOC from phytoplankton and $d_{\text{DOC}} [\text{mg m}^{-3} \text{ d}^{-1}]$ is the degradation of DOC to CO₂.

The generation of allochthonous POC through the death of phytoplankton is given by

$$d_{\text{Chl}} = m C_{\text{PP}}, \quad (8)$$

where $m [\text{d}^{-1}]$ is calculated similarly to the rate of phytoplankton remineralization in MyLake v.1.2. However, it has been redefined as the death rate of phytoplankton.

Autochthonous and allochthonous POC pools convert into DOC by fragmentation with the rates $k_{\text{POC},1}$ and $k_{\text{POC},2}$ $[\text{d}^{-1}]$, respectively, as

$$d_{\text{POC}} = f_{\text{POC}} \sum_{i=1}^2 k_{\text{POC},i} C_{\text{PO},i}, \quad (9)$$

where $C_{\text{PO},i}$ is the concentration of the POC pool i and $f_{\text{POC}} [-]$ is the temperature correction factor for POC fragmentation, given as

$$f_{\text{POC}} = \begin{cases} \theta_{\text{POC}}^{T-20} & T \geq 4^\circ\text{C}, \\ \theta_{\text{POC}}^{-16} \theta_c^{T-4} & T < 4^\circ\text{C}, \end{cases} \quad (10)$$

where θ_{POC} is the temperature adjustment coefficient for POC degradation and θ_c is the temperature adjustment coefficient for organic carbon degradation at temperatures below 4 °C. Different values for θ_{POC} are applied for temperatures above and below 10 °C. The DOC generated from POC_1 is added to the labile pool, and the DOC generated from POC_2 is divided equally between semilabile and refractory pools.

The excretion of DOC from phytoplankton is given by

$$E = r_{\text{ex}} \mu C_{\text{PP}}, \quad (11)$$

where r_{ex} [-] is the DOC excretion fraction and μ [d^{-1}] is the specific growth rate of phytoplankton in MyLake 1.2. In MyLake C, μ is limited by available phosphate. This is in contrast to MyLake v.1.2, where it is the net specific rate of change in chlorophyll *a* concentration, r , that is limited by available phosphate. The excreted DOC is added to the labile pool.

Flocculation relocates a portion of allochthonous DOC into allochthonous POC. It is calculated as

$$F = k_{\text{floc}} \sum_{i=2}^3 C_{\text{DO},i}. \quad (12)$$

The flocculation rate $k_{\text{floc}} = 0.0019 \text{ d}^{-1}$ is set in the model code.

Dissolved organic carbon degradation

The description of DOC degradation is based on the FOKEMA submodule (Holmberg et al., 2014) with some reformulations and refinements. The FOKEMA submodule incorporated into MyLake v.1.2 is based on a three-pool first-order kinetic model for bacterial degradation of DOC by Vähätalo et al. (2010) and on a model for photochemical mineralization by Vähätalo et al. (2000). Each DOC pool has its own bacterial degradability. The degradation rates at 20 °C [d^{-1}] are $k_{\text{DOC},1}$, $k_{\text{DOC},2}$, and $k_{\text{DOC},3}$, respectively. The degradation rate of the refractory pool, $k_{\text{DOC},3}$, is set to 0 d^{-1} in the model code.

The degradation of DOC is calculated as the sum of bacterial degradation d_{DOC} and photochemical mineralization P_{B} . Oxygen limitation has been included through a half-saturation function based on Michaelis–Menten type kinetics. The total degradation of DOC in the water column is calculated as

$$d_{\text{DOC}} = \frac{O_{\text{D}}}{O_{\text{D,sat}} + O_{\text{D}}} f_{\text{DOC}} d_{\text{DOC}(20)} + P_{\text{B}}, \quad (13)$$

where $O_{\text{D,sat}} = 500 \text{ mg m}^{-3}$ is the oxygen half-saturation constant; f_{DOC} is the temperature correction factor; $d_{\text{DOC}(20)}$ [$\text{mg m}^{-3} \text{ d}^{-1}$] is the bacterial DOC degradation at 20 °C; and P_{B} [$\text{mg m}^{-3} \text{ d}^{-1}$] is the photochemical mineralization of DOC. The temperature correction factor is given as

$$f_{\text{DOC}} = \begin{cases} \theta_{\text{DOC}}^{T-20} & T \geq 4^\circ\text{C}, \\ \theta_{\text{DOC}}^{-16} \theta_c^{T-4} & T < 4^\circ\text{C}, \end{cases} \quad (14)$$

where θ_{DOC} is the temperature adjustment coefficient for DOC degradation. Different values for θ_{DOC} are applied for temperatures above and below 10 °C. The bacterial DOC degradation at 20 °C is given according to FOKEMA

as

$$d_{\text{DOC}(20)} = \frac{1}{\Delta t} \sum_{i=1}^3 (1 - e^{-k_{\text{DOC},i}\Delta t}) C_{\text{DO},i}, \quad (15)$$

where $\Delta t = 1$ d is the model time step.

Photochemical mineralization is largely induced by ultraviolet (UV) radiation located in the high-energy region of the solar radiation spectrum (Vähätalo et al., 2000). Because UV radiation is attenuated rapidly in the water column especially in humic lakes, photochemical mineralization is applied only to the topmost 1 m layer. It is calculated as

$$P_B = \frac{M(C)Q_{\text{SW},0}(1 - \alpha)A_s}{V_{0-1}} \int_{\lambda_{\min}}^{\lambda_{\max}} \phi_{\lambda} q_{\lambda} d\lambda, \quad (16)$$

where $M(C) = 12 \text{ g mol}^{-1}$ is the molar mass of carbon, $Q_{\text{SW},0} [\text{W m}^{-2}]$ is the incident shortwave radiative heat flux at the surface, $\alpha [-]$ is the albedo at the water surface, $A_s [\text{m}^2]$ is the lake surface area, $V_{0-1} [\text{m}^3]$ is the volume of the topmost 1 m layer, $\lambda_{\min} = 300 \text{ nm}$ and $\lambda_{\max} = 800 \text{ nm}$ are the minimum and maximum wavelengths contributing to photochemical mineralization, $\phi_{\lambda} [\text{mol C} (\text{mol quanta})^{-1} \text{ nm}^{-1}]$ is the spectrum of apparent quantum yield for photochemical DOC mineralization, and q_{λ} is the monthly spectral scalar photon density above the water surface, in units of $\text{mol quanta m}^{-2} \text{ d}^{-1}$, normalized to an irradiance of 1 W m^{-2} . The file *Qlambda.txt* contains the values for q_{λ} measured in Lake Pääjärvi, Finland, and the values for ϕ_{λ} are included in the model code.

Organic carbon degradation in bottom sediment

Both living sedimentary particulate organic matter SPOM_L and dead sedimentary particulate organic matter SPOM degrade directly to inorganic substances, without an intermediate dissolved phase. The daily degradation of SPOM_L occurs before that of SPOM . The loss of SPOM_L is given in Chl *a* units by

$$d_{\text{Chl, sed}} = k_{\text{Chl, sed}} \frac{O_D}{O_{D, \text{sat}} + O_D} \theta^{T-20} P_{\text{Chl, sed}}, \quad (17)$$

where $k_{\text{Chl, sed}} [\text{d}^{-1}]$ is the degradation rate of SPOM_L and $\theta [-]$ is the temperature adjustment coefficient of phytoplankton mineralization in MyLake v.1.2. The concentration of DO in sediment pore water is equal to that in the corresponding water layer. The degradation of SPOM is calculated in carbon units as

$$d_{\text{POC, sed}} = k_{\text{POC, sed}} \frac{O_D}{O_{D, \text{sat}} + O_D} f_{\text{sed}} C_{\text{PO, sed}}, \quad (18)$$

where $k_{\text{POC, sed}} [\text{d}^{-1}]$ is the degradation rate of SPOM and $f_{\text{sed}} [-]$ is the temperature correction factor for sedimentary POC degradation, given by

$$f_{\text{sed}} = \begin{cases} \theta_{\text{sed}}^{T-20} & T \geq 4^{\circ}\text{C}, \\ \theta_{\text{sed}}^{-16} \theta_c^{T-4} & T < 4^{\circ}\text{C}, \end{cases} \quad (19)$$

where $\theta_{\text{sed}} [-]$ is the temperature adjustment coefficient for sedimentary POC degradation. Different values for θ_{sed} are applied for temperatures above and below 10°C .

However, the amount of DO in the active sediment layer determines the final amount of sedimentary organic matter degradation. If there is not enough DO for maximal degradation, the degradation is restricted by the available DO.

2.2.2 Carbonate system

The lake carbonate system in MyLake C includes the three fractions of dissolved inorganic carbon (DIC): carbon dioxide CO_2 (CO_2 molar density $[\text{mmol m}^{-3}]$ is hereafter denoted as $[\text{CO}_2]_m$), bicarbonate ion HCO_3^- ($[\text{HCO}_3^-]_m$), and carbonate ion CO_3^{2-} ($[\text{CO}_3^{2-}]_m$). The sum of the concentrations of aqueous CO_2 and carbonic acid (H_2CO_3) in the water column is considered as the concentration of CO_2 . The relative abundance of carbonate species is governed by pH, which is represented in MyLake C by the hydrogen ion concentration $[\text{H}^+]$ ($\text{pH} = -\log_{10}[\text{H}^+]$).

The temperature-dependent dissociation constants for HCO_3^- and CO_3^{2-} , given in units of mol kg^{-1} , are calculated according to Roy et al. (1993) as

$$\ln K_1 = 290.9097 - \frac{14554.21}{T} - 45.0575 \ln T, \quad (20)$$

$$\ln K_2 = 207.6548 - \frac{11843.79}{T} - 33.6485 \ln T, \quad (21)$$

respectively, where the water column temperature is given in Kelvin. The molar fractions of carbonates are calculated from $[\text{H}^+]$ by means of the dissociation constants as

$$\psi_{\text{CO}_2} = \frac{[\text{CO}_2]_m}{C_{\text{DI},m}} = \frac{[\text{H}^+]^2}{[\text{H}^+]^2 + K_1[\text{H}^+] + K_1K_2} \quad (22)$$

$$\psi_{\text{HCO}_3} = \frac{[\text{HCO}_3^-]_m}{C_{\text{DI},m}} = \frac{K_1[\text{H}^+]}{[\text{H}^+]^2 + K_1[\text{H}^+] + K_1K_2} \quad (23)$$

$$\psi_{\text{CO}_3} = \frac{[\text{CO}_3^{2-}]_m}{C_{\text{DI},m}} = \frac{K_1K_2}{[\text{H}^+]^2 + K_1[\text{H}^+] + K_1K_2}, \quad (24)$$

where $C_{\text{DI},m}$ $[\text{mmol m}^{-3}]$ is the molar density of DIC. The molar mass of DIC is defined as

$$\begin{aligned} M(C_{\text{DI}}) &= M(\text{CO}_2)\psi_{\text{CO}_2} + M(\text{HCO}_3^-)\psi_{\text{HCO}_3} + M(\text{CO}_3^{2-})\psi_{\text{CO}_3} \\ &= (44.01\psi_{\text{CO}_2} + 61.01\psi_{\text{HCO}_3} + 60.01\psi_{\text{CO}_3}) \text{ g mol}^{-1}. \end{aligned} \quad (25)$$

Hydroxide ion concentration $[\text{OH}^-]$ $[\text{mol l}^{-1}]$ is calculated through the temperature-dependent dissociation constant of water $K_W = [\text{H}^+][\text{OH}^-]$ $[\text{mol}^2 \text{ kg}^{-2}]$ given by Millero (1995)

$$\ln K_W = 148.9802 - \frac{13847.26}{T} - 23.6521 \ln T, \quad (26)$$

where the water column temperature is given in Kelvin. Total alkalinity A $[\text{meq l}^{-1}]$ is defined as

$$A = 0.001 \times ([\text{HCO}_3^-]_m + 2[\text{CO}_3^{2-}]_m) + 1000 \times ([\text{OH}^-] - [\text{H}^+]). \quad (27)$$

The molality of DIC $[\text{mol DIC (kg water)}^{-1}]$ and alkalinity divided by water density $[\text{meq kg}^{-1}]$ are conserved quantities under changes in temperature in the processes of mixing, diffusion, and convection. Thus, the calculations are performed in units of mol kg^{-1} by dividing all the concentrations by water density. The concentration of CO_2 is changed in biological processes that produce or consume CO_2 , in air-water CO_2 exchange, and as the result of inflow and outflow. New carbonate equilibrium is calculated after each of these processes. Alkalinity is

conserved in the input or output of CO_2 through surface flux or stream inflow, but it is altered by biological processes. Ammonium is assumed to be the only nitrogen source in photosynthesis and the only nitrogen compound released in organic matter degradation. Using the Redfield molar ratio of C:N:P of 106:16:1, the change in A due to biological processes is thus (Stumm and Morgan, 1981)

$$\Delta A = 0.001 \times \frac{14}{106M(\text{CO}_2)} \Delta[\text{CO}_2]_{\text{P,D}}, \quad (28)$$

where $\Delta[\text{CO}_2]_{\text{P,D}}$ [mg m^{-3}] is the change in CO_2 concentration due to photosynthesis or organic matter degradation and $M(\text{CO}_2) = 44.01 \text{ g mol}^{-1}$ is the molar mass of CO_2 .

Combining the equations for K_1 , K_2 , K_W , and A gives an equation for the new $[\text{H}^+]$ after the processes affecting water column temperature, CO_2 concentration, or alkalinity:

$$-[\text{H}^+]^4 + (-K_1 - A)[\text{H}^+]^3 + (K_W + K_1(C_{\text{DI}} - K_2 - A))[\text{H}^+]^2 + (K_1(K_W + K_2(2C_{\text{DI}} - A)))[\text{H}^+] + K_1 K_2 K_W = 0. \quad (29)$$

2.2.3 Sinks and sources of CO_2 and DO

DO is produced and CO_2 is consumed through phytoplankton photosynthesis, and DO is consumed and CO_2 is produced through phytoplankton respiration, DOC degradation in the water column, and organic carbon degradation in the bottom sediment. In addition, oxygen and CO_2 are exchanged with the atmosphere, and they enter the lake via stream inflow.

The conceptual in-lake source and sink term for DO is given as

$$S_{\text{DO}} = \Phi - R - D_{\text{DOC}} - D_{\text{sed}} - \frac{F_{\text{O}_2}}{\Delta z}, \quad (30)$$

where Φ [$\text{mg m}^{-3} \text{ d}^{-1}$] is DO production through photosynthesis, R [$\text{mg m}^{-3} \text{ d}^{-1}$] is DO consumption through phytoplankton respiration, D_{DOC} [$\text{mg m}^{-3} \text{ d}^{-1}$] is DO consumption via DOC degradation, D_{sed} [$\text{mg m}^{-3} \text{ d}^{-1}$] is DO consumption via sedimentary POC degradation, F_{O_2} [$\text{mg m}^{-2} \text{ d}^{-1}$] is the air-water flux of oxygen, and Δz [m] is the thickness of the model grid layer. The corresponding term for CO_2 is

$$S_{\text{CO}_2} = D'_{\text{DOC}} + D'_{\text{sed}} + R' - \Phi' - \frac{F_{\text{CO}_2}}{\Delta z}, \quad (31)$$

where D'_{DOC} [$\text{mg m}^{-3} \text{ d}^{-1}$] is CO_2 production through DOC degradation, D'_{sed} [$\text{mg m}^{-3} \text{ d}^{-1}$] is CO_2 production through sedimentary POC degradation, R' [$\text{mg m}^{-3} \text{ d}^{-1}$] is CO_2 production through phytoplankton respiration, Φ' [$\text{mg m}^{-3} \text{ d}^{-1}$] is CO_2 consumption in photosynthesis, and F_{CO_2} [$\text{mg m}^{-2} \text{ d}^{-1}$] is the air-water flux of CO_2 .

Air-water exchange

The fluxes of CO_2 and oxygen between water and the atmosphere are parametrized as the products of the respective concentration differences between the surface water and the atmosphere and the gas exchange velocities k_{gas} [m d^{-1}] as

$$F_{\text{gas}} = k_{\text{gas}}(C_{\text{w,gas}} - C_{\text{eq,gas}}), \quad (32)$$

where $C_{w, \text{gas}}$ [mg m^{-3}] is the concentration of the gas in the topmost layer and $C_{\text{eq}, \text{gas}}$ [mg m^{-3}] is the equilibrium concentration of the gas. Chemical enhancement of CO_2 exchange is not included in MyLake C. The equilibrium concentrations of CO_2 and oxygen are calculated by Henry's law as

$$C_{\text{eq}, \text{gas}} = M(\text{gas})K_{\text{H}, \text{gas}}\chi_{\text{gas}}p_a, \quad (33)$$

where $M(\text{gas})$ [g mol^{-1}] is the molar mass of the gas, $K_{\text{H}, \text{gas}}$ [$\text{mol l}^{-1} \text{atm}^{-1}$] is the solubility constant or Henry's law constant for the gas at surface water temperature, χ_{gas} [$\mu\text{mol mol}^{-1}$] is the mole fraction of the gas in the atmosphere, and p_a [atm] is the atmospheric pressure.

The temperature-dependent solubility constant for CO_2 , $K_{\text{H}, \text{CO}_2}$, is calculated on the basis of the fit by Weiss (1974) in units of $\text{mol kg}^{-1} \text{atm}^{-1}$ as

$$\ln K'_{\text{H}, \text{CO}_2} = -60.2409 + 93.4517 \frac{100}{T_s} + 23.3585 \ln \frac{T_s}{100}, \quad (34)$$

where T_s [K] is the temperature of the topmost water layer. The conversion of the solubility constant to units of $\text{mol l}^{-1} \text{atm}^{-1}$ is performed by multiplying $K'_{\text{H}, \text{CO}_2}$ by the density of the topmost water layer. The corresponding solubility constant for oxygen is calculated according to the fit by Weiss (1970)

$$\ln K_{\text{H}, \text{O}_2} = -58.3877 + 85.8079 \frac{100}{T_s} + 23.8439 \ln \frac{T_s}{100}, \quad (35)$$

where T_s is given in Kelvin. The value of $2.1 \times 10^5 \mu\text{mol mol}^{-1}$ is used as the mole fraction of oxygen in the atmosphere, and the mole fraction of CO_2 is a user-definable parameter $\chi_{\text{CO}_2, 0}$. The atmospheric mole fraction of CO_2 varies seasonally as

$$\chi_{\text{CO}_2} = \chi_{\text{CO}_2, 0} + 4 \sin\left(2\pi \frac{t + 0.310625}{365.2425}\right). \quad (36)$$

The gas exchange velocities (in units of m d^{-1}) for CO_2 and oxygen are calculated the formula by Cole and Caraco (1998):

$$k_{\text{gas}} = 0.24 \times (2.07 + 0.215U_{10}^{1.7}) \left(\frac{Sc_{\text{gas}}}{600}\right)^{-2/3}, \quad (37)$$

where U_{10} [m s^{-1}] is the wind speed at 10 m and Sc_{gas} is the Schmidt number of the gas. The temperature-dependent Schmidt numbers of CO_2 and oxygen are calculated according to Wanninkhof (1992) as

$$Sc_{\text{CO}_2} = 1911.1 - 118.11T_s + 3.4527T_s^2 - 0.041320T_s^3 \quad (38)$$

and

$$Sc_{\text{O}_2} = 1800.6 - 120.10T_s + 3.7818T_s^2 - 0.047608T_s^3, \quad (39)$$

respectively, where T_s is given in degrees Celsius.

The air-water gas fluxes are calculated after the application of biochemical gas sources and sinks within the water column and in the sediment but before the addition of stream loading and the process of wind-induced mixing. Gas influx is added to the topmost water layer, and the subsequent wind-induced mixing then distributes the dissolved gas in the epilimnion. However, a high CO_2 efflux from only the topmost layer may result in a negative concentration, and the carbonate equilibrium cannot be solved correctly. In the case of supersaturated surface

water, the amount of calculated surface flux is first compared with the excess of the gas in the topmost water layer. If there is not enough excess dissolved gas for the calculated gas efflux in the topmost layer, consecutive layers are equilibrated with the atmosphere until the required amount of CO_2 has been transferred.

Processes in the water column

Phytoplankton photosynthesis consumes CO_2 and produces DO within the water column. The rate of apparent photosynthesis – the individual-scale process related to the concept of gross primary production – is defined as the rate of gross carbon fixation subtracted by the rate of photorespiration. The production of DO in apparent photosynthesis is given by

$$\Phi = \frac{M(\text{O}_2)}{M(\text{C})} Q_p \mu_{\text{C}_{\text{PP}}}, \quad (40)$$

where $M(\text{O}_2) = 32 \text{ g mol}^{-1}$ is the molar mass of oxygen and $Q_p [\text{mmol O}_2 (\text{mmol CO}_2)^{-1}]$ is the photosynthetic quotient. The photosynthetic quotient (always > 1) expresses the molar ratio of oxygen released to CO_2 assimilated during photosynthesis. The consumption of CO_2 during apparent photosynthesis is correspondingly

$$\Phi' = \frac{M(\text{CO}_2)}{M(\text{O}_2)} \frac{1}{Q_p} \Phi. \quad (41)$$

The consumption of DO in phytoplankton cellular respiration, or dark respiration, is calculated as

$$R = \frac{M(\text{O}_2)}{M(\text{C})} r_{\text{PP}} \mu_{\text{C}_{\text{PP}}}, \quad (42)$$

where $r_{\text{PP}} [-]$ is the phytoplankton cellular respiration fraction, and the production of CO_2 in phytoplankton respiration is

$$R' = \frac{M(\text{CO}_2)}{M(\text{O}_2)} R. \quad (43)$$

The production of CO_2 through DOC degradation is found simply by expressing the mineralized carbon in CO_2 mass units:

$$D'_{\text{DOC}} = \frac{M(\text{CO}_2)}{M(\text{C})} d_{\text{DOC}}. \quad (44)$$

The consumption of DO in DOC degradation is obtained by

$$D_{\text{DOC}} = \frac{M(\text{O}_2)}{M(\text{CO}_2)} \frac{1}{Q_r} D'_{\text{DOC}}, \quad (45)$$

where Q_r is the respiratory quotient $[\text{mmol CO}_2 (\text{mmol O}_2)^{-1}]$, which expresses the molar ratio of CO_2 production to DO consumption in bacterial respiration.

Processes in bottom sediment

Sedimentary organic matter degradation consumes DO from the overlying water column grid layer. The decrease of DO concentration in layer i via SPOM_L degradation is calculated as

$$D_{\text{Chl, sed}, i} = \frac{1}{Q_r} \frac{M(\text{O}_2)}{M(\text{C})} \frac{s_{\text{C}}}{s_{\text{Chl, sed}}} \frac{V_{\text{sed}, i}}{V_i} d_{\text{Chl, sed}, i}, \quad (46)$$

where V_i is the volume of layer i and $V_{\text{sed},i}$ is the volume of the active sediment layer below the layer i . Correspondingly, the DO concentration decrease in layer i via SPOM degradation is

$$D_{\text{POC},\text{sed},i} = \frac{1}{Q_r} \frac{M(\text{O}_2)}{M(\text{C})} \frac{V_{\text{sed},i}}{V_i} d_{\text{POC},\text{sed},i}. \quad (47)$$

Total DO consumption through sedimentary organic matter degradation is given by

$$D_{\text{sed}} = D_{\text{Chl},\text{sed}} + D_{\text{POC},\text{sed}}. \quad (48)$$

The produced CO_2 is released to the overlying water column grid layer. The increase in water column CO_2 concentration through the total sedimentary organic matter degradation is

$$D'_{\text{sed}} = \frac{M(\text{CO}_2)}{M(\text{O}_2)} Q_r D_{\text{sed}}. \quad (49)$$

3 Other reformulations and developments in MyLake C

3.1 Physical processes

In MyLake C, the attenuation of PAR in the water column is explicitly dependent on the concentrations of both phytoplankton and DOC. The non-chlorophyll-related PAR attenuation coefficient in MyLake v.1.2 has been replaced by a coefficient dependent on DOC concentration, $K_{\text{DOC},\text{P}}$ [m^{-1}], and the averaged DOC-related PAR attenuation coefficient down to depth z is calculated as

$$\bar{K}_{\text{DOC},\text{P}}(z) = \beta_{\text{DOC}} \bar{C}_{\text{DO}}(z), \quad (50)$$

where β_{DOC} [$\text{m}^2 \text{mg}^{-1}$] is the DOC-related specific PAR attenuation coefficient of water and $\bar{C}_{\text{DO}}(z)$ is the average DOC concentration from the surface to depth z . The total PAR attenuation coefficient down to depth z is then calculated as in MyLake v.1.2:

$$\bar{K}_{\text{P}}(z) = \bar{K}_{\text{DOC},\text{P}}(z) + \beta \bar{P}_{\text{Chla},1}(z) + \beta_2 \bar{P}_{\text{Chla},2}(z), \quad (51)$$

where β and β_2 are the optical cross sections of group 1 chlorophyll and group 2 chlorophyll, respectively, and $\bar{P}_{\text{Chla},i}(z)$ is the average group i chlorophyll a concentration from the surface to depth z .

The albedo of snow is set to half of its default value when the snow density ρ_s is greater than $0.9\rho_{s,\text{max}}$, which is related to the fact that heavy snow may be partially melted and refrozen and thus have characteristics close to those of ice. Instead of the constant default value of 250 kg m^{-3} in MyLake v.1.2, the density of fresh snow $\rho_{s,\text{new}}$ [kg m^{-3}] is calculated based on the formula by Hedstrom and Pomeroy (1998) by

$$\rho_{s,\text{new}} = \frac{200}{119.07} (67.92 + 51.25 e^{T_a/2.59}), \quad (52)$$

where T_a [$^{\circ}\text{C}$] is air temperature.

Some additional changes were made in the MyLake C model code in the preliminary manual calibration of a model application to a seasonally ice-covered lake.

- In the ice-snow submodel
 - the frazil ice threshold is set to the value of 1.3 cm, and
 - precipitation is classified as snow only when the average daily air temperature is lower than $-1\text{ }^{\circ}\text{C}$.
- Both daytime and nighttime surface heat fluxes are calculated using the lake surface temperature at the previous time step.
- The average of the temperature profiles at the current time step and the previous time step is used in the calculation of the potential energy required in wind-induced mixing (Eq. 25 in Saloranta and Andersen (2004)) in order to compensate for the error that may be originated from the sequential nature of the surface heat transfer and wind-induced mixing processes in the model.
- River inflow is added above the first water layer heavier than the inflow as in MyLake v.1.2 but not deeper than $z_{\max}/2$ where z_{\max} is the maximum depth of the lake.
- Instead of using linear initial profiles for sediment temperature, the profiles were estimated somewhat more rigorously. The sediment temperature profiles at depths of 2, 3.5, 6, and 10 m were estimated by running a multi-year simulation with the meteorological forcing of the model application and selecting the resulting sediment temperature profiles on the model start date (8 January). The sediment temperature profiles at other depths were linearly interpolated. The values for the thermal diffusivity of the sediment and the specific heat capacity of the sediment have also been altered.

3.2 Particulate organic phosphorus

The description of phosphorus cycling has been extended to include the phosphorus in dead particulate organic matter. The aim was not to describe the phosphorus cycling and simulate the phosphorus concentrations as correctly as possible but to introduce relevant variables and to revise the phosphorus processes so that they are in accordance with the new carbon-related biochemical processes introduced to MyLake C. The parameter values and the initial values related to phosphorus cycling were adjusted so that the phosphorus concentrations remained sensible during the course of the simulations. The description of organic phosphorus needs corrections and additional development if one wants to explicitly simulate phosphorus cycling with MyLake C.

Particulate organic phosphorus (P_{PO}) is integrated into dead particulate organic matter POM. It is included in the inflow concentration of total phosphorus and taken into account in the determination of total phosphorus concentration in the model calculations. Dissolved inorganic phosphorus is produced via the fragmentation of POM (or POC) in the water column and via the degradation of SPOM in the sediment. The amount of particulate organic phosphorus in allochthonous POM is determined by the parameter $s_{\text{P,POM}}$, which is the carbon to phosphorus mass ratio in allochthonous POM. The carbon to phosphorus mass ratio in autochthonous dead POM is the same as in phytoplankton, s_{P} . The total particulate organic concentration in the water column [mg m^{-3}] is thus

$$P_{\text{PO}} = \frac{C_{\text{PO},1}}{s_{\text{P}}} + \frac{C_{\text{PO},2}}{s_{\text{P,POM}}}. \quad (53)$$

The concentration of particulate organic phosphorus in the sediment $P_{PO, sed}$ [mg P (m dry sediment)⁻³] is determined by the parameter $s_{P, sed}$ [[mg C (mg P)⁻¹]], which is the initial carbon to phosphorus mass ratio in dry nonliving organic sedimentary matter (SPOM):

$$P_{PO, sed} = \frac{C_{PO, sed}}{s_{P, sed}}. \quad (54)$$

In MyLake 1.2, the net production or consumption of dissolved inorganic phosphorus by the growth and the mineralization of phytoplankton is calculated through the net change in chlorophyll concentration. In MyLake C, phytoplankton growth consumes dissolved inorganic phosphorus, and dissolved inorganic phosphorus is released from dead particulate organic matter through the fragmentation of dead POC. In other words, dissolved inorganic phosphorus is not released in the transformation of living phytoplankton into dead particulate organic matter in MyLake C.

The mineralization of particulate organic phosphorus in the sediment is calculated separately from the degradation of SPOM. Sedimentary particulate organic phosphorus is mineralized directly to dissolved inorganic phosphorus. The mineralization rate is set in the model code. The degradation of SPOM_L produces dissolved inorganic phosphorus as in MyLake v.1.2. The ratio $s_{P, sed}$ is updated according to the degradation of SPOM and net sedimentation of POM. The mass fraction of phosphorus in sedimenting POM is calculated from the fractions of autochthonous and allochthonous POC in the water column.

3.3 Order of simulation

The biochemical processes are calculated in sequence after the application of heat sources, thermal diffusion, and related convection. The order of biochemical processes is as follows:

- Loss of POC due to fragmentation
- Mineralization and diffusion of dissolved organic phosphorus
- Mineralization of particulate organic phosphorus
- Determination of phytoplankton (chlorophyll *a*) growth and loss rates
- Resuspension, diffusion, and advection of particulate inorganic matter and particulate inorganic phosphorus
- Growth and loss of phytoplankton
 - Determination of the net growth, gross growth, and loss of phytoplankton
 - Excretion of DOC from phytoplankton due to phytoplankton gross growth
- Phytoplankton respiration (CO₂ production and DO consumption) due to phytoplankton gross growth
- Transfer of dead phytoplankton to autochthonous POC
- Net growth, resuspension, diffusion, and advection of phytoplankton
- Loss of dissolved inorganic phosphorus due to phytoplankton growth and diffusion of dissolved inorganic phosphorus
- Loss of DOC due to flocculation
- Increase in POC due to resuspension and DOC flocculation
- Increase in DOC due to POC fragmentation

- Diffusion and advection of POC
- Degradation and diffusion of DOC
- DO production in photosynthesis, DO consumption in DOC degradation, and DO diffusion
- CO₂ consumption in photosynthesis, CO₂ production in DOC degradation, and CO₂ diffusion
- Sediment processes (only carbon-related processes are listed here)
 - Sedimentation of dead SPOM and living SPOM
 - Determination of new $s_{\text{Chl, sed}}$
 - Calculation of the degradation of living SPOM
 - DO consumption due to living SPOM degradation
 - Calculation of the degradation of dead SPOM
 - DO consumption due to dead SPOM degradation
 - CO₂ production due to degradation of living and dead SPOM
 - Mineralization of sedimentary particulate organic phosphorus
 - Calculation of new volume fractions of living and dead SPOM due to sedimentary organic matter degradation
 - Determination of new $s_{\text{P, sed}}$
 - Change in particulate organic phosphorus concentration due to net sedimentation of POM
- Air-water surface flux of oxygen
- Air-water surface flux of CO₂

4 Running a MyLake C model application

4.1 Model code

The MyLake C model code is comprised of 18 MATLAB function files, of which 12 are new, 3 include modifications in comparison to MyLake v.1.2 (*convection_v12_1aIC.m*, *modelinputs_v12_new.m*, and *solvemodel_vC.m*) and 3 remain unchanged from MyLake v.1.2 (*heatflux_v12.m*, *IOflow_v11.m*, and *sedimentheat_v11.m*).

<i>solvemodel_vC.m</i>	Contains most of the model algorithm and numerical procedures.
<i>modelinputs_v12_new.m</i>	Handles the reading of input data, initial conditions, and model parameters from the three Excel files described in Section 4.2.
<i>convection_v12_1aIC.m</i>	Handles the vertical convection caused by unstable vertical water temperature distribution.
<i>heatflux_v12.m</i>	Handles the calculation of surface heat fluxes and other related physical variables. Utilizes the MATLAB Air-Sea Toolbox (https://sea-mat.github.io/sea-mat).
<i>IOflow_v11.m</i>	Handles the addition of stream loading and inflow.
<i>sedimentheat_v11.m</i>	Calculates sediment-water heat exchange and heat diffusion in sediment.
<i>carbondioxideflux.m</i>	Calculates the CO ₂ flux between water and the atmosphere.

<i>carbonequilibrium.m</i>	Calculates the equilibrium state of the dissolved inorganic carbon (carbonate) system.
<i>DIC_convection2.m</i>	Calculates the equilibrium state of the carbonate system after the changes in the DIC and H^+ distributions due to convection.
<i>DIC_diffusion2.m</i>	Calculates the vertical diffusion of DIC and H^+ and the equilibrium state of the carbonate system after the changes in the DIC and H^+ distributions due to the diffusion.
<i>DIC_windmix.m</i>	Calculates the equilibrium state of the carbonate system after the changes due to wind mixing.
<i>DICsystem_bio.m</i>	Calculates the equilibrium state of the carbonate system after the changes in CO_2 concentration and alkalinity in biochemical processes.
<i>DICsystem_new.m</i>	Calculates the equilibrium state of the carbonate system after changes in water column temperature or after the air-water CO_2 flux.
<i>dissconst.m</i>	Calculates the dissociation constants of CO_2 , HCO_3^- , and H_2O .
<i>fokema_new.m</i>	Calculates the degradation of dissolved organic carbon.
<i>IOflow_DIC.m</i>	Calculates the equilibrium state of the carbonate system after the changes in the DIC and H^+ distributions due to inflow.
<i>oxygenflux.m</i>	Calculates the oxygen flux between water and the atmosphere.
<i>relative_oxygen.m</i>	Calculates the relative and absolute saturations of dissolved oxygen.

4.2 Revisions to parameter and input file structures

The three input and parameter data files are updated versions of those described in detail in Saloranta and Andersen (2005).

4.2.1 Meteorological and inflow time series

Rows

1.–2. Header rows (The cell A1 must contain a number)

3.–end Data rows

Columns

1. Year
2. Month
3. Day

4. Global radiation [$\text{MJ m}^{-2} \text{d}^{-1}$]
5. Cloud cover (0–1)
6. Air temperature (at 2 m height) [$^{\circ}\text{C}$]
7. Air pressure [hPa]
8. Wind speed (at 10 m height) [m s^{-1}]
9. Precipitation [mm d^{-1}]
10. Inflow volume [$\text{m}^3 \text{d}^{-1}$]
11. Inflow temperature [$^{\circ}\text{C}$] (if inflow temperature is set to 'NaN', the inflow is assumed to mix with the topmost layer)
12. Inflow concentration of group 2 chlorophyll *a* ($P_{\text{Chla},2}$) [mg m^{-3}]
13. Inflow concentration of suspended inorganic particulate matter (*S*) [kg m^{-3}]
14. Inflow concentration of total phosphorus ($P_{\text{D}} + P_{\text{IP}} + P_{\text{DO}} + (P_{\text{Chla},1} + P_{\text{Chla},2})/y_{\text{c}}$) [mg m^{-3}]
15. Inflow concentration of dissolved organic phosphorus (P_{DO}) [mg m^{-3}]
16. Inflow concentration of group 1 chlorophyll *a* ($P_{\text{Chla},1}$) [mg m^{-3}]
17. Inflow concentration of dissolved organic carbon (C_{DO}) [mg m^{-3}]
18. Inflow concentration of dissolved inorganic carbon (C_{DI}) [mg m^{-3}]
19. Inflow concentration of dissolved oxygen (O_{D}) [mg m^{-3}]
20. Inflow concentration of particulate organic carbon (C_{PO}) [mg m^{-3}]
21. Inflow concentration of hydrogen ion (H^{+}) [mol l^{-1}] ($10^{-\text{pH}}$)

4.2.2 Bathymetry and initial profiles

Rows

- 1.–2. Header rows (The cell A1 must contain a number)
- 3.–end Data rows

Columns

1. Depth levels (m from surface, positive values). The first and the last levels have to be 0 and the lake maximum depth (rounded up to the next multiple of the model grid length), respectively.

2. Horizontal areas [m^2]. The first and the last levels have to be the lake surface area and 0, respectively.
3. Initial profile of temperature [$^{\circ}\text{C}$]
4. Initial profile of group 2 chlorophyll *a* ($P_{\text{Chla},2}$) [mg m^{-3}]
5. Initial profile of suspended inorganic particulate matter (S) [kg m^{-3}]
6. Initial profile of total phosphorus ($P_{\text{D}} + P_{\text{P}} + P_{\text{DO}} + (P_{\text{Chla},1} + P_{\text{Chla},2})/y_{\text{c}}$) [mg m^{-3}]
7. Initial profile of dissolved organic phosphorus (P_{DO}) [mg m^{-3}]
8. Initial profile of group 1 chlorophyll *a* ($P_{\text{Chla},1}$) [mg m^{-3}]
9. Initial profile of dissolved organic carbon (C_{DO}) [mg m^{-3}]
10. Initial profile of dissolved inorganic carbon (C_{DI}) [mg m^{-3}]
11. Initial profile of dissolved oxygen (O_{D}) [mg m^{-3}]
12. Initial profile of particulate organic carbon (C_{PO}) [mg m^{-3}]
13. Initial profile of sediment bulk concentration of total phosphorus ($P_{\text{D}} + P_{\text{P}} + P_{\text{DO}} + P_{\text{Chla}}/y_{\text{c}} + P_{\text{POC}}$) [mg m^{-3} wet weight]
14. Initial profile of sediment volume fraction of dead organic matter [$\text{m}^3 \text{m}^{-3}$ dry weight]
15. Initial profile of sediment volume fraction of inorganic matter [$\text{m}^3 \text{m}^{-3}$ dry weight]
16. Initial profile of pH [-] ($-\log_{10}[\text{H}^+]$)
17. Initial value of total ice thickness [m]
18. Initial value of snow thickness [m]
19. Initial fraction of autochthonous (pool 1) dissolved organic carbon in the water column
20. Initial fraction of semilabile allochthonous (pool 2) dissolved organic carbon in the water column
21. Initial fraction of autochthonous (pool 1) particulate organic carbon in the water column

The initial profile of sediment bulk concentration of chlorophyll *a* is determined from the sediment volume fraction of living organic matter by using a value of $12\,500 \text{ mg Chla} (\text{kg organic matter})^{-1}$ as the initial mass fraction of chlorophyll *a* of living sedimentary organic matter.

4.2.3 Model parameters

Rows

1. Header row (The cell A1 must contain a number)
2. Header row

3. dz [m], model vertical grid length
4. a_k [-], vertical turbulent diffusion parameter during open water periods
5. $a_{k,ice}$ [-], vertical turbulent diffusion parameter during ice-covered periods
6. N_{min}^2 [s^{-2}], minimum stability (buoyancy, Brunt–Vaisala) frequency
7. W_{str} [-], wind sheltering coefficient
8. Lake latitude (decimal degrees)
9. Lake longitude (decimal degrees)
10. α_i [-], albedo of ice
11. α_s [-], albedo of snow
12. I' [$mol\ quantam^{-2}s^{-1}$], light saturation level of photosynthesis for group 2 chlorophyll a
13. f_{PAR} [-], fraction of photosynthetically active radiation (PAR) of the total shortwave energy
14. β [$m^2 mg^{-1}$], optical cross section of group 1 chlorophyll
15. λ_{ice} [m^{-1}], PAR attenuation coefficient for ice
16. λ_{snow} [m^{-1}], PAR attenuation coefficient for snow
17. ϕ_{sld} [-], volume fraction of solids in the sediment
18. I_{scV} [], dimensionless scaling factor for inflow volume
19. I_{scT} [$^{\circ}C$], scaling factor for inflow temperature
20. $I_{scP_{Chla,2}}$ [-], dimensionless scaling factor for inflow concentration of group 2 chlorophyll a
21. I_{scS} [-], dimensionless scaling factor for inflow concentration of suspended inorganic particulate matter
22. $I_{scP_{tot}}$ [-], dimensionless scaling factor for inflow concentration of total phosphorus
23. $I_{scP_{DO}}$ [-], dimensionless scaling factor for inflow concentration of dissolved organic phosphorus
24. $I_{scP_{Chla,1}}$ [-], dimensionless scaling factor for inflow concentration of group 1 chlorophyll a
25. $I_{scC_{DO}}$ [-], dimensionless scaling factor for inflow concentration of dissolved organic carbon
26. $K_{0,nP}$ [m^{-1}], non-PAR attenuation (extinction) coefficient of water (non-chlorophyll-related) (denoted as $\hat{\epsilon}_0$ in MyLake v.1.2)
27. β_{DOC} [$m^2 mg^{-1}$], dissolved organic carbon-related specific PAR attenuation coefficient of water
28. $U_{res,epi}$ [md^{-1}], resuspension rate of dry sediment particles in the epilimnion
29. $U_{res,hypo}$ [md^{-1}], resuspension rate of dry sediment particles in the hypolimnion
30. H_{sed} [m], depth of the mixed, active sediment layer

31. P_{sat} [mg m^{-3}], Langmuir isotherm coefficient
32. F_{max} [mg kg^{-1}], Langmuir isotherm coefficient
33. w_s [m d^{-1}], settling speed of suspended particulate inorganic matter (S)
34. $w_{\text{Chl},1}$ [m d^{-1}], settling speed of organic particulate matter and group 1 chlorophyll a
35. y_c [$\text{mg Chl } a (\text{mg P})^{-1}$], yield coefficient, i.e., chlorophyll a to phosphorus mass ratio
36. m_{20} [d^{-1}], group 1 phytoplankton death rate at 20°C
37. μ'_{20} [d^{-1}], maximal group 1 phytoplankton growth rate at 20°C
38. $k_{\text{Chl},\text{sed}}$ [d^{-1}], degradation rate of living sedimentary particulate organic matter at 20°C
39. $k_{\text{DOP},20}$ [d^{-1}], specific P_{DO} to P_{D} mineralization rate coefficient at 20°C
40. P' [mg m^{-3}], phosphorus half-saturation constant for group 1 phytoplankton
41. I'_2 [$\text{mol quantam}^{-2} \text{s}^{-1}$], light saturation level of photosynthesis for group 2 chlorophyll a
42. β_2 [$\text{m}^2 \text{mg}^{-1}$], optical cross section of group 2 chlorophyll
43. $w_{\text{Chl},2}$ [m d^{-1}], settling speed of group 2 chlorophyll a
44. $m_{20,2}$ [d^{-1}], group 2 phytoplankton death rate at 20°C
45. $\mu'_{20,2}$ [d^{-1}], maximal group 2 phytoplankton growth rate at 20°C
46. P'_2 [mg m^{-3}], phosphorus half-saturation constant for group 2 phytoplankton
47. θ_{DOC} [-], temperature adjustment coefficient for DOC degradation at temperatures at and above 10°C
48. $\theta_{\text{DOC},i}$ [-], temperature adjustment coefficient for DOC degradation at temperatures below 10°C
49. θ_{sed} [-], temperature adjustment coefficient for organic carbon degradation in sediment at temperatures at and above 10°C
50. $\theta_{\text{sed},i}$ [-], temperature adjustment coefficient for organic carbon degradation in sediment at temperatures below 10°C
51. I_{scDI} [-], dimensionless scaling factor for inflow concentration of dissolved inorganic carbon
52. I_{scOD} [-], dimensionless scaling factor for inflow concentration of dissolved oxygen
53. r_{ex} [-], dissolved organic carbon excretion fraction
54. r_{PP} [-], phytoplankton respiration fraction
55. $s_{\text{P,POM}}$ [$\text{mg C} (\text{mg P})^{-1}$], carbon to phosphorus mass ratio in allochthonous particulate organic matter
56. $s_{\text{P,sed}}$ [$\text{mg C} (\text{mg P})^{-1}$], initial carbon to phosphorus mass ratio in dry nonliving organic sedimentary matter
57. $k_{\text{POC,sed}}$ [d^{-1}], degradation rate of dead sedimentary particulate organic matter at 20°C

58. $k_{\text{POC},1}$ [d^{-1}], fragmentation rate of labile (autochthonous) particulate organic carbon at 20 °C
59. $k_{\text{POC},2}$ [d^{-1}], fragmentation rate of semilabile (allochthonous) particulate organic carbon at 20 °C
60. $k_{\text{DOC},1}$ [d^{-1}], degradation rate of labile (autochthonous) dissolved organic carbon at 20 °C
61. $k_{\text{DOC},2}$ [d^{-1}], degradation rate of semilabile dissolved organic carbon at 20 °C
62. θ_c [-], temperature adjustment coefficient for organic carbon degradation at temperatures below 4 °C
63. Q_p [$\text{mmol O}_2 (\text{mmol CO}_2)^{-1}$], photosynthetic quotient
64. Q_r [$\text{mmol CO}_2 (\text{mmol O}_2)^{-1}$], respiratory quotient
65. $\chi_{\text{CO}_2,0}$ [$\mu\text{mol mol}^{-1}$], atmospheric CO_2 mole fraction

Columns

1. Parameter names
2. Parameter values
3. Minimum of the parameter value range (not used in MyLake C)
4. Maximum of the parameter value range (not used in MyLake C)
5. Parameter units

4.3 How to execute a MyLake C model run

In addition to the three Excel files, the file *Qlambda.txt* needs to be loaded as model input. A MyLake C model application can be run using the following MATLAB command:

```
[zz,Az,Vz,tt,Qst,Kzt,Tzt,Czt,Szt,Pzt,Chlzt,PPzt,DOPzt,D0Czt,D0Czt1,D0Czt2,D0Czt3,D0Ctfrac,Daily_BB1t,...
Daily_BB2t,Daily_BB3t,Daily_PBt,DICzt,C02zt,O2zt,O2_sat_relt,O2_sat_abst,P0Czt,B0Dzt,Qzt_sed,...
lambdazt,P3zt_sed,P3zt_sed_sc,His,DoF,DoM,MixStat,Wt,surfaceflux,oxygenflux,C02_eqt,K0t,O2_eqt,...
KO_O2t,C02_ppmt,d02Chlt,P0C1tfrac,d02S0Dt,d02D0Ct,pHt,testi3t,T_sedt]...
= solvemodel_vC(m_start,m_stop,initfile,initsheet,inputfile,'timeseries', parafile,'lake',Qlambda);
```

where `m_start` and `m_stop` [year, month, day] are row vectors of the simulation start and stop dates; `initfile`, `inputfile`, and `parafile` are strings containing the file names (either absolute or relative paths) of the three files containing lake morphometry and initial properties, the time series of meteorological variables and inflow properties, and model parameter values, respectively. Similarly, `initsheet`, `inputsheet`, and `parasheet` are strings containing the Excel worksheet names containing these data.

Model output variables

The model output variables are listed below with units indicated in square brackets. The output matrix dimensions are indicated in round brackets.

zz	Solution depth domain array (length N) [m], i.e., depths at the top of the layers
Az	Layer interface area [m^2] (N)
Vz	Layer volume [m^3] (N)
tt	Solution time domain array (length M), i.e., model day number [d]
Qst	Estimated surface heat fluxes [W m^{-2}] ($[Q_{\text{sw}} Q_{\text{LW}} Q_{\text{sensible}} + Q_{\text{latent}}] \times M$)
Kzt	Predicted vertical turbulent diffusion coefficient [$\text{m}^2 \text{d}^{-1}$] ($N \times M$)
Tzt	Predicted temperature profile [$^{\circ}\text{C}$] ($N \times M$)
Czt	Predicted chlorophyll a (group 2) profile ($P_{\text{Chla},2}$) [mg m^{-3}] ($N \times M$)
Szt	Predicted suspended inorganic particulate matter profile (S) [kg m^{-3}] ($N \times M$)
Pzt	Predicted dissolved inorganic phosphorus (phosphate) profile (P_{D}) [mg m^{-3}] ($N \times M$)
Chlzt	Predicted chlorophyll a (group 1) profile ($P_{\text{Chla},1}$) [mg m^{-3}] ($N \times M$)
PPzt	Predicted profile of phosphorus bound to inorganic particles (P_{IP}) [mg m^{-3}] ($N \times M$)
DOPzt	Predicted dissolved organic phosphorus profile (P_{DO}) [mg m^{-3}] ($N \times M$)
DOCzt	Predicted dissolved organic carbon profile (C_{DO}) [mg m^{-3}] ($N \times M$)
DOCzt1	Predicted fraction of labile (pool 1) dissolved organic carbon of total DOC ($C_{\text{DO},1}/C_{\text{DO}}$) [-] ($N \times M$)
DOCzt2	Predicted fraction of semilabile (pool 2) dissolved organic carbon of total DOC ($C_{\text{DO},2}/C_{\text{DO}}$) [-] ($N \times M$)
DOCzt3	Predicted fraction of refractory (pool 3) dissolved organic carbon of total DOC ($C_{\text{DO},3}/C_{\text{DO}}$) [-] ($N \times M$)
DOCtfrac	Predicted profiles of dissolved organic carbon pools ($C_{\text{DO},1}$, $C_{\text{DO},2}$, $C_{\text{DO},3}$) [mg m^{-3} , mg m^{-3} , mg m^{-3}] ($N \times M \times 3$)
Daily_BB1t	Predicted profile of the daily amount of degradation of labile (pool 1) DOC [mg m^{-3}] ($N \times M$)
Daily_BB2t	Predicted profile of the daily amount of degradation of semilabile (pool 2) DOC [mg m^{-3}] ($N \times M$)
Daily_BB3t	Predicted profile of the daily amount of degradation of refractory (pool 3) DOC [mg m^{-3}] ($N \times M$)
Daily_PBt	Predicted profile of the daily amount of photochemical mineralization of DOC [mg m^{-3}] ($N \times M$)
DICzt	Predicted dissolved inorganic carbon profile (C_{DI}) [mg m^{-3}] ($N \times M$)
CO2zt	Predicted CO_2 profile [mg m^{-3}] ($N \times M$)
O2zt	Predicted dissolved oxygen profile (O_{D}) [mg m^{-3}] ($N \times M$)
O2_sat_relt	Predicted profile of relative saturation of oxygen [-] ($N \times M$)
O2_sat_abst	Predicted profile of absolute saturation of oxygen [-] ($N \times M$)
POCzt	Predicted particulate organic carbon profile (C_{PO}) [mg m^{-3}] ($N \times M$)
Qz_sed	Predicted sediment-water heat flux [W m^{-2}] ($N \times M$)

lambdazt	Predicted average total light attenuation coefficient down to depth z [m^{-1}] ($N \times M$)
P3zt_sed	Predicted concentrations of P_D , P_P , and P_{Chla} in the sediment; volume fraction of dry inorganic matter in dry sediment solids; cumulative gross sedimentation and resuspension (sum of dry inorganic matter and dry living organic matter); fraction of inorganic sedimentation of total net sedimentation; cumulative gross sedimentation of dead particulate organic matter; volume fractions of dry nonliving organic matter and dry living organic matter in dry sediment solids; and cumulative resuspension of dead particulate organic matter [mg m^{-3} , mg kg^{-1} , mg kg^{-1} , -, kg , kg , -, kg , -, kg] ($N \times M \times 11$)
P3zt_sed_sc	Predicted phosphorus resuspension sources for P_D , P_P , and P_{Chla} from the sediment [mg m^{-3}] ($N \times M$)
His	Thicknesses of white ice, snow, and snow ice; temperatures of ice and air; snow density; ice cover existence; and thickness of frazil ice [m , m , m , $^{\circ}\text{C}$, $^{\circ}\text{C}$, kg m^{-3} , true/false, m] ($8 \times M$)
DoF	Predicted freezing dates [model day number]
DoM	Predicted melting dates [model day number]
MixStat	Temporary variables used in model testing, see model code ($X \times M$)
Wt	Meteorological forcing data (columns 4–10 described in Section 4.2.1) ($M \times 7$)
surfaceflux	Predicted CO_2 surface flux (F_{CO_2}) [$\text{mg CO}_2 \text{m}^{-2}$] (M)
oxygenflux	Predicted oxygen surface flux (F_{O_2}) [$\text{mg O}_2 \text{m}^{-2}$] (M)
CO2_eqt	Predicted CO_2 equilibrium concentration ($C_{\text{eq,CO}_2}$) [mg m^{-3}] (M)
K0t	Predicted solubility constant of CO_2 (K_{0,CO_2}) [$\text{mol l}^{-1} \text{atm}^{-1}$] (M)
O2_eqt	Predicted oxygen equilibrium concentration ($C_{\text{eq,DO}}$) [mg m^{-3}] (M)
K0_O2t	Predicted solubility constant of oxygen (K_{0,O_2}) [$\text{mol l}^{-1} \text{atm}^{-1}$] (M)
CO2_ppmt	Predicted atmospheric CO_2 mole fraction (χ_{CO_2}) [$\mu\text{mol mol}^{-1}$] (M)
d02Chlt	Predicted dissolved oxygen production by photosynthesis [$\text{mg m}^{-3} \text{d}^{-1}$] ($N \times M$)
POC1tfrac	Predicted fraction of autochthonous (pool 1) dead particulate organic carbon of total POC [-] ($N \times M$)
d02S0Dt	Predicted dissolved oxygen consumption by organic matter degradation in sediment [$\text{mg m}^{-3} \text{d}^{-1}$] ($N \times M$)
d02D0Ct	Predicted dissolved oxygen consumption by degradation of dissolved organic carbon [$\text{mg m}^{-3} \text{d}^{-1}$] ($N \times M$)
pHt	Predicted profile of water column pH ($-\log_{10}[\text{H}^+]$) [-] ($N \times M$)
testi3t	Temporary variables used in model testing, see model code ($N \times M \times X$)
T_sedt	Predicted profiles of sediment temperature at different depths, see model code ($N \times M \times 4$)

5 Additional model development for gas exchange

In addition to the default procedure for gas exchange calculation, three other formulas for the gas exchange velocity k_{gas} by Heiskanen et al. (2014), MacIntyre et al. (2010), and Tedford et al. (2014) have been implemented in a further developed version of MyLake C.

5.1 Alternative models for the gas exchange velocity

In contrast to Eqs. (32) and (37), the gas exchange velocity k_{gas} is calculated in units of $[\text{m s}^{-1}]$ and the daily air-water flux is calculated as

$$F_{\text{gas}} = 8.64 \times 10^4 \times k_{\text{gas}} (C_{\text{w,gas}} - C_{\text{eq,gas}}). \quad (55)$$

The equation for k_{gas} in the gas exchange model by Heiskanen et al. (2014) is

$$k_{\text{HE}} = ((C_1 U)^2 + (C_2 w_*)^2)^{0.5} S c_{\text{gas}}^{-0.5}, \quad (56)$$

where $C_1 = 1.5 \times 10^{-4}$ and $C_2 = 0.07$ are experimental dimensionless constants, U $[\text{m s}^{-1}]$ is the wind speed at 1.5 m, and w_* $[\text{m s}^{-1}]$ is the penetrative convection velocity, which is calculated according to Imberger (1985) as

$$w_* = \begin{cases} (-\beta z_{\text{AML}})^{1/3} & \text{if } \beta < 0, \\ 0 & \text{if } \beta \geq 0, \end{cases} \quad (57)$$

where z_{AML} [m] is the depth of the actively mixing layer (AML) and β $[\text{m}^2 \text{s}^{-3}]$ is the buoyancy flux. The AML includes the near-surface grid layers in which the water column temperature is within 0.02°C of the temperature in the topmost layer at the instant of the flux calculation. The buoyancy flux is calculated as

$$\beta = \frac{g \alpha_w Q_{\text{eff}}}{\rho_w c_{pw}}, \quad (58)$$

where g $[\text{m s}^{-2}]$ is the gravitational acceleration, α_w $[\text{°C}^{-1}]$ is the thermal expansion coefficient of water*, ρ_w $[\text{kg m}^{-3}]$ is the water density, c_{pw} $[\text{J kg}^{-1} \text{K}^{-1}]$ is the specific heat capacity of water at constant pressure, and Q_{eff} $[\text{W m}^{-2}]$ is the effective surface heat flux. Q_{eff} is defined as the sum of the net surface heat flux and the fraction of net shortwave radiative heat flux that is trapped in the AML, $Q_{\text{SW,AML}}$:

$$Q_{\text{eff}} = Q_{\text{H}} + Q_{\text{L}} + Q_{\text{LW}} + Q_{\text{SW,AML}}. \quad (59)$$

The net surface heat flux includes sensible heat flux Q_{H} , latent heat flux Q_{L} , and net longwave radiative heat flux Q_{LW} , and it is recalculated during the determination of Q_{eff} . The shortwave radiative heat flux at depth z is calculated by

$$Q_{\text{SW}}(z) = Q_{\text{SW}}(0) (f_{\text{PAR}} e^{-K_{\text{P,AML}} z} + (1 - f_{\text{PAR}}) e^{-K_{\text{nP,AML}} z}), \quad (60)$$

where $Q_{\text{SW}}(0)$ is the shortwave radiative heat flux penetrated through the air-water interface, f_{PAR} is the fraction

*The thermal expansion coefficient of water is calculated using the derivative of the water density polynomial used in MyLake as $\alpha_w = -\frac{1}{\rho_w} \frac{d\rho_w}{dT}$.

of PAR of the total shortwave energy, and $K_{P,AML}$ and $K_{nP,AML}$ [m^{-1}] are the total attenuation coefficients of PAR and non-PAR radiation, respectively, in the AML. The net shortwave radiative heat flux trapped in the AML is calculated as in Imberger (1985):

$$Q_{SW,AML} = Q_{SW}(0) + Q_{SW}(z_{AML}) - \frac{2}{z_{AML}} \int_0^{z_{AML}} Q_{SW}(z) dz. \quad (61)$$

The formula for k_{gas} by Tedford et al. (2014) is

$$k_{TE} = c(\nu \varepsilon_{TE})^{0.25} Sc_{gas}^{-0.5}, \quad (62)$$

where ν [$m^2 s^{-1}$] is the kinematic viscosity of water[†], ε_{TE} [$W kg^{-1} = m^2 s^{-3}$] is the total turbulent kinetic energy dissipation rate per unit mass, and $c = 0.5$ is an experimental dimensionless constant. The total turbulent kinetic energy dissipation rate per unit mass is calculated as determined by Tedford et al. (2014):

$$\varepsilon_{TE} = \begin{cases} \frac{0.56 u_{*w}^3}{\kappa z'^3} + 0.77 |\beta| & \text{if } \beta < 0, \\ \frac{0.6 u_{*w}^3}{\kappa z'^3} & \text{if } \beta \geq 0. \end{cases} \quad (63)$$

where u_{*w} [$m s^{-1}$] is the wind-induced water friction velocity, $\kappa = 0.4$ is the von Kármán constant and $z' = 0.15 m$ is a reference depth. u_{*w} is calculated from the atmospheric friction velocity u_{*a} [$m s^{-1}$] as

$$u_{*w} = u_{*a} \left(\frac{\rho_a}{\rho_w} \right)^{0.5}, \quad (64)$$

where ρ_a [$kg m^{-3}$] is the density of air.

In the parameterization by MacIntyre et al. (2010), k_{gas} is calculated from wind speed with a dependence on the direction of the buoyancy flux, that is, depending on if the AML is heating or cooling:

$$k_{MI} = \begin{cases} \frac{1}{3.6 \times 10^5} \times (2.04 U_{10} + 2.0) \left(\frac{Sc_{gas}}{600} \right)^{-0.5} & \text{if } \beta < 0, \\ \frac{1}{3.6 \times 10^5} \times (1.74 U_{10} - 0.15) \left(\frac{Sc_{gas}}{600} \right)^{-0.5} & \text{if } \beta \geq 0. \end{cases} \quad (65)$$

In addition, the Schmidt number exponent is -0.5 instead of $-2/3$ in k_{CC} (Eq. (37)).

The conversion between wind speeds at different heights is performed by assuming a logarithmic wind profile and a ratio of $U_{10}/U_{1.5} = 1.22$.

5.2 New model code

In comparison to the original MyLake C function files that are described in Section 4.1, there are 6 modified files (*solvemodel_vC_gases.m*, *DICsystem_bio_gases.m*, *DICsystem_new_gases.m*, *carbonequilibrium_gases.m*,

[†]The kinematic viscosity of water is calculated from the dynamic viscosity μ following White (2011) as $\ln \frac{\mu}{\mu_0} = -1.704 - 5.306 \frac{273}{T} + 7.003 \left(\frac{273}{T} \right)^2$, where $\nu = \mu/\rho_w$, $\mu_0 = 1.788 \times 10^{-3} kg m^{-1} s^{-1}$, and the water temperature is given in Kelvin.

convection_v12_1aIC_gases.m, and *fokema_new_gases.m*) and 10 new files. There are also 2 function files used in simulation result analysis. The new files are listed below.

<i>CO2flux.m</i>	Calculates the CO ₂ flux between water and the atmosphere using the gas exchange velocity calculated in <i>gasexchcoeff.m</i> .
<i>C_CO2_eq.m</i>	Calculates the equilibrium concentration of CO ₂ .
<i>C_O2_eq.m</i>	Calculates the equilibrium concentration of oxygen.
<i>O2flux.m</i>	Calculates the oxygen flux between water and the atmosphere using the gas exchange velocity calculated in <i>gasexchcoeff.m</i> .
<i>buoyancyflux.m</i>	Calculates the buoyancy flux.
<i>gasexchcoeff.m</i>	Calculates the gas exchange velocity.
<i>schmidtCO2.m</i>	Calculates the Schmidt number of CO ₂ .
<i>schmidtO2.m</i>	Calculates the Schmidt number of oxygen.
<i>thermexp.m</i>	Calculates the thermal expansion coefficient of water.
<i>viscwater.m</i>	Calculates the kinematic viscosity of water.
<i>pclin.m</i>	Calculates the depth of the simulated epilimnion.
<i>z_bio_epilimnion_obs.m</i>	Calculates the depth of the epilimnion based on water column temperature measurements.

5.3 Model execution

A new input argument *gasmodel*, which specifies the applied model for the gas exchange velocity, has been introduced in the execution command. The different options (CC for the default model by Cole and Caraco (1998), Heiskanen for the model by Heiskanen et al. (2014), U_MacIntyre for the model by MacIntyre et al. (2010), and SR_Tedford for the model by Tedford et al. (2014)) are defined along with the model parameter file path. There are also two new output matrices. The execution command is as follows:

```
[zz,Az,Vz,tt,Qst,Kzt,Tzt,Czt,Szt,Pzt,Chlzt,PPzt,DOPzt,D0Czt,D0Czt1,D0Czt2,D0Czt3,D0Ctfrac,Daily_BB1t,...
Daily_BB2t,Daily_BB3t,Daily_PBt,DICzt,C02zt,O2zt,O2_sat_relt,O2_sat_abst,P0Czt,B0Dzt,Qzt_sed,...
lambdazt,P3zt_sed,P3zt_sed_sc,His,DoF,DoM,MixStat,Wt,surfaceflux,oxygenflux,C02_eqt,K0t,O2_eqt,...
K0_O2t,C02_ppmt,d02Chlt,P0C1tfrac,d02S0Dt,d02D0Ct,pHt,testi3t,testi4t,T_sedt,Heff_parts]...
= solvemodel_vC_gases(m_start,m_stop,initfile,initsheet,inputfile,'timeseries', parafile,'lake',...
Qlambda,gasmodel);
```

New model output variables

<i>testi4t</i>	Predicted water column temperature at the instant of air-water gas flux calculation, gas exchange velocity for oxygen, sensible and latent heat fluxes at the instant of air-water gas flux calculation, thickness of the AML, effective heat flux, gas exchange velocity for CO ₂ , and atmospheric friction velocity [$^{\circ}\text{C}$, ms^{-1} , W m^{-2} , W m^{-2} , m , W m^{-2} , ms^{-1} , ms^{-1}] ($N \times M \times 8$)
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Heff_parts	<p>Predicted sensible, latent, and longwave heat fluxes at the instant of air-water gas flux calculation; shortwave radiative heat fluxes at the surface and at the bottom of the AML; and the value of the integral portion of the effective heat flux (Eq. (61)) [W m^{-2}] ($M \times 6$)</p>
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