

# 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 #2 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<sup>A</sup>T<sub>E</sub>Xdiff package for better understanding of what has been changed.

## Anonymous Referee #2

### *General comments*

*It is useful that this paper presents a model comparison that focuses on the factors that would be most important in influencing the heat and gas fluxes from a lake. It was good to see model comparisons focusing on the mixed layer. However, there is a need to clearly state the criteria used to define the mixed layer. I was pleased to see the specific comparison of measured heat fluxes and gas fluxes collected at high resolution with simulated data from two models. This not commonly done and is a unique and valuable aspect of this paper. And for these reasons I think this paper does document important progress in lake model development and does deserve to be accepted for publication following revision.*

*I think for a modeling study such as this there is a need for more information on calibration. How the model was calibrated and what the final error levels were. It doesn't need to be extensive but as a minimum I would like to see a listing of the final calibrated parameter values, as well as a brief description of what each parameter does. A scatter plot of the simulated vs measured temperature. And some statistics on model fit (ie RMSE , MAE etc ) Furthermore, I'm assuming that the model was calibrated against measurements of water temperature, but this may not entirely be the case since there were measurements of gas concentrations and heat fluxes that could in theory also be used for calibration. What was used for calibration should be clearly stated.*

*One of the most important aspects of this paper is the comparison between the simulated gas fluxes with measured data. Therefore, I do think there is a need to better describe the equations governing CO<sub>2</sub> and O<sub>2</sub> concentrations. I was not that familiar with Lake 2.0 but after searching a bit I found that this is not the first time CO<sub>2</sub> and O<sub>2</sub> have been simulated with Lake 2.0, even though this paper may be one of the best verification studies. I would like to see some overview description of the main processes affecting the CO<sub>2</sub> and O<sub>2</sub> concentrations and also more clear references to the original publications where the equations describing these processes are completely defined.*

There were two things that were changed in the version of the model used in this study (the fixed pH value and the equations affecting diffusion in the hypolimnion) and also one assumption (fixed chlorophyll concentration) which I suspect and which later in the paper the authors also suspect leads to errors in the simulated oxygen concentration. I think all three of these should be evaluated in a sensitivity analysis as part of the paper in section 2.4 as was done with the light extinction coefficient.

There are quite a few small language errors in the paper. I have tried to suggest solutions to many in the technical comments. These should not be allowed to take away from the good scientific and technical aspects of this study, so I think it would be good to have paper carefully proofread for language before the final submission.

**Response:** We thank the Reviewer for the positive comments and thorough revision of the manuscript. The paper was edited very carefully and modifications and improvements were made. A Supplementary file was created as well, where more details of LAKE2.0 biogeochemistry processes are described and figures of sensitivity tests are shown. Below, we address every comment and explain the corresponding changes.

## Specific comments

### Comment 1

Abstract - Since you mention the Flake model in the abstract I think you should have a brief statement about how well it worked compared to Lake2.0.

**Response:** The end of the abstract was changed to:

The results demonstrated that both models well captured the seasonal variations in water surface temperature and the internal thermal structure of the Alqueva. The LAKE2.0 model showed slightly better results and satisfactorily captured the seasonal gas regime.

### Comment 2

Line 40 - what do you mean by "to complete the results". Does Flake do something that Lake2.0 does not? Or are you comparing the results of the two models

**Response:** FLake does not do anything more than LAKE2.0, and by "complete" we meant to use its results as a supplement. As we, however, compared the results of two models, the sentence was rewritten:

... FLake model was used as a reference to compare the results of thermodynamic characteristics of the reservoir.

### Comment 3

Lines 98-99 I think you could give a bit more information. What type of errors? How much missing information was there? Linear interpolation?

**Response:** In this particular place of the text by errors we meant missed values. They occurred during the equipment maintenance (short gaps that were filled with linear interpolation) or when the equipment was temporarily dismounted. In the last case, when the gaps in data were larger than 3 hours, data from nearby stations were used instead. For instance, in case of lack in downward radiation data measured at the floating platform we used the values from the weather station on the shore. The corresponding sentence was reworked:

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.

#### Comment 4

*Line 104 Are not these fluxes also occurring through the surface?*

**Response:** They are. The sentence was corrected:

... through a sloping bottom and water-atmosphere surfaces.

#### Comment 5

*Line 105 and unlike Hostetler model I don't know what you mean by unlike Hostetler model. Are you using this model as well? Or our components of this model embedded in Lake2.0?*

**Response:** No, none of the components of Hostetler model is used in the LAKE2.0 and this model did not participate in the experiment. The reference to it was removed from the sentence:

Water temperature profile is simulated explicitly in LAKE2.0 and a number of biogeochemical processes is represented, which makes it capable to reproduce the transfer of CO<sub>2</sub> and CH<sub>4</sub> from and to the atmosphere.

#### Comment 6

*Line 141 the description of photosynthesis is rather unusual. Is it really reasonable to assume that chlorophyll remains constant while photosynthesis is changing? Perhaps this simplification can be justified by the fact that the modeling is mainly looking at gas exchange and not the biology of the lake. However, photosynthesis will affect both O<sub>2</sub> and CO<sub>2</sub>. Assuming a constant chlorophyll concentration could greatly under or over estimate the total photosynthesis in the epilimnion. I think there should be more justification for the constant chlorophyll assumption. Perhaps a sensitivity analysis on how changes in chlorophyll affect the gas flux estimates.*

**Response:** The model uses "pre-defined" values of chlorophyll-a concentration (three options) depending on PAR attenuation coefficient. Assuming this, chlorophyll-a concentration remained constant during almost the whole simulation. However, do avoid any confusion, the sentence on the constant chlorophyll value was removed from the text and the part describing the calculation of the chlorophyll-a from PAR attenuation coefficient was added. We also added a Supplementary material to the article where the model biogeochemical processes are widely described and results of sensitivity tests for pH chlorophyll-a concentration, hypolimnetic diffusivity coefficient, and

PAR attenuation coefficient are provided.

Photosynthesis is given by Haldane kinetics where chlorophyll-a concentration in mixed layer is computed from photosynthetic radiation extinction coefficient (Stefan and Fang, 1994), and assumed zero below.

### Comment 7

Later in lines 150-160 you document a large seasonal variation in the attenuation coefficient. How much of this is due to changes in chlorophyll? Could this variability invalidate the assumption of a constant chlorophyll concentration? Also in this section the model was modified to allow the input of a varying extinction coefficient which is a good idea. However, this could be described more clearly. It is stated that “introduce a new variable, the water extinction coefficient for photosynthetically active radiation (PAR), to the model setup” How does this coefficient differ from the coefficients described in line 120. Perhaps you mean that the existing coefficient described in line 120 was changed from a fixed model coefficient to a time varying one? However I’m still a little confused since PAR is usually considered to be between 400-700 nm and measured as a photon flux density, whereas I would think that the coefficient described on line 120 would have a wider bandwidth and would be measured in terms of watts

**Response:** Attenuation coefficient depends mainly on water turbidity and consequently depends on suspended and dissolved material in water. Higher chlorophyll concentration can indirectly increase the water turbidity and attenuation coefficient. The assumption of a constant chlorophyll concentration is set to mixed layer. The measurements of the attenuation coefficient were done in the layer from surface to 3 meter depth. In table 4 chlorophyll concentrations are presented for surface, 1, 2 and 3 m depth and is noticed that, despite in the September 2018 bloom, the values are almost constant in these depths. Thus, the seasonal variability of attenuation coefficient, accounted in this study through the measurements campaign, is an asset to compute reliable chlorophyll concentrations even if this concentration is set constant in the mixed layer. Supplementary material has a description of the processes that are included in the model.

There are 4 bands of the shortwave radiation in the LAKE2.0 model, and each has its own attenuation coefficient (Table 1). Only the coefficient for PAR range was added as an input variable (the rest remained constants). Corresponding changes were done in the text.

UV	3.13
PAR	variable
NIR	1.73
IR	1.087E+3

Table 1: Attenuation coefficients in LAKE2.0.

Attenuation coefficient units are  $m^{-1}$  while the solar energy was measured in terms of  $Wm^{-2}$  indeed. Conversion of PAR intensity from  $Wm^{-2}$  to  $N_{photons} m^{-2} hour^{-1}$  could be done with the equation (20) and (21) provided in the Supplementary material.

### Comment 8

Lines 165-166 need to be made clearer.

**Response:** The sentence was removed from the paragraph.

*Comment 9*

Starting at line 177 there are two changes to the model described one concerning pH and the other concerning hypolimnetic diffusivity. Sensitivity analysis should be done for both of these and these results would be better presented in the section starting on line 150

**Response:** The paragraph concerning diffusion hypolimnion was moved to the Section 2.4. Figures for the model sensitivity tests for this coefficient as well as for pH and chlorophyll-a concentration values were added to the Supplementary materials.

*Comment 10*

Line 191 this information is better place in the section on observational data (see comment above).

**Response:** Corresponding changes were done (see response to Comment 3).

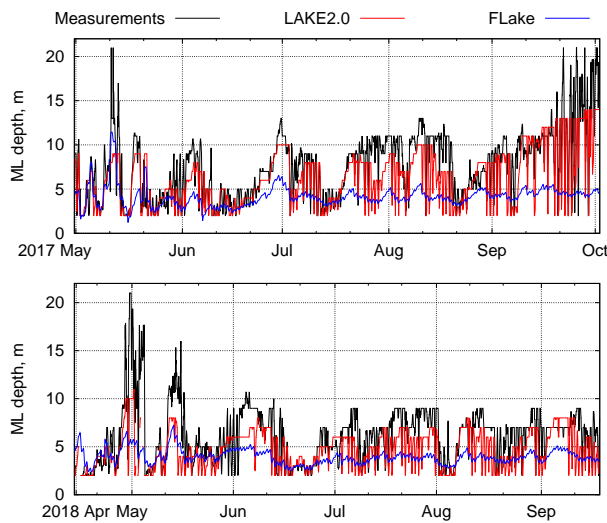
*Comment 11*

Line 207 Model simulations of the mixed layer depth (MLD) are discussed. The method for defining the MLD should be described in the methods section. Also in figure 4 it would be good to show a plot of the variations in the MLD over time. In the caption of fig 4 describe what the dashed horizontal lines represent.

**Response:** A new paragraph with a discussion on ML depth results was added to the end of Section 3.1 **Water temperature**. A method for the estimation of ML depth is defined there and the results are shown. A new figure with time series of the evolution of ML depth is introduced as well.

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 (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 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.

Caption for the Fig. 4 was corrected as well.



### Comment 12

Line 232 states “water temperature of thermocline beneath the ML at any depth” Don’t you mean water temperature of the hypolimnion?

**Response:** That is right in general, however, particularly here we were speaking about the  
 5 FLake model outputs. FLake does not represent meta- and hypolimnion, instead it has mixed layer and thermocline below it (a layer of water with negative temperature gradient down to the bottom). In FLake, this thermocline is described as parametrized curve which form is similar for every lake (this concept of self-similarity is the essence of this model). Depth-normalized curve is defined by the shape factor parameter, thus, if one knows it plus temperatures on the top and  
 10 bottom of the thermocline, it is possible to compute temperature at any depth of this curve. The sentence was reworked:

FLake provides ML depth, shape factor for the thermocline curve, ML and bottom temperature. Using these values it is possible to access water temperature of thermocline at any  
 15 depth.

### Comment 13

Line 252 states “Present results show comparable differences between the FLake and the LAKE2.0 models and EC measurements over lakes (Stepanenko et al., 2014; Heiskanen et al., 2015)” To me  
 20 present studies means the study being described in this paper. Do you mean something like other recent studies?

**Response:** This is a mistake in the text. Now Present results show ... is changed to Recent works showed ...

### Comment 14

25 Lines 255-259 Is it possible to estimate the depth of the horizontal flows from the surface temperature of the inflowing river? It seems like this would be most significant if the inflows are

*moving through the surface layer.*

**Response:** The LAKE2.0 model is capable to include the effects of inflow/outflow rivers, however, we did not include this option during the experiment: firstly, there are no regular measurements on the tributary rivers, secondly, we assumed that their effect is not significant. Our assumption was based no the following simple estimation.

We can write the thermal balance of the mixed layer in the following form:

$$\rho c V \frac{\partial T_{ML}}{\partial t} = q \rho c (T_{river} - T_{ML}) + S_{lake}(-H - LE + radiation),$$

where  $\rho$  is water density,  $c$  — water heat capacity,  $V$  — volume of the ML,  $T_{ML}$  and  $T_{river}$  are ML and river temperature, respectively,  $q$  is the inflow rate,  $m^3 s^{-1}$ ,  $S_{lake}$  — area of the lake surface,  $H, LE, radiation$  — sensible, latent heat and radiation fluxes. The part  $q \rho c (T_{river} - T_{ML})$  shows the amount of heat brought by the river.

$q$	$36 \text{ m}^3 \text{ s}^{-1}$	provided by EDIA for April 2020
$\rho$	$999 \text{ kg m}^{-3}$	—
$T_{ML}$	$16.5 \text{ }^\circ\text{C}$	average of the measurements in April 2020
$T_{river}$	$17.5 \text{ }^\circ\text{C}$	no data originally, assumed as an average daytime air temperature
$c$	$4185 \text{ J kg}^{-1} \text{ K}^{-1}$	—
$S_{lake}$	$2.5 \times 10^8 \text{ m}^2$	—
$H$	$30 \text{ W m}^{-2}$	average value for April
$LE$	$80 \text{ W m}^{-2}$	„

Table 2: Example of values for the heat capacity estimation.

Using corresponding values given in Table 2, we compared  $q \rho c (T_{river} - T_{ML})$  with  $S_{lake} H$  and  $S_{lake} LE$  and found out that the heat brought by the river tributary is only about 2% of heat lake losses from sensible heat and 0.8% of latent heat.

### Comment 15

*Line 270 In the second week of May, CO2 probe accidentally dismounted from the platform and remained. - I think you should just remove these data from the plot You clearly do not believe they are meaningful and have a good explanation for this.*

**Response:** Figure 8 was remade and Fig. 9 was combined with Fig. 8. Corresponding changes have been made in the paragraph.

### Comment 16

*Lines 298-299 Chlorophyll concentrations are given in mg/l should these be ug/l (10-6g/l)? The mg/l concentrations that are given are very high and would be considered typical of a highly eutrophic lake. They would also certainly greatly affect the O2 concentration I have the same concern for the values in table 4.*

**Response:** A mistake was made cholorophyll-a units: it  $\text{mg m}^{-3}$ . Corrections were made in text and in the Table 4.



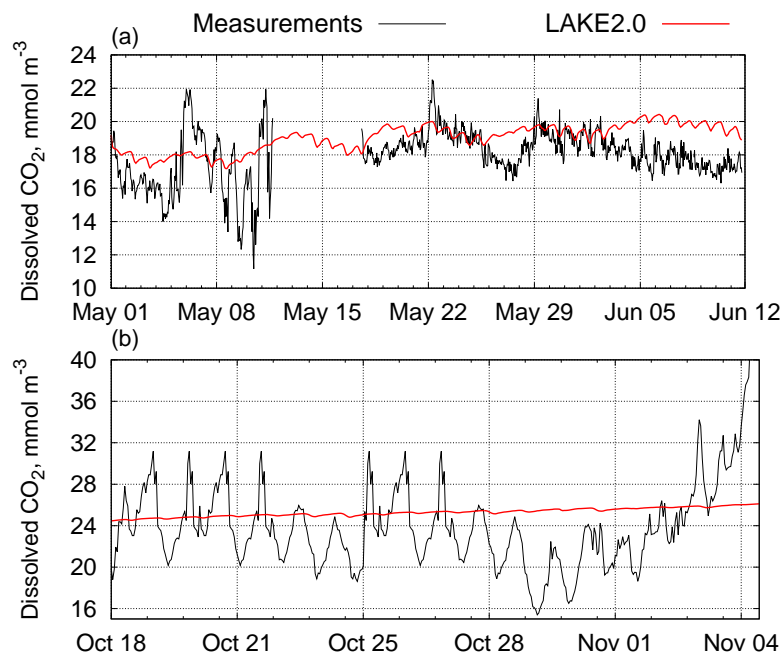


Figure 1: Result figure discussed in Comment 15

### Comment 17

Line 322 You state “Such errors could be due to the sporadic input of measured wind speed, which values change rapidly” First I would suggest sporadic nature rather than input. But I also think this needs more of an explanation Are we talking about errors in both latent and sensible heat? And what is the mechanism by which sporadic winds are increasing model error?

**Response:** No, here we were speaking only about latent heat. We noticed that latent heat in the model is sensitive to strong increase of wind speed. In such cases, a local peak of latent heat in the model may occur, which usually does not coincide with the measurements. Corresponding sentence was rephrased to become clearer:

Such errors 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.

### Comment 18

Line 325 You state “On the second year of the experiment (October 2018, when the probe was returned to the platform), simulated CO<sub>2</sub> values did not show big errors despite the fact that pH value remained constant during the whole simulation period.” But was not the pH also constant during the first year? Were there larger errors in the first year due to the fixed pH?

**Response:** Yes, the value of pH remained constant during the whole simulation. Here we wanted to point out that, despite that fact, the simulated values of CO<sub>2</sub> have not "gone far" from the observations after 18 months of the simulation, in the end of October 2018. The corresponding

sentence was rephrased:

On the 18th month of the experiment (October 2018, when the probe was returned to the platform), the simulated CO<sub>2</sub> values did not show large residuals despite the fact that pH value remained constant during the whole simulation.

### Comment 19

*Line 334 This final paragraph needs to be reworked First I think you should be stressing that the Lake 2.0 model was shown to accurately simulate the heat fluxes and gas fluxes from the ML. I think this is one of the major model developments being described here. Secondly, I don't think you should start out by say that Flake is good model — Im sure this is true but it is not the purpose of this paper. You should be stating that Lake 2.0 is as good or better than Flake as you have shown in some of the comparisons in the paper. Finally in terms of using these two models to improve weather predictions you state that Flake has lower computational demands. By why not give some numbers on this? How much slower is Lake 2.0? Is it realistic to think it could be used to support weather prediction in the future?*

**Response:** The final paragraph was reworked. We removed the part about computational performance. FLake model is used in several NWP systems, thanks to its simplicity and satisfactory representation of the evolution of the lake surface temperature, which is the most important parameter from the point of view of weather forecasting and, therefore, support weather prediction. We do not state that LAKE2.0 would support it in future, but it can be used in many tasks in fields of ecology, biogeochemistry, etc.

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.

## Technical details

*Line 1 (Suggested change) The Alqueva reservoir (southeast of Portugal) being the largest artificial lake in Western Europe and a strategic freshwater supply in the region. The reservoir is of scientific interest and monitored in order to maintaining the quality and quantity of water and evaluate its impact on the regional climate. To support these tasks we conducted numerical studies of the thermal and gas regimes in the lake.*

Suggestions were considered and the sentence was corrected.

*(Suggested change)supplemented by the data observed at the weather stations and the floating platforms deployed during the field campaign of the ALOP (ALentejo Observation and Prediction System) project. One-dimensional model LAKE2.0 was used for the numerical studies.*

5      Weather stations and floating platform were deployed and established before the ALOP. Other corrections were done.

*line 8 this parameterization » this model?*  
Corrected.

10      *Line 14 participants » regulators*  
Corrected.

*Line 20 allow to use them » allows them to be used*  
15      Corrected.

*Line 25 models are important models is important*  
Corrected.

20      *Line 30 for the lake ecosystem vital activity » regulating lake ecosystem processes*  
Corrected.

*Line 39 allowing to reproduce the concentrations » that simulates the concentrations*  
Corrected.

25      *Line 43 spelling (hypolimnion) forced with the observed data » forced with the observed meteorological data*  
Corrected.

30      *Line 49 spreading along 83 km over » spreading over 83 km of of Guadiana » of the Guadiana*  
Corrected.

*Line 51 the capacity of water » the storage capacity of water*  
Corrected.

35      *Line 59 in favourable position. » into a favourable position. Rainfall seasons normally last from » Seasonal rainfall normally occurs between*  
Corrected.

40      *Lines 64-65 Geographical and climatological factors make the Alqueva reservoir a vital source of fresh water needed to support the population and economy in the region, while on the other hand, an increasing anthropogenic*  
Corrected.

45      *Line 71 air columns, over the water-atmosphere interface, and in the shores » air columns, at the water-atmosphere interface, and on the shores*  
Corrected.

Line 73 4 floating platforms » four floating platforms

Corrected.

Line 76 was settled on the platform » was deployed on the platform

Corrected.

Line 77 an eddy-covariance system, Campbell Scientific Irgason, provides data for atmospheric  
» an eddy-covariance system, Campbell Scientific provides data of atmospheric

Corrected.

Line 89 and for punctually vertical profiles » and was occasionally used to collect vertical profiles

Corrected.

Line 94 were obtained in automatic regime and transferred » were automatically downloaded  
and transferred

Corrected.

Line 96 weather stations and conduct measurements, to collect » weather stations, to conduct  
more detailed measurements, and to collect

Corrected.

Line 125 condition » conditions

Corrected.

Line 126 condition is » conditions are

Corrected.

Line 161 (Suggested change) In addition to LAKE2.0, The FLake model was used to simulate  
water temperature for the chosen period. FLake model (Mironov,

Corrected.

Line 162 a two-layer representation of the temperature profile » a two-layer representation of  
the lake's thermal structure

Corrected.

Line 196 (Suggested change) Water temperature is a crucial factor for Numerical Weather  
Prediction (NWP) applications, and as a regulator of lake ecosystem activity, and their ecosystems.

Corrected.

Line 237 its integral energy » the simulated heat content of the entire water column.

Corrected.

Line 245 is capable to calculate » are capable of calculating

Corrected.

*Line 246 and the profile 7 represents » and figure?? shows.*

Corrected.

*Line 270 are represented quite good » are represented quite well*

Corrected.

*Line 292 In November the turnover happens » In November, following turnover*

Corrected.

*Line 312 Alqueva reservoir with using the LAKE2.0 » Alqueva reservoir using the LAKE2.0*

Corrected.

*Line 316 correlation coefficients are 0.99 for both » correlation coefficients for the relationship between simulated and measured temperature are 0.99 for both*

Corrected.

*Line 317 FLake shows overestimation about 1.5 » FLake shows an overestimation of about 1.5*

Corrected.

*Line 318 show the same rate of overestimation » show the same level of overestimation*

Corrected.

*Line 324 good accordance » good corospondance.*

Corrected.

*Line 328 of modernisation of LAKE2.0 » inclusion of a more complete description of the process regulating photosynthesis and respirations in the LAKE2.0 model*

Corrected.

*Line 329 (Suggested change) Although measured oxygen concentrations are well simulated values of O2 over short time intervals, the annual Alqueva oxygen cycle cannot be reproduced because the model does not respond to changes in algal concentration (underestimation of O2 values) and winter minimum (high overestimation). Winter overestimation is supposedly due to the relatively low water temperatures. Why above is it supposedly? Are you not sure?*

Corrected. We say "supposedly" because it remains the principal hypothesis for explanation of such big residuals. The depth of the reservoir of the used bathymetry might be the cause as well, either everything in place to a certain extent.

# 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 CO<sub>2</sub> and O<sub>2</sub> 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).

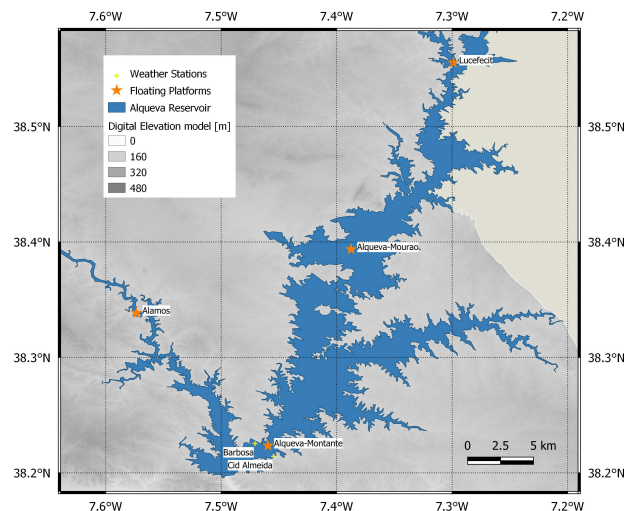
A realistic representation of the thermal and gas regimes by lake models ~~are~~ is important for solving current and prognostic tasks. For example, high accuracy of the calculations of sensible and latent heat fluxes, momentum, and water surface temperature is required for atmospheric models, where 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 ( $\text{CO}_2$ ,  $\text{O}_2$ ,  $\text{CH}_4$ ) 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  $\text{O}_2$ ,  $\text{CO}_2$ , and  $\text{CH}_4$  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 km<sup>2</sup>, the maximum depth is 92 m, the average depth is 16.6 m, and the ~~storage~~ capacity of water is estimated at 4.15 km<sup>3</sup>, 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](http://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<sup>-2</sup> (one of the highest in Europe) and the daily maximum in summer often may exceed 1000 Wm<sup>-2</sup> (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 CO<sub>2</sub> 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 LAKE2.0<sup>1</sup> 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 CO<sub>2</sub> and CH<sub>4</sub> 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

<sup>1</sup> 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,  $\rho_{w0}$  — 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  $\lambda_t = c_w \rho_{w0} \nu_T$  ( $\nu_T$  — turbulent coefficient of thermal diffusivity,  $\text{m}^2\text{s}^{-1}$  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 CH<sub>4</sub> oxidation act as CO<sub>2</sub> 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<sup>-1</sup> (August 2017) to a maximum of 1.519 m<sup>-1</sup> (July 2018) with an average value of 0.643 m<sup>-1</sup> (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  $\rho$  is density of water. In LAKE2.0 model equation 2 is presented as  $K_{z,LAKE2.0} = \alpha K_z$ , where  $\alpha$  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, CO<sub>2</sub>, O<sub>2</sub>, CH<sub>4</sub>, 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  $\rho$  is density of water. In LAKE2.0 model equation 2 is presented as  $K_{z, LAKE2.0} = \alpha K_z$ , where  $\alpha$  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.

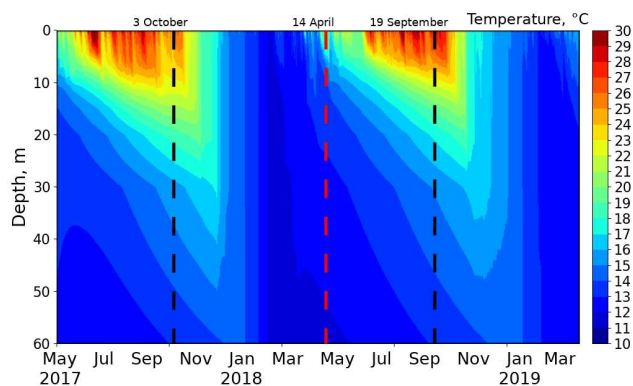
### 3 Results and discussion

#### 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.

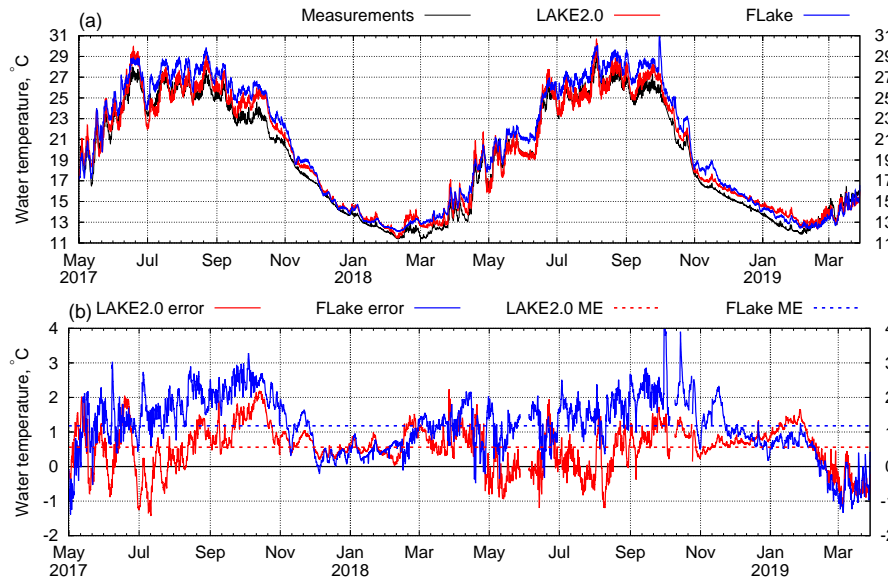


**Figure 2.** Time-depth Hovmöller diagram of the LAKE2.0 simulated water temperature in the Alqueva reservoir based on hourly data. Dashed lines indicate the end (black) and the beginning (red) of stratification.

Water temperature in ~~these months in~~ upper layers increases up to  $30^{\circ}\text{C}$  in warm period, and in the hottest months (July-September) reaches  $25^{\circ}\text{C}$  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

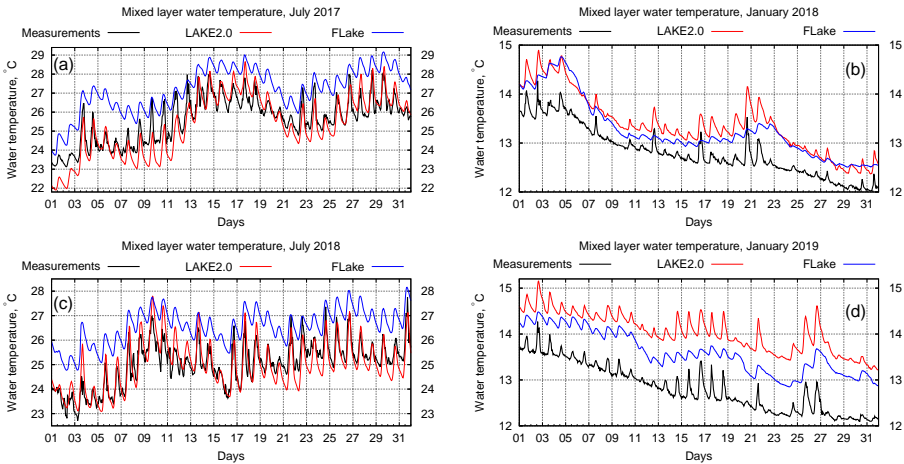


better for warm periods while FLake results are better for cold. Both models demonstrate almost identical correlation for the selected periods.

**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	<b>0.99</b>	<b>0.99</b>	<b>0.56</b>	<b>1.18</b>	<b>0.74</b>	<b>1.27</b>

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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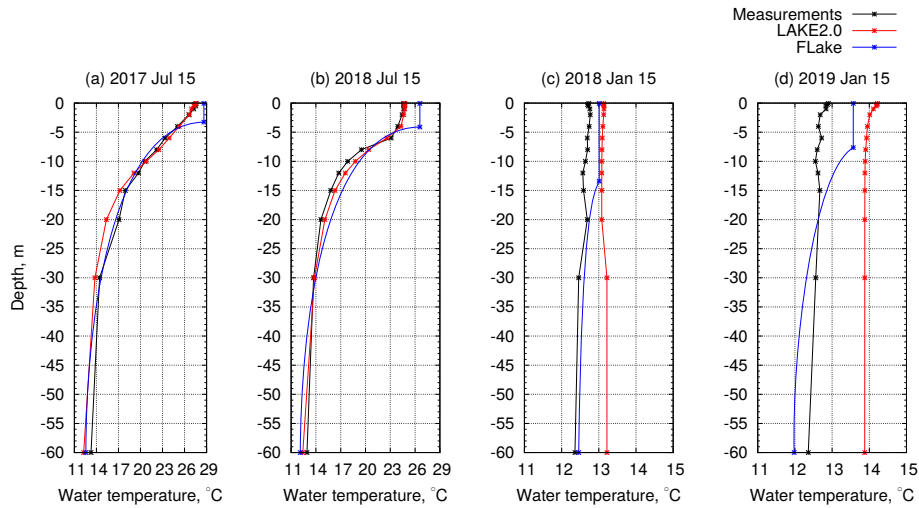
are -0.23 and -0.04 °C for 2017 and 2018 correspondingly) while FLake provides an overestimation of 1-2 degrees and an underestimation of the daily amplitude. Correlation coefficients in this case are 0.94/0.88 (LAKE2.0) and 0.90/0.89 (FLake) correspondingly. Diurnal ML temperature variations can reach 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.

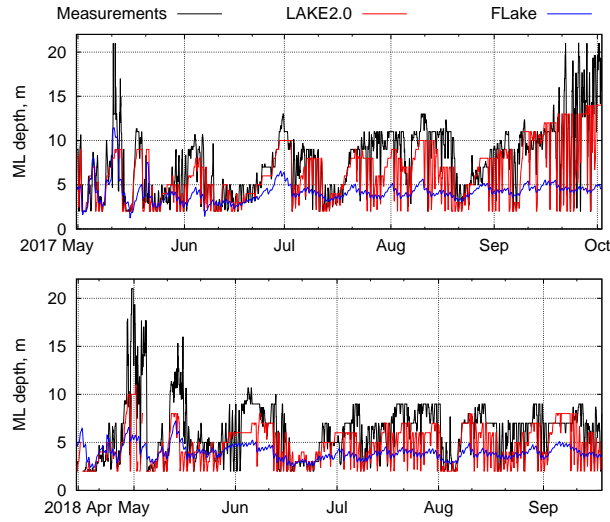
Temperature distribution with depth is another significant parameter for lake thermodynamics. LAKE2.0 model simulates water temperature at pre-defined depth levels; ~~FLake provides a~~. FLake provides ML depth, shape factor for the thermocline curve, ML and bottom temperature. Using these values it 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.

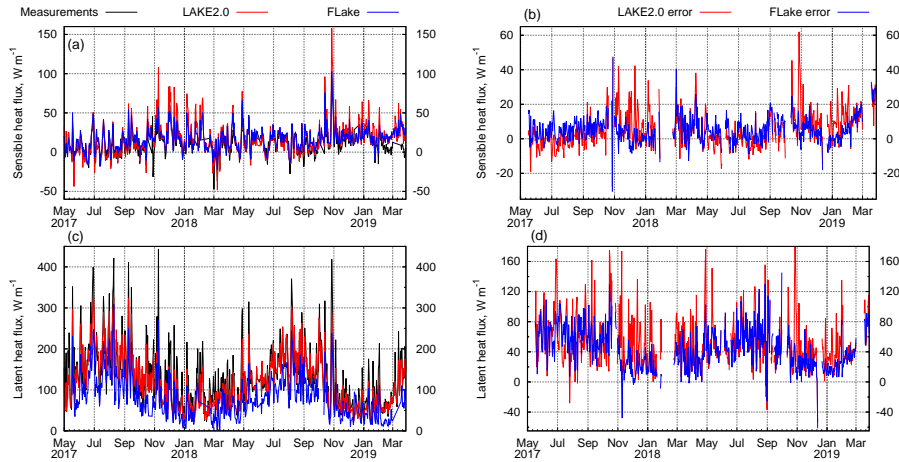
### 3.2 Heat fluxes

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  $\text{Wm}^{-2}$ ) 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, $\text{Wm}^{-2}$	5.51	5.36	52.93	43.46
MAE, $\text{Wm}^{-2}$	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.

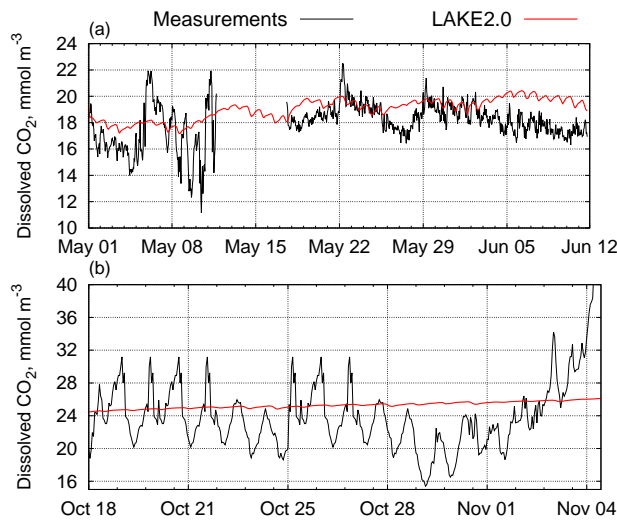
In terms of latent heat fluxes the LAKE2.0 model results are worse than the FLake when compared to the ~~Eddy-covarienee~~ eddy-covariance (EC) measurements. However, it should be noted that several studies have indicated that the ~~eddy-covarienee~~ eddy-covariance EC systems tend to underestimate the 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 CO<sub>2</sub> 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 CO<sub>2</sub> 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 CO<sub>2</sub> concentration on water in the first months of the ALOP field campaign in comparison with LAKE2.0 simulated results.



**Figure 8.** Timeseries of dissolved CO<sub>2</sub> 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 CO<sub>2</sub> 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. In the second week of May, CO<sub>2</sub> 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 CO<sub>2</sub> in water at 25 cm depth for the period 18 October – 5 November.~~ 8 (b)). In this period, LAKE2.0 simulated values of CO<sub>2</sub> 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.

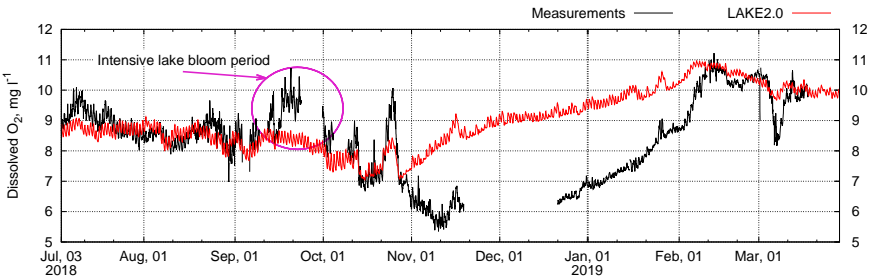
Thus, we can conclude that in long-time simulations LAKE2.0 model represents CO<sub>2</sub> trends quite well. The model failed to reproduce diurnal cycle of the surface carbon dioxide concentration which calls for inquiry of parameterizations of photosynthesis and respiration in the model. However, 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 O<sub>2</sub> in water at 25 cm depth for the period July 3, 2018 — March 29, 2019 at the Alqueva reservoir.

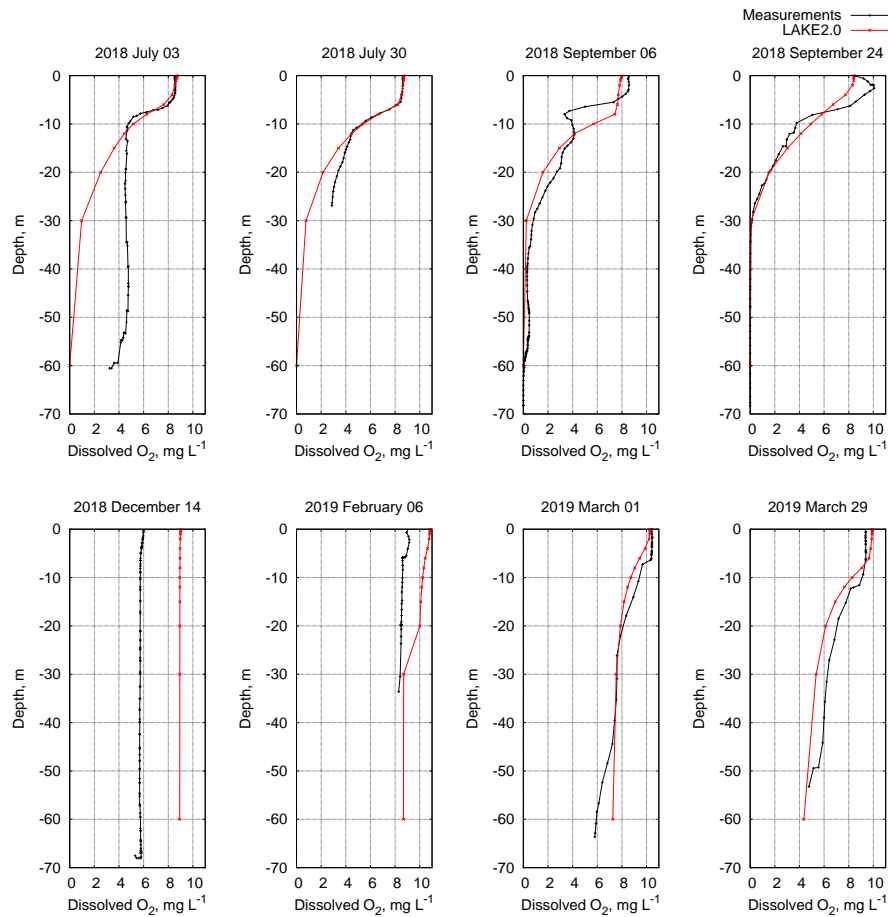
- 5 way during the first two months until the middle of September when a microalgal bloom occurred. It caused an intensive production of O<sub>2</sub> in water that can not be represented by the LAKE2.0 which does not have an explicit representation of algae, and the bloom does not affect atmospheric 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~~mg l<sup>-1</sup> mg l<sup>-1</sup>. 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<sup>-3</sup> 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 <sup>-3</sup>										
	'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  $14.036 \text{ mg l}^{-1}$  at the surface, and came back to values of  $2.309 \text{ mg m}^{-3}$  in November. ~~LAKE2.0 model solves DO concentration assuming a constant chlorophyll-a concentration of  $2.3 \text{ l}^{-1}$ .~~ 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  $1.3 \text{ mg m}^{-3}$ . 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  $2.5 \text{ mg l}^{-1}$ . March profiles (1 and 29) show good similarity in measured and simulated values.



**Figure 10.** Profiles of dissolved  $\text{O}_2$  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 CO<sub>2</sub> and O<sub>2</sub> 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<sup>-2</sup> (LAKE2.0) and 6.75 Wm<sup>-2</sup> (FLake). Latent heat flux results of both models in terms of MAE are worse: 53.99 Wm<sup>-2</sup> (LAKE2.0) and 45.6 Wm<sup>-2</sup> (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 CO<sub>2</sub> 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 CO<sub>2</sub> 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 -O<sub>2</sub> ~~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 -O<sub>2</sub> 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](mailto:miakunin@uevora.pt), [m.yakunin89@gmail.com](mailto: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.

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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  $\text{CH}_4$ , oxygen  $\text{O}_2$  and carbon dioxide  $\text{CO}_2$ . 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  $\text{CO}_2$  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/m<sup>3</sup> 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 "CO<sub>2</sub>" subscript because carbon atoms are supplied to or removed from DIC of a solution in a form of CO<sub>2</sub>.

In the following, the parameterizations of processes related to O<sub>2</sub> and CO<sub>2</sub> dynamics are described, whereas formulations for CH<sub>4</sub> 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 CO<sub>2</sub> 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  $\nu_w$  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:

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



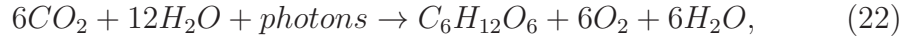
where  $H_{sec} = 3600$  s and  $S_{PAR}^*$  is PAR intensity in  $W/m^2$ . The coefficient transforming from J to Einstein (Einstein is an energy of Avogadro number of photons),  $T_{J \rightarrow Eins}$ , is estimated assuming the uniform distribution of energy in PAR region, which yields:

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

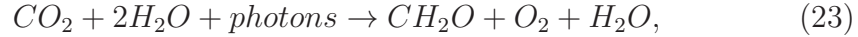
with  $N_A, h_P, c$  denoting Avogadro number, Planck constant and the light speed in vacuum, respectively, all in SI units.

The treatment of chlorophyll-a concentration  $\rho_{Chl-a}$  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
$C_P$	$\text{h}^{-1}$	9.6
$\theta_P$	n/d	1.036
$T_0$	$^{\circ}\text{C}$	20
$T_{00}$	$^{\circ}\text{C}$	10
$\mu_{O_2}$	g/mol	32
$H_{sec}$	s	3600
$C_{PAR}$	Einstein/( $\text{m}^2 \cdot \text{h}$ )	0.687
$\theta_{PAR}$	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.
$\lambda_{PAR}$	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  $\mu_\beta$  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
$\theta_{\mu_\beta}$	n/d	1.085
$\theta_{k_c}$	n/d	1.103
$T_{\mu_\beta}$	K	25
$T_{k_c}$	K	20
$\mu_{\beta,0}$	mol/(m <sup>2</sup> *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  $\tau_{Dh}$  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,  $\Delta = \rho_p/\rho_{w0} - 1$ ,  $\rho_p$  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  $1.25 \text{ g/cm}^3$  (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,  $\alpha$ , 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

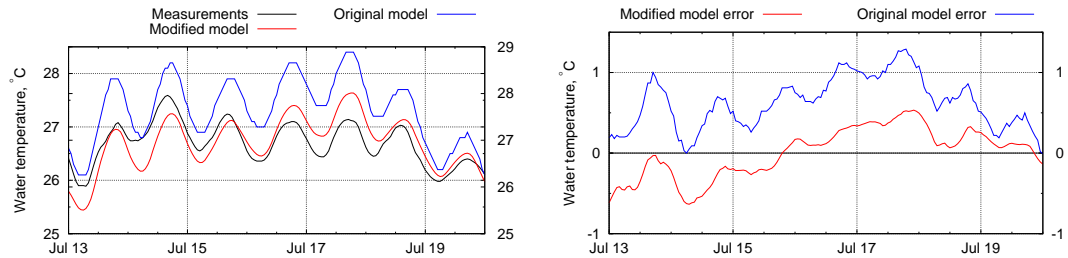


Figure S1: ML water temperature, original and modified model results and their errors when compared to the observations.

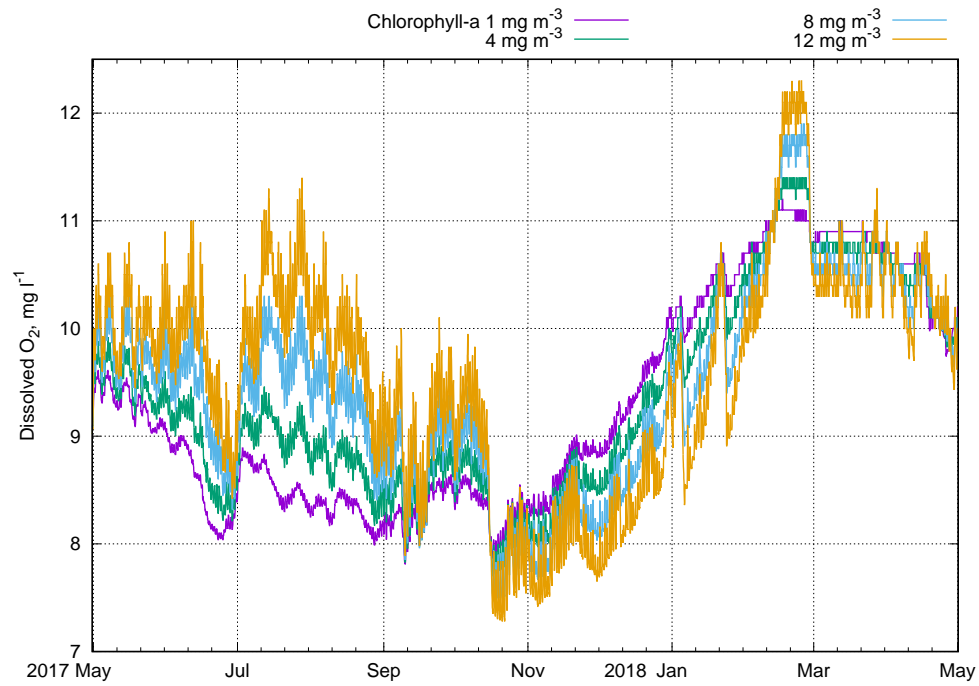


Figure S2: DO concentration at different chlorophyll-a concentration values.

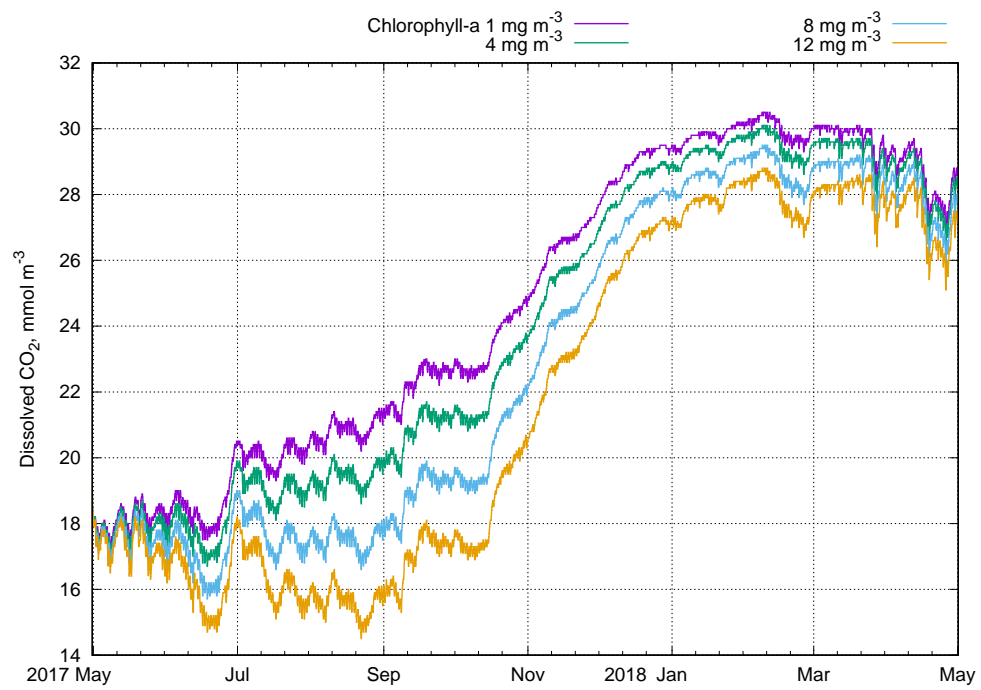


Figure S3:  $CO_2$  concentration at different chlorophyll-a concentration values.

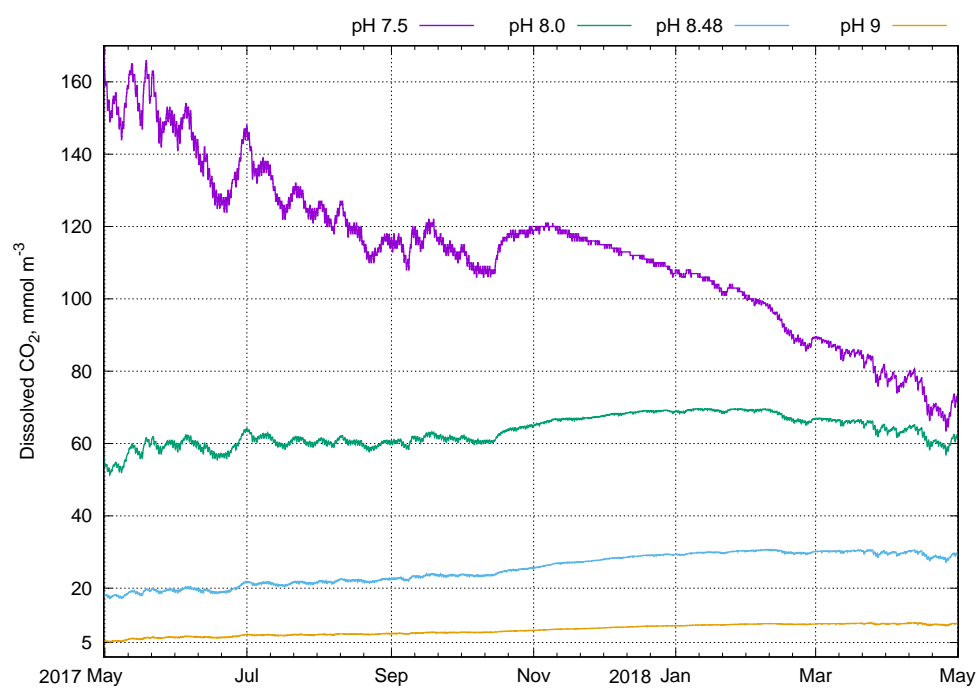


Figure S4: Dissolved  $\text{CO}_2$  concentrations at different pH values.

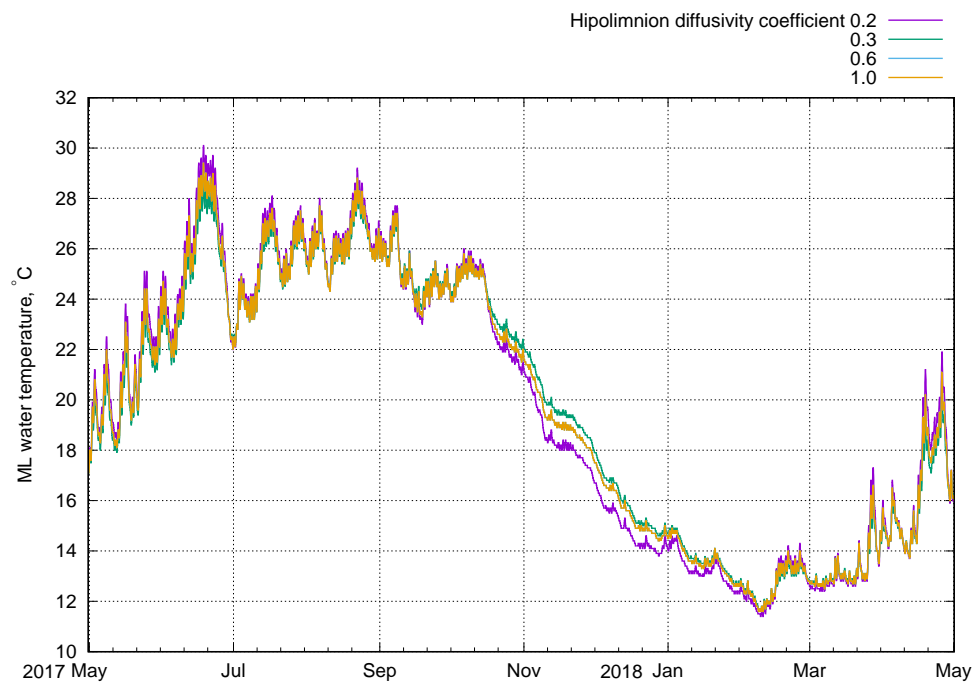


Figure S5: ML temperature at different hypolimnetic diffusivity coefficient values.



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