

Numerical study of the seasonal thermal and gas regimes of the large artificial reservoir in Western Europe using LAKE2.0 model

AUTHORS' RESPONSES TO THE REFEREE #1 COMMENTS

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Introduction. Document structure

This document contains authors' responses to the comments of the Anonymous Referee. The document structure is the following:

- Referee's comments are numbered and given in *italic font*. General, specific, and technical comments come separately.
- Authors' response follows the comment and starts after "**Response:**" with normal font.
- The text from the article itself (if some changes are done, and if it is reasonable to provide it) is typed with **typewriter font** and separated from the response with an extra blank line.
- *Technical comments and mistakes* are not numbered, and authors' response follows immediately.

Reviewed manuscript with all the corrections is given after all responses. It contains the changes and proposals of **two** Referees and was prepared using L^AT_EXdiff package for better understanding of what has been changed.

Anonymous Referee #1

General comments

In their paper the authors show measurements and numerical simulation results with the two layer model FLake and the onedimensional model LAKE2.0. The authors compare temperature and heat fluxes and dissolved gases such as CO₂ and O₂. In general, the results of Lake2.0 are better than FLake. This is no surprise and FLake is a simpler approach. Lake2.0 reproduces temperatures in general with an error of 1° C. The simulation of dissolved gases in general is good. However the daily variation is missing because the model does not reflect biological activity completely enough and during deep recirculation modelled oxygen lies higher than measured.

The accuracy of temperature stratification of 1° C indicates careful set-up of the model, and can only be achieved by considering the variable light absorption during the year. The good agreement between modelled dissolved oxygen and measurements during the stratification period indicates that the oxygen concentration in the surface layer is controlled mainly by exchange with the atmosphere, as biological processes are not reflected in the model; as a consequence during winter and during strong blooms the modelled oxygen is not as good anymore. I suspect there could be an upwelled oxygen demand during deep recirculation that is not included in the model.

This manuscript is significant as it shows that temperature of reservoirs can well be represented with 1 d models: Lake2.0 is an option. Modelling oxygen and carbon dioxide is possible with simple assumptions (without biological model); however for representation of oxygen during deep recirculation and during algal blooms as well the daily variation of CO₂, a more detailed model is necessary: Scientific significance 2.3; Scientific quality: the modelling is well done; the improvement of absorption was a smart step; the manuscript gives a competent impression; measurements suited for checking simulation: scientific quality 1.6. Scientific reproducibility. 1,5 see below Presentation quality: 2; English writing: in general good: see comments below. the fonts in Figures are generally too small: especially: Figs. 1, 2, 5, 7; number of figures is appropriate.

Response: We thank the Reviewer for the positive comments about the article. The paper was re-edited very carefully and modifications and improvements were made. Below, we address every comment and explain the corresponding changes in the manuscript.

5 Important issues

Comment 1

I would recommend not to use a contour plot to judge onset and end of stratification: the authors claim stratification starts iend of April: Fig.11 indicates clearly, the reservoir was stratified on 2019 March 1st and 29th. An earlier onset of stratification explains the better oxygen simulation in Fig 10 from ca. Feb 8th. Better look at temperature tracks of sensors of different depths.

Response: We carefully analysed the water temperature data and used the definition of lake summer stratification given in Wetzel R. G. *Limnology*, Saunders College Publishing, 2nd edition, 1983, p 75, which implies it when a stratum of thermal discontinuity exists between epilimnion and hypolimnion (usually accepted as a change of $>1^{\circ}\text{C}$ per metre. These led us to rework the second paragraph of section 3.1 concerning the stratification periods and update Fig. 3. However, we consider the figure with time-depth temperature diagram more demonstrative than time series of water temperature on various depth. The reworked part is the following:

According to the definition given in (Wetzel, 1983), summer stratification period is characterized by a stratum of thermal discontinuity (metalimnion) which separates an upper layer of warm circulating water (epilimnion) and cold and relatively undisturbed water below (hypolimnion). The stratum of thermal discontinuity is usually defined as a change of $>1^{\circ}\text{C}$ per metre. Summer stratification periods are clearly seen in Fig. 1 (marked with dashed lines). The simulation began in a stratified conditions which lasted until 3 October 2017 while in 2018 stratification lasted from 14 April to 19 September.

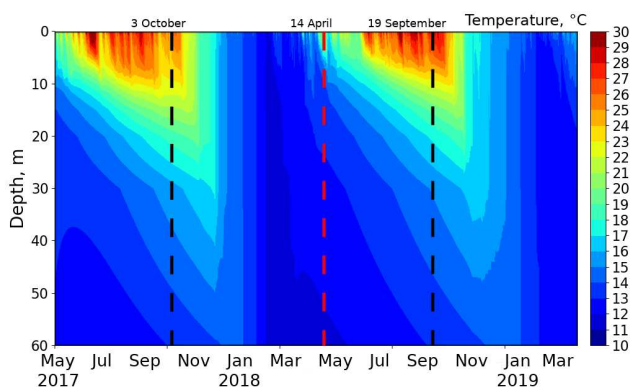


Figure 1: Time-depth Hovmöller diagram of the LAKE2.0 simulated water temperature in the Alqueva reservoir based on hourly data. Dashed lines indicate the end (black) and the beginning (red) of stratification.

Comment 2

At two places the pH dependence of CO₂ solubility is mentioned, e.g. line 177. Do the authors indicate the Henry coefficient depends on pH; or does this refer to the much stronger pH dependence of the carbonate equilibrium? Has bicarbonate been modelled, or DIC (dissolved inorganic carbon)?
 5 – connected with this: I cannot really follow what the altered pH on line 179 may indicate.

Response: We decided to add a supplementary material to the article where details on the biogeochemical processes are provided widely. You may find it attached to this file after the article.

Evolution and vertical distribution of three dissolved gases are considered in the LAKE2.0 model, which are methane CH₄, oxygen O₂ and carbon dioxide CO₂. However, dissolved carbon dioxide is supposed to be always in carbonate equilibrium, so that it contributes to concentration of dissolved inorganic carbon (DIC), $C_{DIC} = C_{CO_2} + C_{HCO_3^-} + C_{CO_3^{2-}}$, and it is the change of DIC that reflects the number of carbon atoms in CO₂ molecules added to (or lost by) a solution from (to) atmosphere, bubbles, respiring organisms or decaying organic matter (see Section 1.2 in Supplementary).
 15

In addition, the content of dissolved organic carbon (DOC), particulate organic carbon (both living, POCL, and dead, POCD) are calculated. POCL includes carbon atoms contained in phytoplankton and zooplankton.

Comment 3

There could be a mention of the two most common 1D lake models: DYRESM (Imberger) and GLM (e.g. Bruce et al. of Hipsey et al.)
 20

Response: We added a references to these models along with the FLake model in the **Introduction**:

One-dimensional lake models, e.g. the FLake model (Mironov et al., 2010), DYRESM (Imberger and Patterson, 1981), GLM (Hipsey et al., 2019), play a major role in this process.
 25

Technical details

Line 8: capable OF
 Corrected.

Line 98 : BEING used
 Corrected.
 30

Line 125: are -> is
 Corrected.
 35

Line 137 "into account" to the end of phrase
 Corrected.

Line 147. Check sentence

Reworked:

To calculate the dissolved carbon dioxide concentration in water, the same type of prognostic equation is used as for other gases.

Line 155: unit is missing

Added m^{-1} .

Line 162: THE chose period

Corrected.

Line 165 capital T

The sentence was removed.

Line 173: comma after stage?

Added.

Line 185: how is density rho calculated (including solutes?)

Solutes were not included in the current experiment (Alqueva is a freshwater lake), and the ρ was calculated with the dependence on water temperature according to (McCutcheon, S. C., Martin, J. L., & Barnwell, T. O. (1993). *Water Quality. In Handbook of Hydrology* (pp. 11.11-11.73)).

Line 191: comma after hours (possibly also before bigger)

The sentences were reworked:

A linear interpolation was used to fill the gaps in data smaller than 3 hours. The gaps longer than 3 consecutive hours were substituted with the corresponding values from the land weather stations (Barbosa and Cid Almeida).

Caption Fig. 4: include the information of 6-hours mean

Added.

Caption Fig. 4: errors-> temperature difference

Corrected.

Line 221: that -> which

Corrected.

Line 237. Remove "is"

Removed.

Line 251: covariAnce

Corrected.

Line 255: constant -> continuous

Corrected.

Line 266: which WAS SET TO A VALUE OF 8.48, which correspondED . . .

5 Corrected.

Figure 8: remove useless data between 10 and 17 March (or explain what can be seen)

Removed. Figure 8 was remade.

Line 274 comma after period

10 Added.

Line 270: good -> well

Corrected.

Numerical study of the seasonal thermal and gas regimes of the large artificial reservoir in Western Europe using LAKE2.0 model

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Abstract.

The Alqueva reservoir (southeast of Portugal) ~~being is~~ the largest artificial lake in Western Europe and ~~a~~ strategic freshwater supply in the region. The reservoir is of scientific interest in terms of monitoring and maintaining the quality and quantity of water and its impact on the regional climate. To ~~solve support~~ these tasks we conducted numerical studies of the thermal and gas regimes in the lake over the period from May 2017 to March 2019, supplemented by the data observed at the weather stations and ~~the~~ floating platforms during the field campaign of the ALOP (ALentejo Observation and Prediction System) project. One-dimensional model LAKE2.0 was used for the numerical studies. Being highly versatile and adjusted to the specific features of the reservoir, this ~~parameterization is capable to simulate~~ model is capable of simulation of its thermodynamic and biogeochemical characteristics. Profiles and time series of water temperature, sensible and latent heat fluxes, concentrations of CO₂ and O₂ reproduced by the LAKE2.0 model were validated against the observed data and were compared with the thermodynamic simulation results obtained with the FLake model. The results demonstrated that ~~LAKE2.0 model has good ability in capturing both models well captured~~ the seasonal variations in ~~the~~ water surface temperature and the internal thermal structure of the Alqueva ~~reservoir~~. The LAKE2.0 model showed slightly better results and satisfactorily captured the seasonal gas regime.

1 Introduction

Inland water bodies are active and simultaneously sensitive ~~participants~~ regulators of the weather and climate processes of the Earth, changing the temperature, wind, precipitation in the surrounding areas; their thermal and gas regimes, in turn, can serve as a response to ecosystem status or climate change (Bonan, 1995; Adrian et al., 2009; Samuelsson et al., 2010). In modern climate/weather models lakes and reservoirs became large-scale structures and are taken into account explicitly (Bonan, 1995), their parameterizations are intensively embedding in these models (~~Mironov et al., 2010; Salgado and Le Moigne, 2010; Dutra et al., 2010;~~ Salgado and Le Moigne, 2010; Dutra et al., 2010; Subin et al., 2012). One-dimensional lake models ~~play a major role in this~~

~~process~~, e.g. the FLake model (Mironov et al., 2010), DYRESM (Imberger and Patterson, 1981), GLM (Hipsey et al., 2019), play a major role in this process. Their simplicity, computational efficiency, and reliability of the simulation results allow ~~to use them~~ them to be used not only in studies of the dynamics of single lakes but also in the climate-related tasks of long-term numerical simulations, where vast territories with huge number of water bodies should be taken into account. As a result, the number of numerical studies connected with the vertical thermodynamics and biogeochemistry of lakes and their interaction with the atmosphere increases (Thiery et al., 2014; Heiskanen et al., 2015; Le Moigne et al., 2016; Ekhtiari et al., 2017; Su et al., 2019).

A realistic representation of the thermal and gas regimes by lake models ~~are~~ is important for solving current and prognostic tasks. For example, high accuracy of the calculations of sensible and latent heat fluxes, momentum, and water surface temperature is required for atmospheric models, where these parameters are the boundary conditions (Bonan, 1995; Mironov et al., 2010; Dutra et al., 2010; Salgado and Le Moigne, 2010; Balsamo, 2013). On the other hand, an adequate simulation of the water temperature profiles would be a very interesting new output of weather prediction and earth system models because the temperature is a key factor for ~~the lake ecosystem vital activity~~ lake ecosystem processes. This information might be useful for water quality management and for better representation of the gas emissions (CO_2 , O_2 , CH_4) from lakes to the atmosphere which are relevant to various atmospheric processes (Walter et al., 2007).

Fully filled only in 2004, the Alqueva reservoir is in the spotlight of many studies connected with its ecosystem vital activity and ecology (Penha et al., 2016; Tomaz et al., 2017; Pereira et al., 2019), water quality (~~Potes et al., 2012, 2018; Novais et al., 2018~~) (Potes et al., 2011, 2012, 2018; Novais et al., 2018), and lake-atmosphere interactions (Lopes et al., 2016; Policarpo et al., 2017; Potes et al., 2017; Iakunin et al., 2018). The aim of the present work is a numerical study of the seasonal variations of thermal and gas regimes of the reservoir which was held under the ALOP (ALentejo Observation and Prediction systems) project, where an extensive field campaign and lake model simulations were combined. For the latter we used one-dimensional model LAKE2.0 (Stepanenko et al., 2016), that features the biogeochemical block ~~allowing to reproduce~~ that simulates the concentrations of O_2 , CO_2 , and CH_4 in water. In addition, well-established in weather and climate studies FLake model was used as a reference to ~~complete~~ compare the results of thermodynamic characteristics of the reservoir. Before starting the numerical simulations, the LAKE2.0 model has been adapted to the features of the Alqueva reservoir including the introduction of the realistic values of the water acidity and light extinction coefficients and adequate value of the coefficient of the ~~hypolimnion~~ hypolimnion turbulent mixing rate. Both models were forced with the observed meteorological data at the reservoir which contributed to increase the reliability of the results. The simulation covered the period from May 2017 to April 2019 and its results as well as the possibility to apply LAKE2.0 model in operational mode might be used in future studies of weather and climate, and biochemical related tasks.

2 Methods

2.1 Object of study

The Alqueva reservoir is located in the southeast of Portugal spreading ~~along over~~ 83 km ~~over the of~~ former valley of ~~the~~ Guadiana river (Fig 1). Established in 2002 to cover the region's water and electricity needs, its surface covers an area of

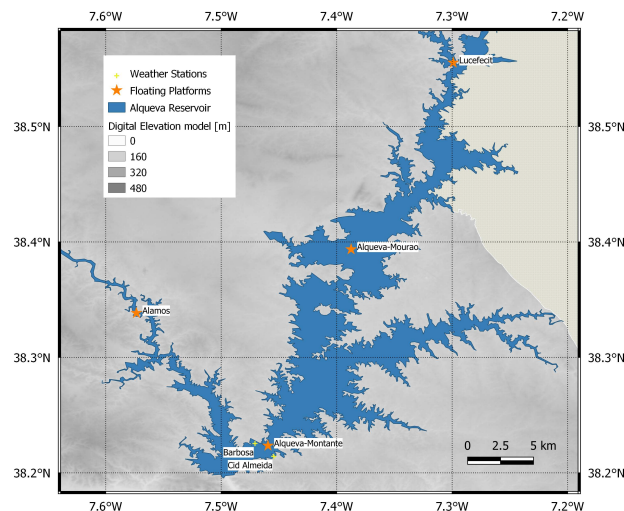


Figure 1. Location of the Alqueva reservoir and ALOP stations. The map was built using digital elevation model ASTER GDEM 2 (<https://asterweb.jpl.nasa.gov/gdem.asp>).

- 5 250 km², the maximum depth is 92 m, the average depth is 16.6 m, and the ~~storage~~ capacity of water is estimated at 4.15 km³, which make it the largest reservoir in Western Europe.

Long periods of drought that could last for more than one consecutive year (Silva et al., 2014) are typical in this part of the Iberian Peninsula. The Alqueva region is characterized by a hot-summer Mediterranean climate (*Csa* type according to the Köppen climate classification) with a small area of semi-arid climate (*BSk* type). In summer, maximum daily air temperature
10 ranges between 31 and 35 °C (July and August) while the record values may reach 44 °C. Winter period (December-February) in the region is relatively mild and wet with average air temperature of 10.3 °C. Nevertheless, even in January the air temperature can reach maximum value of 24 °C during long periods of stable conditions when the Azores Anticyclone settles ~~in~~
~~into a~~ favourable position. ~~Rainfall seasons normally last from October to~~ ~~Seasonal rainfall normally occurs between October~~
~~and~~ May. The annual average values of the accumulated precipitation (1981-2010 normals from www.ipma.pt) registered at
15 the weather station in Beja located 40 km away from the reservoir is 558 mm. Mean daily values of the incident solar radiation at the surface are about 300 Wm⁻² (one of the highest in Europe) and the daily maximum in summer often may exceed 1000 Wm⁻² (Iakunin et al., 2018).

2.2 Observed data

Geographical and climatological factors make the Alqueva reservoir a vital source of fresh water ~~for living and economical purposes needed to support the population and economy~~ in the region. ~~On~~, while on the other hand, an increasing anthropogenic and heat stress negatively affects the lake ecosystem (Penha et al., 2016). Monitoring the quantity and quality of water in the reservoir became an essential scientific task. This task is addressed in the framework of the ALOP project related to the observations and numerical experiments on the study of processes of the atmosphere - Alqueva reservoir system. Models of different spatial and time scales were used in the ALOP numerical experiments.

The ALOP field campaign was focused on measurements of physical, chemical, and biological parameters in the water and air columns, ~~over~~ at the water-atmosphere interface, and ~~in~~ on the shores of the reservoir. In present work the following facilities were used and equipped to obtain the required data for the numerical simulations during the field campaign: ~~4~~ four floating platforms (Montante, Mourão, Alamos, and Lucetfecit) and two dedicated weather stations in the margins (Barbosa and Cid Almeida), their locations are marked with circles in Fig 1. The principal scientific site on the lake was the Montante floating platform which is located in the southern and deeper part (74 m) of the reservoir (38.2276° N, 7.4708° W). The following equipment was ~~settled~~ deployed on the platform during the whole field campaign continuously providing measurements:

- an eddy-covariance system, Campbell Scientific ~~Irgason~~, provides data ~~for~~ of atmospheric pressure, air temperature, water vapour and carbon dioxide concentrations, 3D wind components, linear momentum, sensible heat, latent heat, and carbon dioxide fluxes;
- albedometer (Kipp & Zonen CM7B) and pyrradiometer (Philipp Schenk 8111) in order to measure upwelling and downwelling shortwave and total radiative fluxes;
- set of 14 probes (Campbell Scientific 107) to measure the water temperature profile at the following depths: 5 cm, 25 cm, 50 cm, 1 m, 2 m, 4 m, 6 m, 8 m, 10 m, 12 m, 15 m, 20 m, 30 m, and 60 m.

Two probes were installed at the platform to assess water quality. A multiparametric probe (Aqua TROLL 600, IN-SITU, USA) that provided information about dissolved oxygen concentration and pH values, among other parameters, was mounted on the platform at 25 cm depth on the 3rd of July 2018 and worked until the end of the campaign. It was also used to make profiles during regular maintenance visits to the platform. A Pro-Oceanus Mini CO2 Analog Output probe was also mounted on the platform at 25 cm depth to measure dissolved CO₂ concentration continuously and ~~for punctually~~ was occasionally used to collect vertical profiles. Installed in the beginning of the campaign, the probe was working until the middle of June 2017 when it failed. It has been repaired and installed again in October 2017 but another problem occurred in November and probe was removed definitely.

Two land weather stations (Barbosa and Cid Almeida) were installed on opposite shores with the floating platform in the middle, between them (38.2235° N, 7.4595° W and 38.2164° N, 7.4545° W, correspondingly, green circles in Fig. 1). The equipment of both weather stations is listed in Table 1. Data from the Montante floating platform, Barbosa, and Cid Almeida weather stations were ~~obtained in automatic regime~~ automatically downloaded and transferred daily to the server in the Institute

of Earth Sciences (ICT), University of Évora. An important part of the campaign were the regular field trips to the reservoir for the cleaning and maintenance of the instrumentation on the platforms and weather stations~~and conduct measurements,~~ to conduct more detailed measurements, and to collect water samples at several depths and bottom sediments.

Table 1. Weather stations equipment

Measured parameter	Station	
	Barbosa	Cid Almeida
Albedometer	N/A	Philipp Schenk 8104
Air temperature and humidity	Campbell Scientific CS 215	Thies Clima 1.1005.51.512
Wind Speed	Gill Instruments WindSonic 1405-PK-021	Vector Instruments A100R
Wind Direction	„	Vector Instruments W200P

For further work, the data collected during the field campaign was treated before being used as a forcing for atmospheric and/or lake modelling related tasks. ~~Gaps, errors, and missed data were carefully interpolated~~ Missed data (gaps in data smaller than 3 hours) were carefully filled using linear interpolation. Longer gaps were substituted with values from closest weather stations.

2.3 LAKE2.0 model

For the simulation of the thermodynamic and biogeochemical processes in the Alqueva reservoir the LAKE2.0¹ model was chosen. A detailed description of the LAKE2.0 model may be found in Stepanenko et al. (2016), briefly the model equations are formulated in terms of water properties averaged over a lake's horizontal cross-section, thus introducing into the model fluxes of momentum, heat, and dissolved gases through a sloping bottom ~~surface~~ and water-atmosphere surfaces. Water temperature profile is simulated explicitly in LAKE2.0 ~~, and unlike Hostetler model (Hostetler and Bartlein, 1990), and~~ a number of biogeochemical processes is represented, which makes it capable to reproduce the transfer of CO₂ and CH₄ from and to the atmosphere.

Governing equations for the basic processes of the lake dynamics in the model are obtained using horizontally averaged Reynolds advection-diffusion equation for the quantity f which may be one of the velocity components, temperature, turbulent kinetic energy (TKE), TKE dissipation, or gas concentration:

$$c\partial_t \bar{f} = \underbrace{A^{-1}\partial_z(Ak_f\partial_z\bar{f})}_I - \underbrace{A^{-1}\partial_z(A\bar{F}_{nz})}_{II} + \underbrace{R_f(\bar{f}, \dots)}_{III}, \quad (1)$$

where term I describes turbulent diffusion, thermal conductivity or viscosity, term II is the divergence of non-turbulent flux of f , term III represents the horizontally averaged sum of sources and sinks, \bar{F}_{nz} is the non-turbulent flux of f , k_f is the

¹ Available at <http://tesla.parallel.ru/Viktor/LAKE/wikis/LAKE-model>

turbulent diffusion coefficient (thermal conductivity coefficient for temperature, viscosity for momentum) for f quantity. The LAKE2.0 model successfully represents conditions in the well-mixed upper layer of lakes (epilimnion).

In water, $k-\epsilon$ parameterization for computing turbulent fluxes is used. In ice and snow, a coupled transport of heat and liquid water is reproduced (Stepanenko et al., 2019). In bottom sediments, vertical transport of heat is implemented in a number of
5 sediment columns, originating from different depths.

Water temperature profile in the model is driven by equation (1) with substitution $f \rightarrow T$, where $c = c_w \rho_{w0}$, c_w — water specific heat, ρ_{w0} — mean water density, $\overline{R_f} = 0$ represents heat flux from the sediments, $\overline{F_{nz}}(z) = S_{rad}$ — downward short-wave radiation flux attenuating according to Beer–Lambert law in four wavebands (infrared, near-infrared, photosynthetically active, ultraviolet) with ~~prescribed~~corresponding extinction coefficients. Heat conductance is a sum of molecular and turbulent
10 coefficients, $k_T = \lambda_m + \lambda_t$, where $\lambda_t = c_w \rho_{w0} \nu_T$ (ν_T — turbulent coefficient of thermal diffusivity, m^2s^{-1} derived from the $k-\epsilon$ parameterization).

To solve the equation (1) for water temperature, top and bottom boundary conditions should be defined. The top boundary ~~condition~~conditions are represented by a heat balance equation, involving net radiation and a scheme for turbulent heat fluxes in the surface atmospheric layer based on Monin–Obukhov similarity theory (Monin and Obukhov, 1954). Bottom boundary
15 condition is set at the water-sediments interface and is based on the continuity of both heat flux and temperature at the interface. Bottom sediments are represented with one-dimensional multilayer model which includes heat conductivity, liquid moisture transport (diffusion and gravitational percolation), ice content, and phase transitions of water.

Lake hydrodynamics is described by (1) applied to horizontal momentum components with $F_{nz} = 0$, $c = 1$, and R_f representing Coriolis force and bottom friction. The Coriolis force has to be included in the momentum equations for lakes with
20 horizontal size that exceeds the internal Rossby deformation radius (Patterson et al., 1984).

Wind stress which is computed by Monin–Obukhov similarity theory is applied as a top boundary condition for momentum equations, bottom friction is set by logarithmic law with prescribed roughness length. Friction at a sloping bottom (term R_f) is calculated by quadratic law with tunable drag coefficient.

LAKE2.0 model uses $k-\epsilon$ model (Canuto et al., 2001) to compute turbulent viscosity, temperature conductivity and diffusivity. It takes ~~into account~~ both shear and buoyancy production of turbulent kinetic energy into account; an equation for
25 dissipation rate is a highly parametrized one with several constants calibrated in idealized flows.

Biochemical oxygen demand (BOD) is caused by degradation of dissolved organic carbon (DOC) and dead particulate organic carbon (POCD). The dynamics of the latter two, together with living particulate organic carbon (POCL) is represented by the model from Hanson et al. (2004) adapted to the 1D framework. Photosynthesis is given by Haldane kinetics where
30 chlorophyll-a concentration ~~is assumed to be constant in the mixed layer, assumed zero below and in mixed layer is~~ computed from photosynthetic radiation extinction coefficient (Stefan and Fang, 1994) ~~—an external model parameter~~and assumed zero below. The model does not take into account the nutrients concentrations explicitly. The fluxes of dissolved gases to the atmosphere are calculated using Henry’s law and surface-renewal model (Stepanenko et al., 2016), involving subsurface turbulent kinetic energy dissipation rate, provided by the $k-\epsilon$ closure.

To calculate the dissolved carbon dioxide concentration in ~~a water~~water, the same type of prognostic equation is used as ~~that~~ for other gases. In LAKE2.0, sedimentary oxygen demand and BOD, respiration, and CH₄ oxidation act as CO₂ producers, while photosynthesis is the only sink of carbon dioxide in the water column. More detailed equations and comments on the biogeochemical processes in the model are given in the Supplemental materials.

5 2.4 Model modifications and sensitivity tests

The given version of the LAKE2.0 model used ~~a constant~~constant values for light extinction coefficient in water for IR, NIR, PAR, and UV bands. This could lead to significant errors, especially in long term simulations, because ~~this parameter controls these parameters control~~ the vertical distribution of solar energy in different water layers ~~and has a~~. Light extinction coefficient for PAR (400-700 nm) demonstrates big annual variability in the Alqueva reservoir, as shown in Potes et al. (2012). ~~On the other hand, light extinction coefficient was constantly measured, and it was measured constantly~~ during the ALOP field campaign. Since April 2017 until March 2019 it varied from a minimum of 0.247 m^{-1} (August 2017) to a maximum of 1.519 m^{-1} (July 2018) with an average value of 0.643 m^{-1} (12 measurements). Thus, prior to the simulation, it was decided to upgrade the LAKE2.0 model and introduce a new variable, the ~~water-light~~extinction coefficient for photosynthetically active radiation (PAR) to the model setup. During the initialisation, the model reads the available values of this coefficient and does a linear interpolation for every model ~~timestep~~time step. Although the model results are not very sensitive to ~~water extinction coefficient~~it, the proposed modification allowed to improve the results in some periods by about 1 degree as exemplified in the Fig. ~~22-S1 in the Supplementary materials~~ for a selected period.

~~Water temperature in mixed layer, original and modified model results and their errors when compared to the observations made at the Montante platform.~~

Water pH significantly affects the solubility of carbon dioxide (Fig. S4 in the Supplementary materials), but its value is a model scalar constant. In reality, observations show that pH tends to decrease near the bottom and has a seasonal variation, changing from 7.8 to 8.8 during the years (2017-2019) in the mixed layer. After averaging the measurements, pH constant inside the model code was altered from 6.0 to 8.48 for a better representation of real processes. Another modification has been done to the hypolimnetic diffusivity parameterization. According to Hondzo and Stefan (1993) for lakes of regional scale hypolimnetic eddy diffusivity rate K_z is related to stability frequency N^2 and the lake area A_s :

$$K_z = c_1 (A_s)^{c_2} (N^2)^{c_3}, \quad (2)$$

where $c_1 = 8.17 \times 10^{-4}$, $c_2 = 0.56$, $c_3 = -0.43$ are empirical constants, $N^2 = -(\partial\rho/\partial z)(g/\rho)$, z is depth, g is acceleration of gravity, and ρ is density of water. In LAKE2.0 model equation 2 is presented as $K_{z,LAKE2.0} = \alpha K_z$, where α is a calibration coefficient that allows to adapt this parameterization to the specific features of a given lake. In a series of sensitivity experiments it was found out that for simulation of thermal regime on the Alqueva reservoir the value of $\alpha = 0.3$ provides the best representation of the heat diffusion from the surface to the depth of the lake (see the comparison in Fig. S5 of the Supplementary).

2.5 FLake model

In addition to LAKE2.0, [the](#) FLake model was used to simulate water temperature for [the](#) chosen period. FLake model (Mironov, 2008) is based on a two-layer representation of the ~~temperature profile and on the integral energy budgets for the two layers~~ [lake's thermal structure](#). The upper layer is assumed to be well mixed and the structure of the deep stratified layer is described using the concept of self-similarity of the temperature-depth curve. ~~the mean water temperature during the simulation run and apart of it provides mixed layer and bottom temperature, thermocline shape factor, and mixed layer depth in the output.~~ [The](#) FLake model is widely used in climate and numerical weather prediction studies (Salgado and Le Moigne, 2010; Samuelsson et al., 2010; Le Moigne et al., 2016; Su et al., 2019) to simulate the feedback of freshwater lakes on the atmospheric boundary layer, and in the intercomparison experiments with other parameterizations. In particular, FLake has been applied in studies of the Alqueva reservoir by Iakunin et al. (2018), Potes et al. (2012), and Salgado and Le Moigne (2010).

2.6 Simulation setup

The simulation conducted in the present study covered 23 months from the 1st of May 2017 to the 29th of March 2019 with 1 hour timestep for input and output data. In the setup stage, specific features of the Alqueva reservoir were prescribed: the series of PAR extinction coefficients for the simulation period, the morphometry of the lake bottom expressed via dependence of horizontal cross-section area on depth and the initial profiles of water temperature, CO₂, O₂, CH₄, and salinity (the last two profiles were set to zero due to the lack of the observation data).

~~Water pH significantly affects the solubility of carbon dioxide, but its value is a model scalar constant. In reality, observations show that pH tends to decrease near the bottom and has a seasonal variation, changing from 7.8 to 8.8 during the years (2017-2019) in the mixed layer. After averaging the measurements, pH constant inside the model code was altered from 6.0 to 8.48 for a better representation of real processes. Another modification has been done to the hypolimnetic diffusivity parameterization. According to Hondzo and Stefan (1993) for lakes of regional scale hypolimnetic eddy diffusivity rate K_z is related to stability frequency N^2 and the lake area A_s :~~

$$\underline{K_z = c_1 (A_s)^{c_2} (N^2)^{c_3}},$$

~~where $c_1 = 8.17 \times 10^{-4}$, $c_2 = 0.56$, $c_3 = -0.43$ are empirical constants, $N^2 = -(\partial \rho / \partial z)(g / \rho)$, z is depth, g is acceleration of gravity, and ρ is density of water. In LAKE2.0 model equation 2 is presented as $K_{z, LAKE2.0} = \alpha K_z$, where α is a calibration coefficient that allows to adapt this parameterization to the specific features of a given lake. In a series of sensitivity experiments it was found out that for simulation of thermal regime on the Alqueva reservoir the value of $\alpha = 0.3$ provides the best representation of the heat diffusion of heat from the surface to depth of the lake.~~

Both LAKE2.0 and FLake models were initialized with ALOP data measured at the Montante, in the reservoir floating platform and ran in standalone version. Atmospheric forcing input data were taken from the Montante platform observations. ~~Gaps in data smaller than 3 hours were filled with a linear interpolation. In case of gaps bigger than 3 consecutive hours data~~

was substituted with the corresponding values from the land weather stations (Barbosa and Cid Almeida). Comparison between LAKE2.0 and FLake models was made in terms of water temperature and heat fluxes over the water surface.

3 Results and discussion

3.1 Water temperature

- 5 Water temperature is a crucial factor for Numerical Weather Prediction (NWP) applications, ~~for lakes vital activity, and their ecosystems~~ and as a regulator of lake ecosystem activity. It is a key parameter of the lake-atmosphere interactions. Thus, detailed representation of the evolution of the water temperature at various depths is an important task.

~~Figure 2 shows the temporal evolution of the LAKE2.0 simulated water temperature in the reservoir over the whole chosen period. Time-depth Hovmöller diagram of the LAKE2.0 simulated water temperature in the Alqueva reservoir based on hourly data. The summer period,~~

- ~~According to the definition given in (Wetzel, 1983), summer stratification period is characterized by a strong thermal stratification of water, is clearly seen on~~ stratum of thermal discontinuity (metalimnion) which separates an upper layer of warm circulating water (epilimnion) and cold and relatively undisturbed water below (hypolimnion). The stratum of thermal discontinuity is usually defined as a change of $>1^{\circ}\text{C}$ per metre. Summer stratification periods are clearly seen in Fig. 2. ~~It begins in late April and ends in November.~~ (marked with dashed lines). The simulation began in a stratified conditions which lasted until 3 October 2017 while in 2018 stratification lasted from 14 April to 19 September.

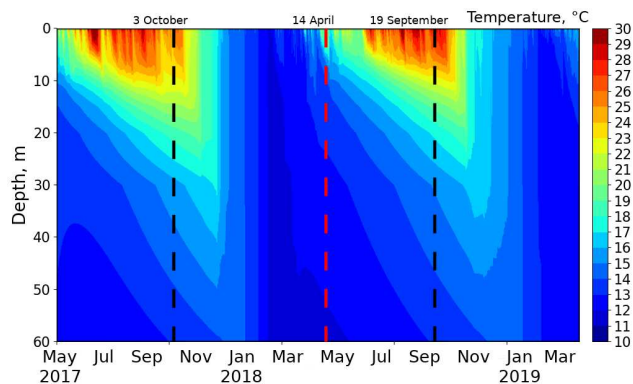


Figure 2. Time-depth Hovmöller diagram of the LAKE2.0 simulated water temperature in the Alqueva reservoir based on hourly data. Dashed lines indicate the end (black) and the beginning (red) of stratification.

Water temperature in ~~these months in~~ upper layers increases up to 30°C in warm period, and in the hottest months (July-September) reaches 25°C at 10 m depth. ~~Autumn turnover occurs in the end of October — beginning of November. In winter turnover period,~~ water temperature becomes uniform at depths up to 30 meters ~~and by the middle of December.~~ Since December,

when the lake shows no temperature stratification. During this period temperature decreases, it gradually cooling from 19 to 12 °C (in late February). In the end of April spring stratification occurs again and the cycle repeats.

The temperature of water in the mixed layer (ML) is of a particular interest in many studies. The LAKE2.0 provides water temperature at different depths defined in the model setup, and ML thickness, assuming that ML temperature is constant (not including surface skin effect). As in the real mixing layer ML the temperature is not exactly constant, measurements from the sensor at 0.5 m depth were chosen for the comparison we have chosen the water temperature at 50 cm deep comparison. On the whole simulation period ML depth in the reservoir was never less than 70 cm. Figure 3 (a) shows LAKE2.0 simulated results in comparison with measured values and FLake results of ML temperature. To smooth hourly fluctuations in such long-term simulation, moving average was used with 6-hour period.

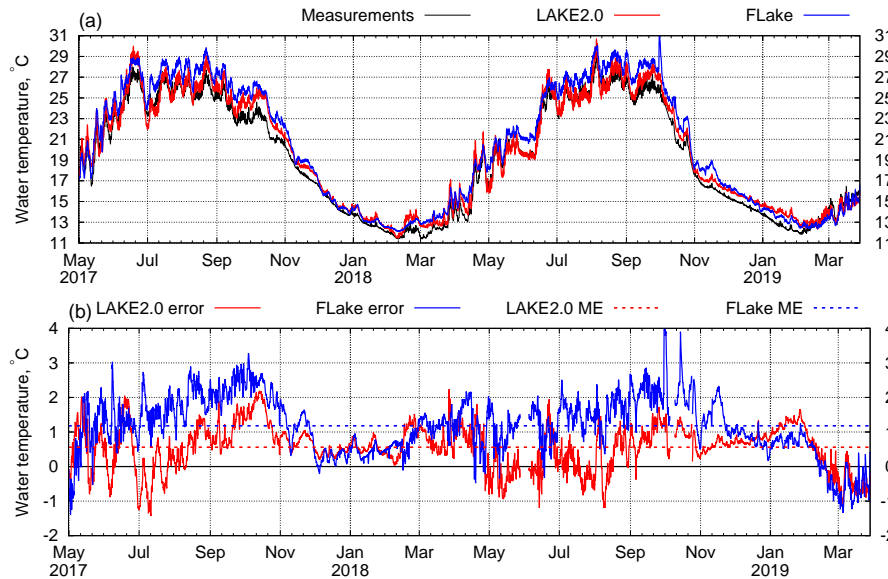


Figure 3. Top: time series (6-hours moving average) of the Alqueva water temperature in mixed layer: measured (black curve), and modelled using the LAKE2.0 (red curve), and the FLake (blue curve). Bottom: errors of temperature differences between observations and LAKE2.0 (red curve) and FLake (blue curve) models relatively to the observations at the Alqueva reservoir, 6-hours moving average. Dashed lines show corresponding mean errors for LAKE2.0 and FLake.

Differences between the two model results and the measurements (errors) are shown in Fig. 3 (b). In the period of March–November of both years when the lake is stratified, the LAKE2.0 model demonstrates better results, while during the cold periods (November–March) both models shows similar error rates. Statistic of the comparison is presented in Table 2. Overall, mean absolute errors for the whole simulation period are 1.27 °C for FLake and 0.74 °C for LAKE2.0. Mean errors of the LAKE2.0 and FLake models for the simulation period are 0.56 and 1.18 °C correspondingly (shown as dashed lines in Fig. 3 (b)), which means that both models tend to slightly overestimate ML temperature. The LAKE2.0 model results are

better for warm periods while FLake results are better for cold. Both models demonstrate almost identical correlation for the selected periods.

Table 2. Statistical results of ML water temperature intercomparison.

Time periods	Correlation		Mean error, °C		MAE, °C	
	LAKE2.0	FLake	LAKE2.0	FLake	LAKE2.0	FLake
May '17 – Oct '17	0.95	0.96	0.52	1.57	0.79	1.63
Nov '17 – Feb '18	0.99	0.99	0.61	0.63	0.61	0.64
Mar '18 – Oct '18	0.99	0.99	0.48	1.50	0.69	1.51
Nov '18 – Feb '19	0.98	0.98	0.83	0.92	0.83	0.92
All period	0.99	0.99	0.56	1.18	0.74	1.27

For more detailed analysis of the surface water temperature evolution we chose four months, July 2017/18 and January 2018/19, ~~that~~ which represent stratified and non-stratified lake state to see the daily cycles of the ML water temperature (Fig. 4). It is seen that LAKE2.0 model shows exceptionally good results in summer months (Fig. 4 (a), average mean errors

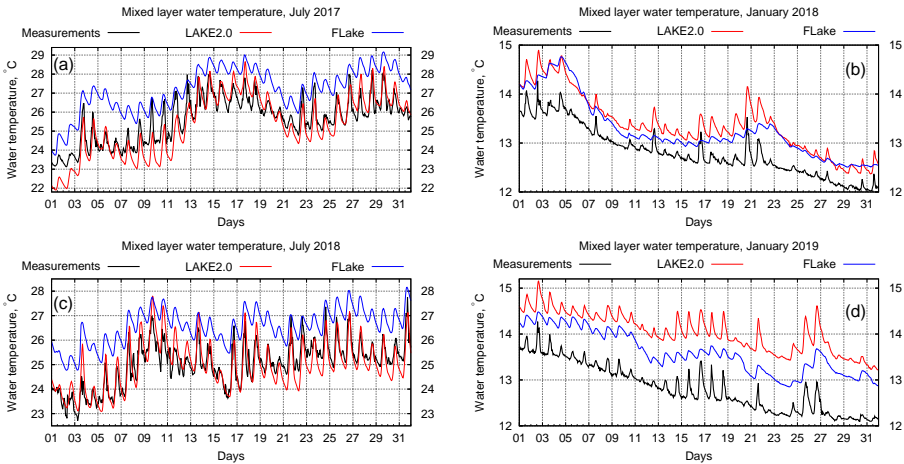


Figure 4. Timeseries of mixed layer water temperature for July 2017/2018 (a,c) and January 2018/2019 (b,d).

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are -0.23 and -0.04 °C for 2017 and 2018 correspondingly) while FLake provides an overestimation of 1-2 degrees and an underestimation of the daily amplitude. Correlation coefficients in this case are 0.94/0.88 (LAKE2.0) and 0.90/0.89 (FLake) correspondingly. Diurnal ML temperature variations can reach 3 degrees and generally are well represented by LAKE2.0 model. In January the water temperature profile in the reservoir is homogeneous, daily amplitude is not so high (Fig. 4 (b)), and FLake model shows a smaller overestimation (0.95 correlation for both months and mean errors of 0.45/0.78 °C). LAKE2.0 results show a positive offset, average mean error for January 2018 is 0.78 °C and correlation is 0.97. In January 2019 LAKE2.0

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mean error is 1.22 °C but, in general, the shape of the curve is similar to the measured and daily variations of temperature is represented quite goodwell.

Temperature distribution with depth is another significant parameter for lake thermodynamics. LAKE2.0 model simulates water temperature at pre-defined depth levels; ~~FLake provides a~~. FLake provides ML depth, shape factor for the thermocline curve, ML and bottom temperature. Using these values it is possible to access ~~the~~ water temperature of thermocline ~~beneath~~ ~~the ML~~ at any depth. Simulation results are shown in Fig. 5 for the following cases: 15 July 2017, 15 January 2018, 15 July 2018, and 15 January 2019 on 12:00 UTC each.

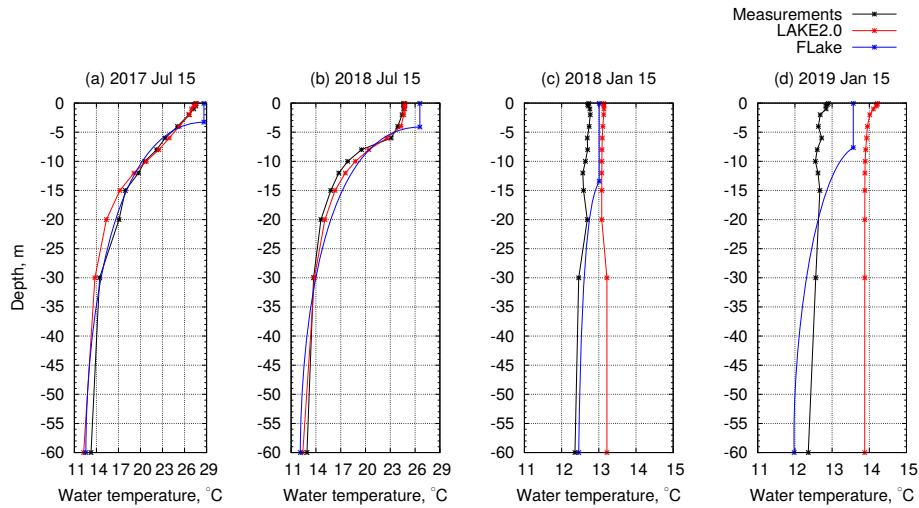


Figure 5. Water temperature profiles for 15 July 2017 (a), 15 January 2018 (b), 15 July 2018 (c), and 15 January 2019 (d), 12:00 UTC each.

Summer water temperature profiles are well represented by both models, although FLake shows an overestimation in the ML. In winter, on the other hand, LAKE2.0 overestimates water temperature through whole water column. Although LAKE2.0 reproduces the short-term (daily and weekly scales) thermal evolution of the ML very well, its integral energy is the simulated heat content of the entire water column seemed to be higher than in reality. The errors are higher on the second year of the simulation in the results of winter 2018/19, exceeding 1 degree. The modelled water column tends to heat slightly more than the actual water column (Fig. 5 (c), (d)). This behaviour may be due to a small misrepresentation of the energy balance at the lake surface or at the bottom and requires additional tests that could eliminate such systematic errors and improve the results, especially in cold periods.

The other important parameter which is essentially connected with lake vertical thermal structure is depth of mixed layer. To estimate it we assumed that ML ends at a point of half of the maximum temperature gradient (but not less than 0.5°C). Such criterion was used for observed data and LAKE2.0 results. In Flake, the ML depth is a major diagnostic variable, updated each time step using a sophisticated formulation, that treats both convective and stable regimes (see Mironov et al. (2010)). Time series of the ML depth for the 2017 and 2018 Alqueva's stratification periods are shown in Fig. 6. Curves of ML depth calculated from measurements and LAKE2.0 results coincide quite well. However, since the simulated water

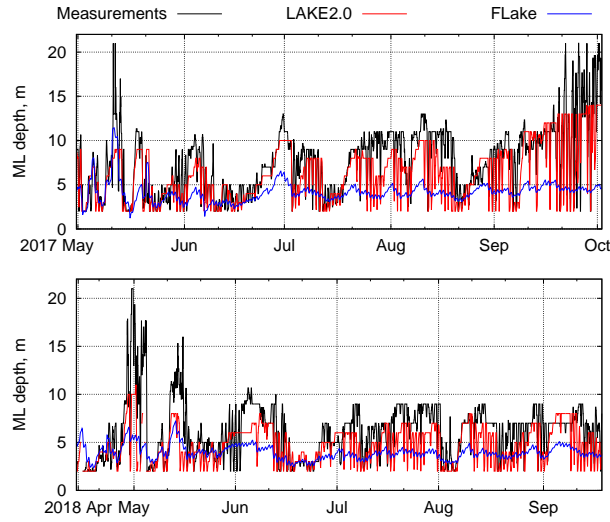


Figure 6. Evolution of ML depth during stratification periods (moving average with six-hours window).

temperature profiles are more smooth, LAKE2.0 ML depth has more "downward" peaks in the figure. Although FLake tends to underestimate ML depth, the general pattern of it correlates with measurements.

3.2 Heat fluxes

Sensible and latent heat fluxes play an important role in lake-atmosphere interaction, determining the rates of heat accumulation by water bodies or evaporation from the surface and consequently have effects on the local climate and on the establishment of thermal circulations (see for example Iakunin et al. (2018)). The LAKE2.0 model (as well as the FLake) ~~is capable to calculate~~ are capable of calculating heat fluxes and ~~the figure 7 represents shows~~ the daily averaged results of the simulation of these variables.

Sensible heat flux is well represented by both models (Fig. 7 (a,b)) which is supported by low mean errors (see table 3) and high correlation coefficient. Latent heat flux, however, is overestimated by LAKE2.0 and FLake models (by 53-43 Wm^{-2}) although both models demonstrate high correlation (0.92) with the measurements.

Table 3. Sensible and latent heat flux errors and correlation coefficients

	Sensible heat		Latent heat	
	LAKE2.0	FLake	LAKE2.0	FLake
Mean error, Wm^{-2}	5.51	5.36	52.93	43.46
MAE, Wm^{-2}	8.38	6.85	53.40	44.02
Corr. coefficient	0.88	0.87	0.92	0.92

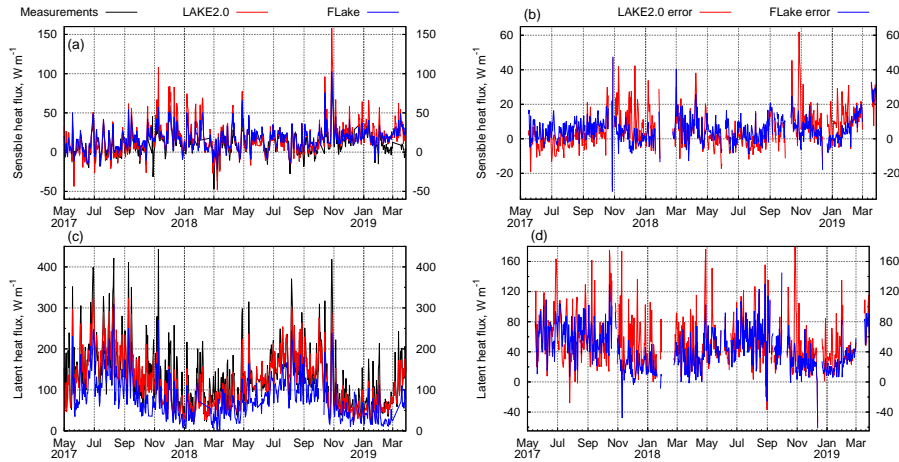


Figure 7. Daily averaged sensible (a) and latent (c) heat fluxes with corresponding errors (b, d). Black curve represents the measured values, red curve is associated with LAKE2.0 results, and blue curve is with FLAKE results.

In terms of latent heat fluxes the LAKE2.0 model results are worse than the FLake when compared to the ~~Eddy-covarienee~~ eddy-covariance (EC) measurements. However, it should be noted that several studies have indicated that the ~~eddy-covarienee~~ eddy-covariance EC systems tend to underestimate the heat fluxes (e.g. Twine et al., 2000). ~~Present results show~~ Recent works showed comparable differences between the FLake and the LAKE2.0 models and EC measurements over lakes (Stepanenko et al., 2014; 5 Heiskanen et al., 2015) in which the relative differences of about 35% were noticed. The differences between model and EC observations can also come from the model errors due to the fact that the Alqueva reservoir is an open lake with a ~~constant~~ continuous inflow and outflow of Guadiana river. The horizontal flows, not represented in one-dimensional vertical models, can add or remove energy from the water body. Also, the water level of the Alqueva changes significantly during the year due to drought periods and discharges through the dam. It decreased on up to 7 meters in 2018 that corresponds the loss of 35% of 10 total volume of water. The models cannot take into an account those changes while they could be a major source of errors in heat flux computations.

3.3 Dissolved carbon dioxide

The diffusion of CO₂ from the atmosphere to water and its further dissociation are of major importance to photosynthetic organisms which depends on the availability of inorganic carbon (Wetzel, 1983). Dissolved inorganic carbon constituents also 15 influence water quality properties such as acidity, hardness, and related characteristics.

The solubility of CO₂ in water depends on several factors such as pH, water temperature, etc. Observations indicate that pH may vary from 8.8 at the surface level to 7.4 at the bottom, while in the model it is a constant parameter which value was set to a value of 8.48 which ~~corresponds~~ corresponded to the mean pH value during the simulation period. Figure 8 reveals

the dynamics of CO₂ concentration on water in the first months of the ALOP field campaign in comparison with LAKE2.0 simulated results.

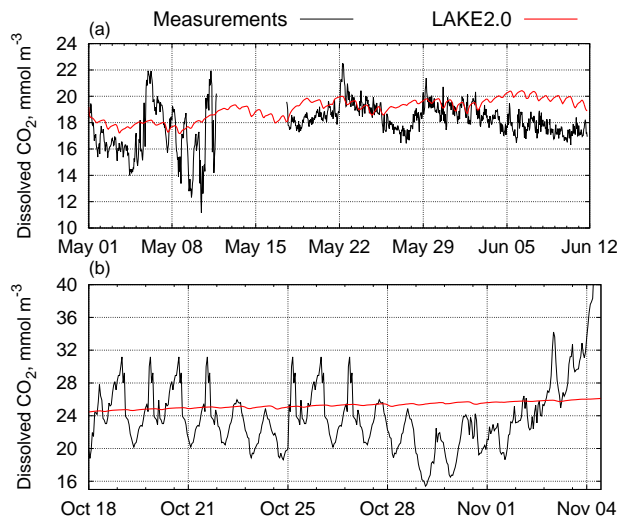


Figure 8. Timeseries of dissolved CO₂ in water at 25 cm depth

In general, the LAKE2.0 values are smoother than the observations as the model does not react to the changes in CO₂ so fast but the mean values are well represented. On May 20-26 and in the beginning of June (subplots in Fig. 8 (a)) daily cycles are represented quite ~~good~~well. In the second week of May, CO₂ probe accidentally dismantled from the platform and remained floating in the water on the connecting cord until the next field work trip (17th of May). ~~This explains the rapid changes in measured values in this period.~~ On the 12th of June the probe failed and it was dismantled and removed from the Montante platform. Later on the 18th of October the probe was mounted on the platform again and it was working in a test mode for three weeks (Fig. ~~??~~). ~~Timeseries of dissolved CO₂ in water at 25 cm depth for the period 18 October – 5 November.~~ 8 (b)). In this period, LAKE2.0 simulated values of CO₂ do not show much daily variations and have an increasing trend due to autumn water cooling. Small daily biases in simulated values coincide with peaks in measured data.

Thus, we can conclude that in long-time simulations LAKE2.0 model represents CO₂ trends quite well. The model failed to reproduce diurnal cycle of the surface carbon dioxide concentration which calls for inquiry of parameterizations of photosynthesis and respiration in the model. However, the diurnal means are well captured which is enough in perspective of using the model in climate applications.

3.4 Dissolved oxygen

Dissolved oxygen (DO) is essential to all aerobic organisms living in lakes or reservoirs. To understand the distribution, behaviour, and growth of these organisms it is necessary to know the solubility and dynamics of oxygen distribution in water. The rates of supply of DO from the atmosphere and from photosynthetic inputs, and hydromechanical distribution of oxygen

are counterbalanced by consumptive metabolism. The rate of oxygen utilization in relation to synthesis permits an approximate evaluation of the metabolism of the lake as a whole (Wetzel, 1983).

The concentration of DO in the Alqueva reservoir was measured continuously on the Montante platform since July 3rd 2018. Comparison of measured and model values are shown in Fig. 9. The model represents DO concentration in a realistic

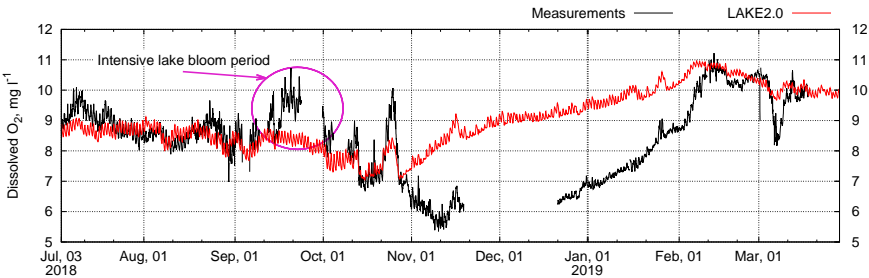


Figure 9. Timeseries of dissolved O₂ in water at 25 cm depth for the period July 3, 2018 — March 29, 2019 at the Alqueva reservoir.

- 5 way during the first two months until the middle of September when a microalgal bloom occurred. It caused an intensive production of O₂ in water that can not be represented by the LAKE2.0 which does not have an explicit representation of algae, and the bloom does not affect atmospheric forcing. Then, until the end of October, the model showed good results but in November the observations demonstrated a decrease of oxygen concentration which was not followed by the model, in fact, the model predicted an increase until the beginning of February. In November ~~the turnover happens, following turnover.~~
- 10 water temperature decreases and does not change significantly with ~~depths~~depth; under this conditions concentration of oxygen producing organisms decreases so does DO that falls from 8-9 to ~~6~~6 mg l⁻¹ mg l⁻¹. The model does not reflect this decrease in photosynthesis but largely increases DO concentration following the decrease of water temperature (oxygen is more soluble in colder water). When in the middle of February temperature returns to stratified regime DO concentration in the model and measurements coincide again.
- 15 The photosynthesis rate can be linked to chlorophyll-a measurements (Table 4) which were done during the field work at the Alqueva reservoir. In July 2018, when DO measurements began, concentration of chlorophyll-a ranged from 1.754 to 2.98 ~~-1~~ mg m⁻³ in water ML (0-3 m). Further, when autumn bloom occurred in September, chlorophyll concentration significantly

Table 4. Chlorophyll-a measurements at the Alqueva

Depth	Chlorophyll-a concentration, mg m ⁻³										
	'17 Jul	Sep	Nov	'18 Jan	Apr	Jun	Jul	Sep	Nov	19' Jan	Feb
Surface	1.11	7.60	1.03	2.55	12.189	5.796	2.678	14.036	2.309	No pigments	1.2
1 m	0.00	6.33	0.78	2.33	12.695	4.344	1.754	6.279	1.385	—	—
2 m	1.11	6.65	1.03	2.44	11.573	3.989	2.124	7.849	1.847	—	—
3 m	2.77	6.65	0.96	1.99	9.973	3.022	2.980	9.603	1.385	—	—

increased and reached 14.036 mg l^{-1} at the surface, and came back to values of 2.309 mg m^{-3} in November. ~~LAKE2.0 model solves DO concentration assuming a constant chlorophyll-a concentration of 2.3 l^{-1} .~~ ALOP field campaign ended in December 2018 but the work on stations and the Montante platform maintenance continued, so in January and February 2019 samples from water surface layer were taken. The sample of January 15 showed no traces of chlorophyll-a in water which is related to very low DO concentration in this period (Fig. 9). The measurements of chlorophyll-a in water sample taken on 2nd of February showed the value of 1.3 mg m^{-3} . It corresponds to the relative increase of oxygen producers in water, and hence, DO concentration.

Analysis of DO profiles (Fig 10) shows similar results. Distribution of oxygen with depth are well represented by the model for July and September profiles, while in December and February with no stratification in temperature and oxygen LAKE2.0 model overestimates DO on up to 2.5 mg l^{-1} . March profiles (1 and 29) show good similarity in measured and simulated values.

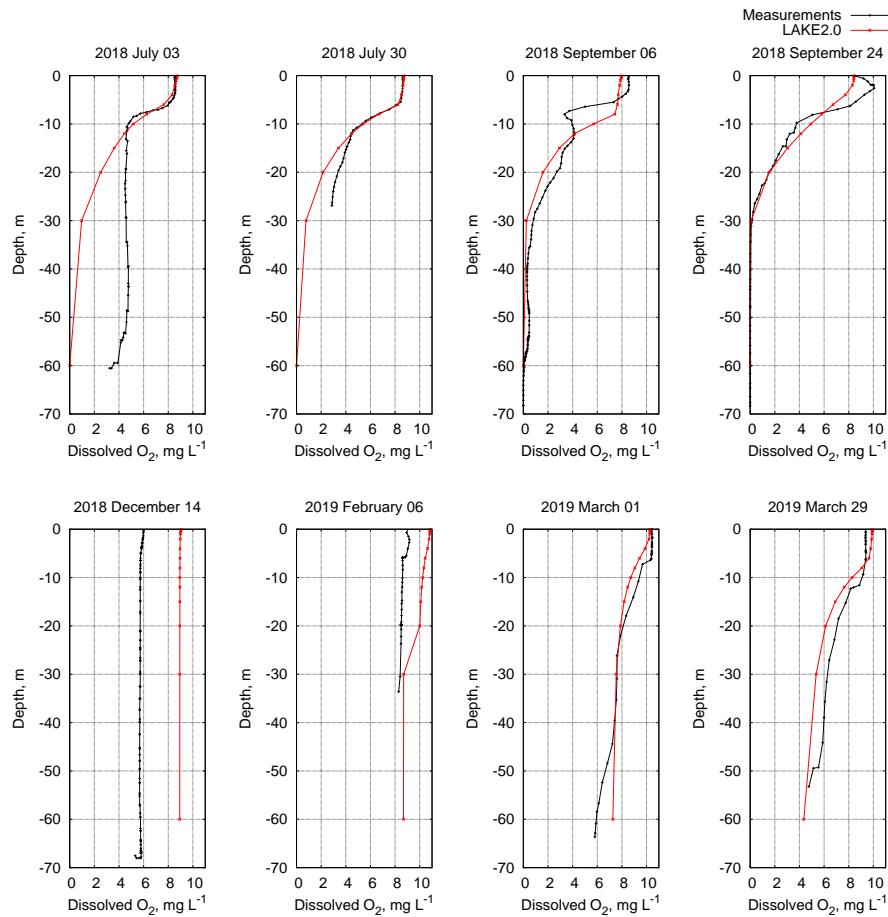


Figure 10. Profiles of dissolved O_2 in water measured during the field campaign (Black) and model values (red).

4 Conclusions

Numerical studies of the seasonal variations of the thermal and gas regimes in the Alqueva reservoir ~~with~~ using the LAKE2.0 and the FLake models are presented in this work. Simulated profiles and timeseries of water temperature, sensible and latent heat fluxes, concentrations of dissolved CO₂ and O₂ were compared with observed data. The seasonal variations of the ML water temperature are well represented by both models. Mean absolute errors are 0.74 °C and 1.27 °C for LAKE2.0 and FLake models correspondingly and the correlation coefficients for the relationship between simulated and measured temperature are 0.99 ~~for~~ both. The LAKE2.0 model overestimates ML water temperature only by 0.5 °C during the warm periods (March – October), while FLake shows ~~overestimation~~ an overestimation of about 1.5 degrees. In the cold periods (November – February) both models show the same ~~rate level~~ of overestimation of ML temperature about 0.6-0.9 °C.

The model errors of the seasonal variations in sensible and latent heat fluxes are the following. Sensible heat MAEs are 7.71 Wm⁻² (LAKE2.0) and 6.75 Wm⁻² (FLake). Latent heat flux results of both models in terms of MAE are worse: 53.99 Wm⁻² (LAKE2.0) and 45.6 Wm⁻² (FLake). Such errors ~~could be due to the sporadic input of measured wind speed, which values change rapidly~~ occur mainly in periods when the wind increases suddenly. Strong single high hourly wind input data cause high latent heat simulated values, not always confirmed by the observations.

LAKE2.0 simulated dissolved carbon CO₂ timeseries demonstrated a good ~~aeoordance~~ correspondence with the observations in mean values, however the model significantly underestimated the magnitude of diurnal cycle. On the ~~second year~~ 18th month of the experiment (October 2018, when the probe was returned to the platform), the simulated CO₂ values did not show ~~big errors~~ large residuals despite the fact that pH value remained constant during the whole simulation ~~period~~.

Dissolved oxygen, reproduced by the model, reveals the need of ~~modernisation of~~ inclusion of a more complete description of the processes regulation photosynthesis and respirations in the LAKE2.0 model before operational use. Although ~~the measured oxygen concentrations are well~~ simulated values of -O₂ ~~may coneur with measurements in over~~ short time intervals, the annual Alqueva oxygen cycle cannot be reproduced because the model does not respond to ~~algae bloom~~ changes in algal concentration (underestimation of -O₂ values) and winter minimum (high overestimation). Winter overestimation is supposedly due to ~~the~~ relatively low water temperatures. Nevertheless, high versatility and flexibility of the LAKE2.0 model gives good opportunities for elimination this flaws with the aim of adequate modelling of seasonal variations in gas regime of the lake.

~~The performed simulation confirms that the FLake model is a good option to be used to forecast lake surface water temperature namely in Numerical Weather Prediction in which the running time is critical~~ Performed simulations showed that LAKE2.0 model accurately simulates the lake thermal regime and the heat and gas fluxes from the ML. In terms of water temperature profile, LAKE2.0 demonstrated better performance than the FLake model. The results are encouraging as to the ability of the LAKE2.0 model to represent the evolution of physicochemical profiles inside the lakes, and may be used operationally in the future, coupled with weather prediction models, to forecast variables useful in the management of water quality and aquatic ecosystems. Similarly, the results indicate that the LAKE2.0 model could be used in climate modelling to estimate the impacts of the climate change on the thermal and gas regimes of the lake.

Code and data availability. The current versions of the models used in the work as well as the atmospheric forcing data can be obtained at <https://doi.org/10.5281/zenodo.3608230> or upon request from the author (Maksim Yakunin, miakunin@uevora.pt, m.yakunin89@gmail.com). The source code of the FLake model is available for download at the website (<http://www.flake.igb-berlin.de/site/download>). The source code of the latest versions of the LAKE2.0 model is available at the website (<http://tesla.parallel.ru/Viktor/LAKE/wikis/LAKE-model>).

5 *Competing interests.* The authors declare that they have no conflict of interest.

Acknowledgements. The work is co-funded by the European Union through the European Regional Development Fund, included in the COMPETE 2020 (Operational Program Competitiveness and Internationalization) through the ICT project (UID / GEO / 04683/2019) with the reference POCI-01-0145-FEDER-007690 and also through the ALOP project (ALT20-03-0145-FEDER-000004). Victor Stepanenko was supported by Russian Science Foundation (grant 17-17-01210).

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Supplement to the paper by Maksim Iakunin
et al. "Numerical study of the seasonal
thermal and gas regimes of the large artificial
reservoir in Western Europe using LAKE2.0
model"

May 10, 2020

1 Representation of biogeochemical processes in LAKE model

1.1 Governing equations for dissolved gases and or- ganic carbon in a water column

Evolution and vertical distribution of three dissolved gases are considered in the LAKE2.0 model, which are methane CH_4 , oxygen O_2 and carbon dioxide CO_2 . However, dissolved carbon dioxide is supposed to be always in carbonate equilibrium, so that it contributes to concentration of dissolved inorganic carbon (DIC), $C_{DIC} = C_{\text{CO}_2} + C_{\text{HCO}_3^-} + C_{\text{CO}_3^{2-}}$, and it is the change of DIC that reflects the number of carbon atoms in CO_2 molecules added to (or lost by) a solution from (to) atmosphere, bubbles, respiring organisms or decaying organical matter (see Section 1.2).

In addition, the content of dissolved organic carbon (DOC), particulate organic carbon (both living, POCL, and dead, POCD) are calculated. POCL includes carbon atoms contained in phytoplankton and zooplankton.

The species listed above obey the following equation system:

$$\frac{\partial C_{CH_4}}{\partial t} = \text{Dif}_A(C_{CH_4}) + B_{CH_4} - O_{CH_4}, \quad (1)$$

$$\frac{\partial C_{O_2}}{\partial t} = \text{Dif}_A(C_{O_2}) + B_{O_2} + P_{O_2} - R_{O_2} - D_{O_2} - S_{O_2} - O_{O_2}, \quad (2)$$

$$\frac{\partial C_{DIC}}{\partial t} = \text{Dif}_A(C_{DIC}) + B_{CO_2} - P_{CO_2} + R_{CO_2} + D_{CO_2} + S_{CO_2} + O_{CO_2}, \quad (3)$$

$$\frac{\partial \rho_{DOC}}{\partial t} = \text{Dif}(\rho_{DOC}) + E_{POCL} - D_{DOC}, \quad (4)$$

$$\frac{\partial \rho_{POCL}}{\partial t} = \text{Dif}(\rho_{POCL}) + P_{POCL} - R_{POCL} - E_{POCL} - D_{h,POCL}, \quad (5)$$

$$\frac{\partial \rho_{POCD}}{\partial t} = \text{Dif}(\rho_{POCD}) - \frac{\partial(w_g \rho_{POCD})}{\partial z} - D_{POCD} + D_{h,POCL}. \quad (6)$$

where $\text{Dif}_A(\bullet) \equiv \frac{1}{A} \frac{\partial}{\partial z} (A k_s \frac{\partial \bullet}{\partial z})$, $\text{Dif}(\bullet) \equiv \frac{\partial}{\partial z} (k_s \frac{\partial \bullet}{\partial z})$ are diffusion operators, w_g is a sedimentation velocity of POCD particles. Equations (4)-(6) do not contain A , because they are not derived by horizontal averaging, but follow from assumption of horizontal homogeneity of respective biogeochemical variable. This is caused by uncertainty of estimating the flux of these substances at the sloping interface between water and sediments. The r.h.s of these equations represent diffusion (assuming $k_s = k_{s,t} + k_{s,m}$ with the same eddy diffusivity $k_{s,t}$ and molecular diffusivity $k_{s,m}$ for all species; molecular diffusivity is not included in POCL and POCD equations), sources and sinks due to the following processes:

- dissolution/exsolution of gases at the bubble-water interface (B_{CH_4} , B_{O_2} and B_{CO_2});
- photosynthesis (P_{O_2} , P_{CO_2} , P_{POCL});
- respiration (R_{O_2} , R_{CO_2} , R_{POCL});
- biochemical oxygen demand in the water column (D_{O_2} , D_{CO_2} , D_{DOC} , D_{POCD});
- sedimentary oxygen demand (S_{O_2} , S_{CO_2});
- methane aerobic oxidation in the water column (O_{CH_4} , O_{O_2} , O_{CO_2});
- death of living species ($D_{h,POCL}$)

All variables in the above list are positive definite, excepting B_{CH_4} , B_{O_2} and B_{CO_2} that may be either positive or negative. All concentrations in (1)-(3) are expressed in mol/m³ that allows for simple relations of sinks and sources in different equations based on stoichiometry of the respective reactions. Organic carbon variables DOC, POCL and POCD in (4)-(6) are molar concentrations of carbon atoms contained in these organic groups. Terms B_{CO_2} , P_{CO_2} , R_{CO_2} , D_{CO_2} , S_{CO_2} , O_{CO_2} in (3) possess "CO₂" subscript because carbon atoms are supplied to or removed from DIC of a solution in a form of CO₂.

In the following, the parameterizations of processes related to O₂ and CO₂ dynamics are described, whereas formulations for CH₄ processes are presented in (Stepanenko et al., 2016).

The formulations for photosynthesis, respiration, biochemical oxygen demand and sedimentary oxygen demand basically adopted from (Stefan and Fang, 1994) and (Hanson et al., 2004).

1.2 Carbonate equilibrium

Carbonate equilibrium means the equilibrium in the following reactions:



Involving kinetic constants of these reactions yields, that the DIC reads

$$C_{DIC} \equiv C_{CO_2} + C_{HCO_3^-} + C_{CO_3^{2-}} = C_{CO_2} [1 + k_1 10^{pH} + k_1 k_2 10^{2pH}]. \quad (9)$$

Here, the constants are given by Arrhenius equation:

$$k_i = k_{i0} \exp \left[-\frac{E_{act,i}}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right], \quad i = 1, 2, \quad (10)$$

R – universal gas constant, $k_1 = 4.3 \cdot 10^{-7}$ mol/l, $k_2 = 4.7 \cdot 10^{-11}$ mol/l, $E_{act,1} = 7.66 \cdot 10^3$ J/mol, $E_{act,2} = 1.49 \cdot 10^4$ J/mol. Thus, C_{CO_2} is readily calculated given C_{DIC} value, and vice versa, where pH is an external parameter.

Carbon atoms are added or removed from carbonate equilibrium system in a form of CO₂ during respiration, photosynthesis and organic chemical

and physical processes, hence the change of C_{DIC} equals to number of CO_2 consumed or produced. This explains the sense of terms in equation (3). For obtaining CO_2 flux across bubble surface or CO_2 diffusive flux to the atmosphere, C_{CO_2} is needed and is calculated from (9).

1.3 Boundary conditions for dissolved gases in a water column

The top boundary condition (at the lake-atmosphere interface) for any dissolved gas concentration in the case of open water has the form:

$$\left. \frac{k_s}{h} \frac{\partial C}{\partial \xi} \right|_{\xi=0} = F_C, \quad (11)$$

where C is C_{CH_4} , C_{O_2} or C_{CO_2} , and F_C is the diffusive flux of a gas into the atmosphere, positive upwards. This flux is calculated according to the widely used parameterization:

$$F_C = k_{ge}(C|_{\xi=0} - C_{ae}), \quad (12)$$

with C_{ae} being the concentration of the gas in water equilibrated with the atmospheric concentration and described by Henry law and k_{ge} , m/s, denoting the gas exchange coefficient, the so-called "piston velocity". The latter is written as:

$$k_{ge} = k_{600} \sqrt{\frac{600}{Sc(T)}}, \quad (13)$$

with the Schmidt number $Sc(T)$ having individual values for different gases and being temperature-dependent. The k_{600} coefficient has been a subject of numerous studies, and a number concepts have been put forward to quantify it (Donelan and Wanninkhof, 2002). The proper computation of this coefficient should account for the effects of a number of factors such as turbulence in adjacent layers of water and air, wave development and breaking, cool skin dynamics. The surface renewal model (MacIntyre et al., 2010; Heiskanen et al., 2014), used in LAKE2.0 model, "integrates" those effects through the near-surface dissipation rate of turbulent kinetic energy:

$$k_{600} = \frac{C_{1,SR}(\epsilon|_{\xi=0}\nu_w)^{\frac{1}{4}}}{\sqrt{600}}, \quad (14)$$

where ν_w designates molecular viscosity of water, $C_{1,SR} = 0.5$ is an empirical constant. TKE dissipation rate is available directly from $k - \epsilon$ closure.

When a lake is covered by ice, $F_C = 0$, which neglects contribution of diffusion through ice cracks.

1.4 Photosynthesis

The intensity of photosynthesis in terms of oxygen molecules production is expressed as:

$$P_{O_2} = \frac{P_{max} L_{min} \rho_{Chl-a}}{H_{sec} \mu_{O_2}}. \quad (15)$$

The denominator here serves to convert units in the r.h.s. from $\text{mg}/(\text{l}^*\text{h})$ to $\text{mol}/(\text{m}^3 \text{ s})$. The P_{max} value expresses limitation of oxygen production by temperature in a form:

$$P_{max} = C_P \theta_P^{(T-T_0)}, \quad (16)$$

so that C_P is a value of P_{max} at the reference temperature $T = T_0$. The limitation of oxygen production by the available photosynthetically active radiation PAR (S_{PAR}) is given by the Haldane kinetics:

$$L_{min} = \frac{S_{PAR}(1 + 2\sqrt{C_{Lmin,1}/C_{Lmin,2}})}{S_{PAR} + C_{Lmin,1} + S_{PAR}^2/C_{Lmin,2}}. \quad (17)$$

The PAR intensity delivering maximum to a limiter L_{min} ($=1$) is $S_{PAR} = \sqrt{C_{Lmin,1}C_{Lmin,2}}$. In the model, these coefficients are specified as (Stefan and Fang, 1994; Megard et al., 1984):

$$C_{Lmin,1} = C_{PAR} \theta_{PAR}^{(T-T_0)}, \quad (18)$$

$$C_{Lmin,2} = H(T - T_{00})C_{Lmin,2,>T_{00}} + [1 - H(T - T_{00})]C_{Lmin,2,<T_{00}}, \quad (19)$$

with $H(\bullet)$ denoting a Heavyside function, and T_{00} standing for another reference temperature. It is seen from (17), that $L_{min} \rightarrow 0$ if $S_{PAR} \rightarrow 0$ and $S_{PAR} \rightarrow \infty$, i.e. PAR inhibits photosynthesis at both low and high values of its intensity. The PAR intensity S_{PAR} is expressed in a number of photons per square meter per hour, so that:

$$S_{PAR} = H_{sec} T_{J \rightarrow E} S_{PAR}^*, \quad (20)$$

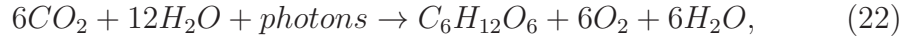
where $H_{sec} = 3600$ s and S_{PAR}^* is PAR intensity in W/m^2 . The coefficient transforming from J to Einstein (Einstein is an energy of Avogadro number of photons), $T_{J \rightarrow Eins}$, is estimated assuming the uniform distribution of energy in PAR region, which yields:

$$T_{J \rightarrow Eins} = \frac{\lambda_{PAR}}{N_A h_P c}, \quad (21)$$

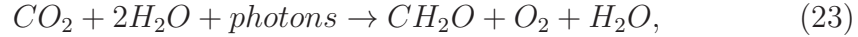
with N_A, h_P, c denoting Avogadro number, Planck constant and the light speed in vacuum, respectively, all in SI units.

The treatment of chlorophyll-a concentration ρ_{Chl-a} is given in Section 1.10.

Finally, from the gross photosynthesis reaction:



or, in a shortened form:



we see that the carbon dioxide consumption equals oxygen production, i.e. $P_{CO_2} = P_{O_2}$.

Equation (22) also implies that $P_{POCL} = P_{CO_2}$.

1.5 Respiration

P.Hanson et al. (Hanson et al., 2004) assume, that respiration is performed by "living particles", i.e. POCL, only in epilimnion, and may be scaled by gross primary production (i.e., photosynthesis rate), $R_{POCL} = \alpha_{POCL} P_{POCL}$, $\alpha_{POCL} = 0.8$. In contrast, we assume that this process happens at all depths where enough oxygen *in situ* to be used in respiration is available, with the same scaling. Evidently,

$$R_{O_2} = R_{CO_2} = \alpha_{POCL} P_{POCL}. \quad (24)$$

1.6 Biochemical oxygen demand (BOD)

We treat biochemical oxygen demand as a consumption of oxygen during degradation of dead organic particles (POCD) D_{POCD} and dissolved organic

Table 1: Constants in photosynthesis model

Constant	Units	Value
C_P	h^{-1}	9.6
θ_P	n/d	1.036
T_0	$^{\circ}\text{C}$	20
T_{00}	$^{\circ}\text{C}$	10
μ_{O_2}	g/mol	32
H_{sec}	s	3600
C_{PAR}	Einstein/($\text{m}^2 \cdot \text{h}$)	0.687
θ_{PAR}	n/d	1.086
$C_{Lmin,2,>T_{00}}$	Einstein/($\text{m}^2 \cdot \text{h}$)	15.
$C_{Lmin,2,<T_{00}}$	Einstein/($\text{m}^2 \cdot \text{h}$)	5.
λ_{PAR}	m	$5.5 * 10^{-7}$ (550 nm)

carbon (DOC) D_{DOC} , following (Hanson et al., 2004); they suggest that $D_{POCD} = \rho_{POCD}/\tau_{POCD}$, $D_{DOC} = \rho_{DOC}/\tau_{DOC}$ with time scales $\tau_{POCD} = 20D_{sec}$, $\tau_{DOC} = 200D_{sec}$ (D_{sec} is a number of seconds in a day). Thus, the BOD rate is:

$$D_{O_2} = D_{CO_2} = \left(\frac{\rho_{POCD}}{\tau_{POCD}} + \frac{\rho_{DOC}}{\tau_{DOC}} \right). \quad (25)$$

1.7 Sedimentary oxygen demand (SOD)

The sedimentary oxygen demand appears as a sink in (2) and in essence is the contribution of the vertical flux of O_2 at the lake's bottom to the horizontally averaged oxygen concentration:

$$S_{O_2} = -\frac{F_{SOD}}{A} \frac{\partial A}{\partial z}. \quad (26)$$

Basing on the argument that SOD is controlled by both diffusion (governed by Fickian law) and biochemical consumption (described by Michaelis-Menten kinetics), (Walker and Snodgrass, 1986) derive:

$$F_{SOD} = \mu_{\beta} \frac{C_{O_2}}{k_{O_2,SOD} + C_{O_2}} + k_c C_{O_2}, \quad (27)$$

where μ_β is proportional to organics oxidation potential rate in sediments, and k_c is the mass transfer coefficient. Both are thought to be exponentially dependent on temperature:

$$\mu_\beta = \mu_{\beta,0} \theta_{\mu_\beta}^{T-T_{\mu_\beta}}, k_c = k_{c,0} \theta_{k_c}^{T-T_{k_c}}. \quad (28)$$

The stoichiometry of SOD is assumed to be close to that of BOD (??), therefore, $S_{CO_2} = S_{O_2}$. Additionally, the flux of O_2 due to SOD at the lake bottom, F_{SOD} , is used as the bottom (lake deepest point) boundary condition for the oxygen equation (2).

Table 2: Constants in sedimentary oxygen demand model

Constant	Units	Value
θ_{μ_β}	n/d	1.085
θ_{k_c}	n/d	1.103
T_{μ_β}	K	25
T_{k_c}	K	20
$\mu_{\beta,0}$	mol/(m ² *s)	$0.5/(\mu_{O_2} D_{sec}), [\mu_{O_2}] = g/mol$
$k_{c,0}$	m/s	$0.045/D_{sec}$

1.8 Exudates and death rate of POCL

Hanson et al. suggest exudation to be scaled with photosynthesis rate, $E_{POCL} = \beta_{POCL} P_{POCL}$, $\beta_{POCL} = 0.03$ and the death rate to be defined as $D_{h,POCL} = \frac{P_{POCL}}{\tau_{Dh}}$, where time scale τ_{Dh} ranges from $1.1D_{sec}$ in hypolimnion to $33D_{sec}$ in epilimnion.

1.9 Sedimentation of organic particles

In the current model version we use the Stokes sedimentation velocity below the mixed layer:

$$w_s = \frac{4}{3A} \frac{\Delta g d^2}{\nu_m}, \quad (29)$$

and the high-Reynolds-number limit of this variable

$$w_s = \sqrt{\frac{4}{3B}\Delta g d} \quad (30)$$

in the mixed layer. Here, $\Delta = \rho_p/\rho_{w0} - 1$, ρ_p is a particle's density, and d – its diameter, the typical values for constants may be chosen as $A = 30.0$, and $B = 1.25$ (Song et al., 2008), and the density of organic particles as 1.25 g/cm^3 (Avnimelech et al., 2001).

1.10 Chlorophyll-a dynamics

The chlorophyll-a dynamics in the model follows a simple scheme suggested in (Stefan and Fang, 1994), where chlorophyll-a density is calculated as:

$$\rho_{Chl-a} = \rho_{Chl-a,0} H(H_a - z), \quad (31)$$

where the active layer, H_a , is a maximum value between mixed-layer depth, H_{ML} , and the photic zone depth, H_{PZ} . The mixed-layer depth is defined as the depth of maximum Brunt-Väisälä frequency, and the photic zone depth is estimated as the depth at which the PAR irradiance drops to 10% of its surface value. The mean chlorophyll-a concentration in the active layer, $\rho_{Chl-a,0}$, is assigned according to a trophic status of the lake: $2 * 10^{-3} \text{ mg/l}$ for oligotrophic lakes, $6 * 10^{-3} \text{ mg/l}$ for mesotrophic lakes and $15 * 10^{-3} \text{ mg/l}$ for eutrophic lakes. In turn, the trophic status is formally defined from the water turbidity. The Secchi disk values of 2 m and 3.5 m are used to distinguish between eutrophic and mesotrophic, mesotrophic and oligotrophic states, respectively. These thresholds are expressed in the model through light extinction coefficient values, α , using Poole and Atkins formula (Poole and Atkins, 2009):

$$\alpha = \frac{k_{PA}}{z_{SD}}, \quad (32)$$

where z_{SD} is the Secchi disk depth and $k_{PA} = 1.7$. The above chlorophyll-a scheme is identical to that of (Stefan and Fang, 1994), excepting for it does not take into account the annual cycle of $\rho_{Chl-a,0}$.

2 Sensitivity tests

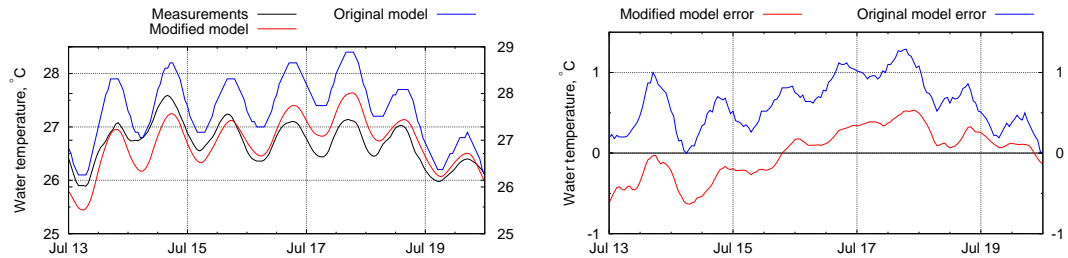


Figure S1: ML water temperature, original and modified model results and their errors when compared to the observations.

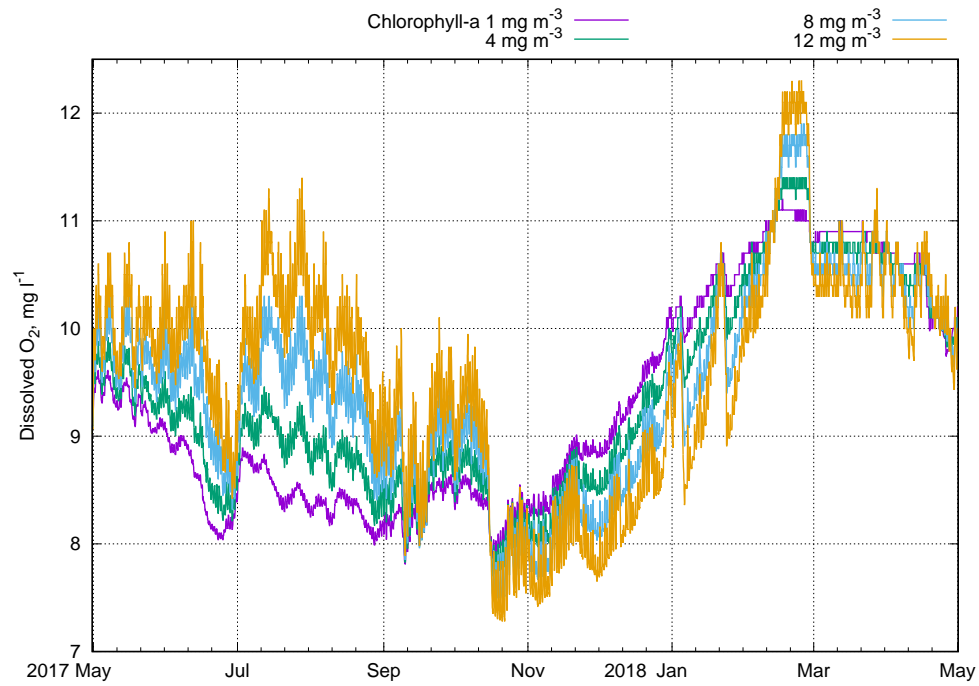


Figure S2: DO concentration at different chlorophyll-a concentration values.

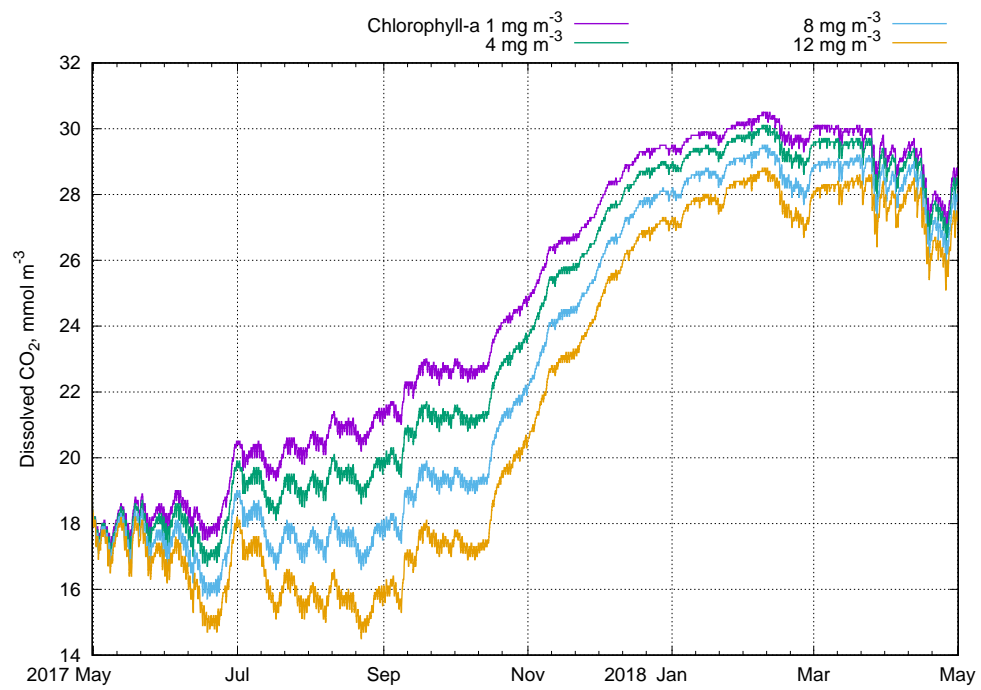


Figure S3: CO_2 concentration at different chlorophyll-a concentration values.

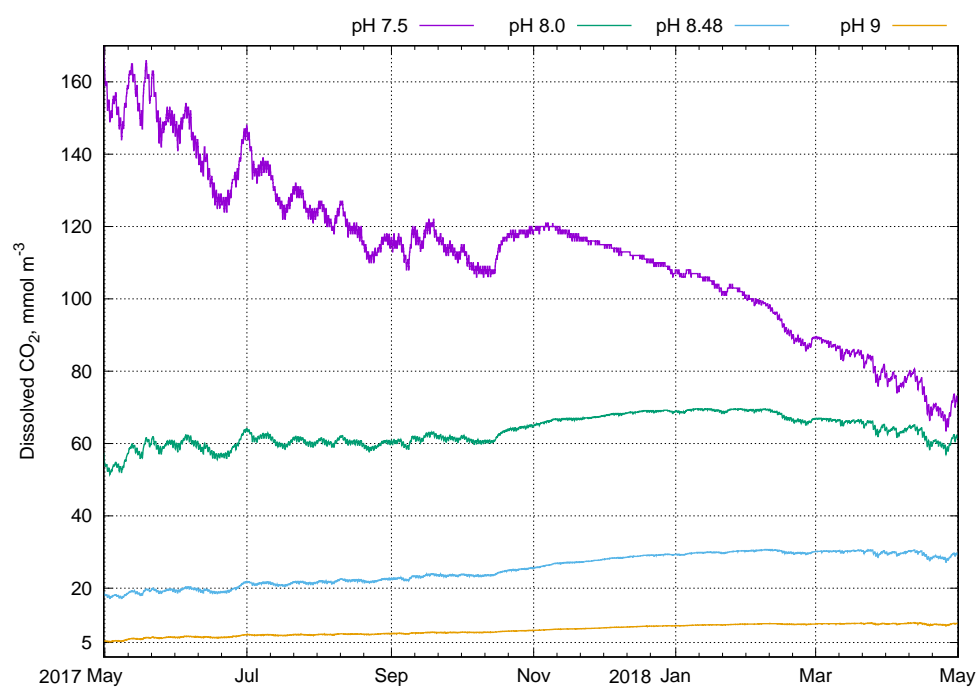


Figure S4: Dissolved CO_2 concentrations at different pH values.

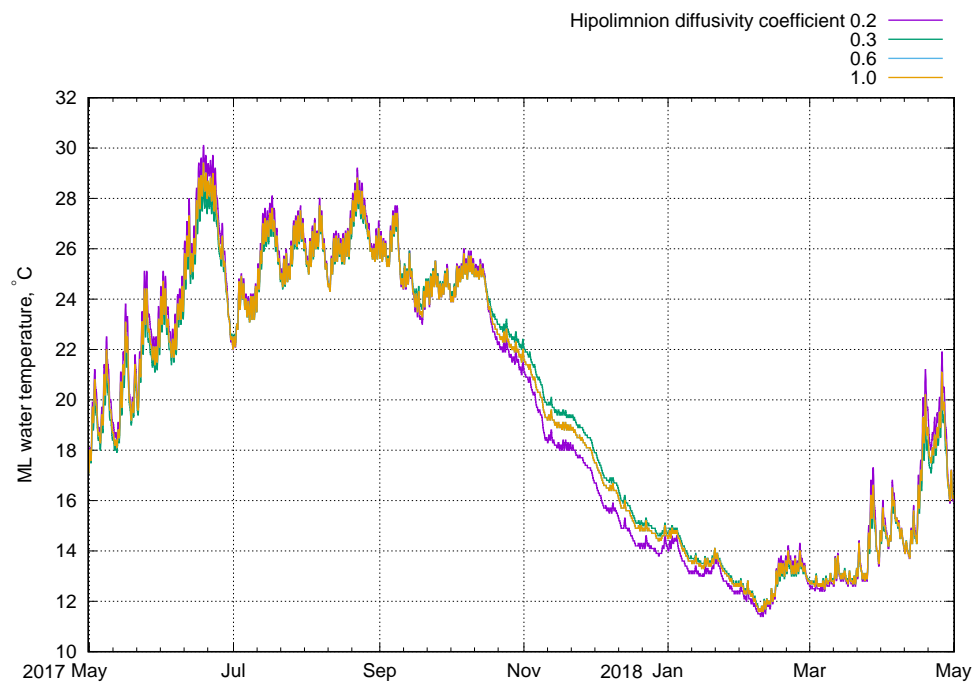


Figure S5: ML temperature at different hypolimnetic diffusivity coefficient values.

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