bg-2019-95
Author responses to comments

We would like to thank the editor and the two referees for the effort and time they put in to review our manuscript. We are grateful for their careful and considered comments and have made every attempt to fully address these comments in the revised manuscript.

In the following list, the points raised by the referees are written in **bold** characters, whereas our responses are shown in blue characters and the text excerpts indicating the corresponding changes made to the manuscript are shown in orange characters. The line numbers within our responses correspond to those in the revised manuscript file.

A separate list of major structural changes and figure/table revisions is included after the point-by-point responses to the referee comments.

Referee #1

Overall, I find this to be useful work. Exercises such as this are not done as often as they should be. However, I am concerned about the model calibration and the overall message of the manuscript. I am unsure what overall message the authors are advocating. They do a comparison of the different parameterizations in a 1D model and leave it at that. The manuscript also has organizational issues which make it difficult to follow. To make this work more impactful, I suggest a section on modeling advice.

Please do not be discouraged by this review. I feel this work can be useful with some reorganization and reframing of the overall message. I very much look forward to reading a revised version.

Our study is essentially a gas exchange model intercomparison study. The performance of the four parameterizations of CO_2 transfer velocity applied in this study has been estimated in prior studies by comparing the results to directly measured CO_2 fluxes and gas transfer velocities. In our study, we performed a corresponding comparison between the CO_2 transfer velocities and fluxes obtained through (a) lake model simulations and (b) calculation using measured CO_2 concentrations and other relevant variables. In addition, the aim of our study is to assess the capability of the lake model MyLake C to simulate lake inorganic carbon cycling especially under the conditions of high simulated CO_2 effluxes.

We have restructured the Methods section according to the Referee's suggestions and included further discussion on modeling advice and the overall conclusions of the study regarding the modeling of lake carbon cycling.

Specific Comments
I am concerned about the model calibration. During the calibration step, the entire ecosystem is changed for each parametrization. I understand the calibration was intended to capture the surface CO2 concentration. I would consider tuning the model capture some aspect of the ecosystem such as chlorophyll concentration.

We performed the model calibration against water column CO_2 concentration, and the aim of the calibration was indeed to optimize the simulated near-surface CO_2 concentration because air-water CO_2 exchange is governed by the air-water CO_2 concentration difference.

In the study, four different individual calibrations of the model application were performed. Because the lake model simulates a rather complex coupled physical-biogeochemical system and the statistical inference method used in the calibration tries to find an optimal parameter set using a relatively high number of free parameters, the individual parameter sets often tend to differ from each other. In other words, each statistical calibration yields a unique description

of the lake carbon cycling. This is one of the reasons why the aim of the calibration procedure was not to try to reproduce the actual in-lake carbon cycling but rather to compare different possible ways to generate an optimal water column CO_2 concentration.

There are many possible drivers of in-lake CO_2 concentration variation, for example, phytoplankton processes, microbial degradation processes, and external loading of carbon species. Because phytoplankton is only one of the contributing factors and it is known that MyLake is not highly capable of simulating short-term phytoplankton dynamics correctly, different factors were considered equal in the calibration. In addition, comprehensive data on water column CO_2 concentration were available, whereas chlorophyll *a* measurements had not been performed in the lake during the study period.

It was also not clear why these specific parameterizations were chosen. Some rationale for choosing these specific parameterizations is needed. Admittedly, I am not familiar with most of these parameterizations, so the modeling community could benefit from a description of each. I suggest a section on "gas exchange parameterizations" where you start with a paragraph stating the gas exchange parameterizations and the parameters that go into them. I suggest putting all the parameters in a table with units. Additional sections can be descriptions of each parameterization and where it is currently being used (ie which models use them and which studies use them). Lastly, why wasn't Wanninkhof 1992 used in this comparison? Wann.1992 is the parametrization incorporated into ocean models such as the CESM and MITgcm. MITgcm has been used to in studies of the Great Lakes. Also, the chosen parameterizations are completely different from those used in marine environments (for example, Wrobel and Piskosub Ocean Sci., 12, 1091–1103, 2016). I can't think of any reason why there are different parameterizations for freshwater and marine systems.

We selected the four parameterizations, or gas exchange models, because the performance of these parameterizations has been assessed against direct CO_2 flux measurements in Lake Kuivajärvi in previous studies by Heiskanen et al. (2014), Mammarella et al. (2015), and Erkkilä et al. (2018). Consequently, also the simulations performed in our study could be indirectly compared with direct measurements in the study lake. We have include the reasoning in the text.

P3 L24–27: "The four gas exchange models were selected because their performance in estimating air–water CO_2 fluxes in a small boreal lake has been extensively assessed in previous studies by Heiskanen et al. (2014), Mammarella et al. (2015), and Erkkilä et al. (2018) by comparing the calculated fluxes with direct CO_2 flux measurements."

The model by Wanninkhof (1992) is a wind-based parameterization, similarly to the parameterization by Cole and Caraco (1998). We chose to select the simple parameterization by Cole and Caraco (1998) to represent the parameterizations that are based only on wind speed in our study. Wind speed-based parameterizations have been shown to be inadequate in small lakes, and the use of more sophisticated parameterizations has been recommended (Heiskanen et al., 2014; Erkkilä et al., 2018).

Different parameterizations of air-water gas exchange for freshwater and marine systems are needed because the main drivers of near-surface turbulence are different in these systems. It has been shown that thermal convection is a larger source of mixed-layer turbulence than wind shear especially in lakes with a small surface area and a sheltered location (Read et al., 2012). (This may be the case also in oceanic regions with low to intermediate winds and strong insolation (see McGillis et al., 2004).) Thus, it has been suggested, for example, in the two aforementioned studies, that parameterizations relying only on wind speed may be insufficient under such conditions. Many boreal lakes are small in area, and also convective processes may have an essential role in air-water gas exchange in these lakes. By contrast, all the parameterizations in Wrobel and Piskozub (2016) are based solely on wind speed or include also gas

transfer by bubbles. We have clarified the limited applicability of wind-based parameterizations in the Introduction:

P2 L17–18: "Buoyancy flux is relatively more important in small, wind-sheltered lakes, and parameterizations of the gas transfer velocity that are based solely on wind speed may not be applicable under such conditions (Read et al, 2012)."

We have revised the manuscript to include a more detailed description of the applied parameterizations and related parameters according to the Referee's suggestions. The main parameters are tabulated in Table 1 and their descriptions are given, followed by the descriptions of the gas exchange models and their prior usage. However, as far as we know, the models by MacIntyre et al. (2010) and Tedford et al. (2014) have not been widely used in other studies, let alone having been integrated into biogeochemical models. Furthermore, we consider that the model by Cole and Caraco is so well-established and widely known in the field that there was no need to review its usage further.

I suggest a section providing modeling advice. Differences in gas transfer velocity and CO2 flux using each method are mentions, but there is no consensus on which parametrization the community should be using. I also suggest highlighting more the impact the choice of these parametrizations has on global efflux from lakes.

We have concluded that it is not a trivial task to judge which parameterization is most suitable for integration into MyLake C. None of the four model versions with different gas transfer velocity parameterizations surpassed the other ones in the study because of the complex interplay between the near-surface water CO_2 concentration and air-water CO_2 flux in the simulations. However, many experimental studies have shown that traditional, wind-based parameterizations often yield too low fluxes when compared to estimates based on direct measurements. Thus, we find that it is recommended to strive to use the more sophisticated gas exchange models provided that the lake biogeochemical model can be made adaptable to higher CO_2 losses and that the parameters related to the convection-based parameterizations can be simulated correctly.

We have added section 4.4, which contains a more detailed discussion on our recommendations on the selection of the gas exchange model. We have also stated more clearly also in the Discussion that the estimates of global gas efflux will be higher if more correct gas exchange parameterizations are used.

P22 L31–P23 L2: "The issues raised in our study concerning lacustrine carbon budgets can also be generalized to a larger scale. The application of advanced gas exchange models has been shown to lead to increased estimates of CO_2 emissions from boreal inland waters. Thus, higher estimates of net terrestrial ecosystem production and carbon flux from land to inland waters are required to close the regional carbon budget. Also, the use of advanced, possibly more correct gas exchange models in the assessment of global gas efflux from freshwaters may result in higher estimates of the impact of freshwater ecosystems on global carbon cycling."

Technical corrections
- Make it clear GEM stands for gas exchange model. It took me a minute to realize this.

GEM is actually intended to stand for an individual MyLake C version that uses one of the four different gas exchange models/parameterizations. When the actual model/parameterization (that is, the formula) is discussed, the phrase "gas exchange model" is used in the text.

We have clarified the usage of the abbreviation GEM in the manuscript. The abbreviation has originally been defined at its first occurrence in section 2.2.4. We have also repeated the definition of the abbreviation at the beginning of the Results and Discussion sections.

P12 L3–5: "Even though the differences between the formulations of the gas exchange models incorporated into MyLake C are rather notable, the resultant CO_2 concentrations did not differ

substantially between the GEMs, that is, between the simulations with the MyLake C versions using different gas exchange models (Fig. 1).”

P17 L15–17: “There was less variation between the air–water CO_2 fluxes simulated with different GEMs, that is, simulated with the MyLake C versions using different gas exchange models, than between the CO_2 fluxes calculated with the corresponding different gas exchange models on the basis on measured surface heat fluxes and air–water CO_2 concentration gradients (Table 3).”

- Add a table stating all the parameters with units used in each GEM
We have added the table (Table 1) as suggested.

- Figures 3 and 5 I suggest a cross plot off to the right with a list of summary statistics (correlation, bias, RMSE, Nash-Sutcliffe efficiency, etc.)
We have included a cross plot containing also some summary statistics along with each subplot in Figures 3 and 5.

- I suggest a paragraph of modeling advice. How does this work advance modeling of the carbon cycle in lakes?
We believe that this work addresses the issue of the selection of the gas transfer parameterization to be used in biogeochemical lake models. It is clear – on the basis of many previous experimental studies – that traditional wind-based gas exchange parameterizations tend to give too low gas fluxes and that more advanced models with higher flux estimates should be used. However, our study suggests that it is not a straightforward task to simply use a better gas exchange model in a lake model because it may bring about difficulties in the simulation of in-lake carbon cycling, particularly in the generation of sufficient gain of CO_2 in the water column. Thus, we conclude that further development related to the mathematical description of in-lake carbon processes and to the modeling or other means of estimation of external inorganic and organic carbon loading are still needed.
Please see also our answer to the prior Specific Comment that is related to this comment.

- In the last paragraph of section 2.1.1 make it clear where the temperature dependent solubility comes into play. For this section I suggest looking at Wanninkhof et al. 2009 in annual review of marine science vol1:213-244.
We agree that there are different ways to describe the air-water concentration difference at equilibrium by using different solubility coefficients (for example, Henry's law solubility constant, Ostwald solubility coefficient, and Bunsen solubility coefficient). We have clarified that we meant the temperature dependence of the Henry's law solubility constant K_H:
P4 L11–12: “[…] where K_H is the temperature-dependent aqueous-phase solubility (also known as the Henry's law constant) of CO_2 at surface water temperature, […]
P7 L26–27: “[…] and the temperature dependence of the aqueous-phase solubility K_H is calculated according to Weiss (1974).”

- In section 2.1.2 It is unclear where the approximation U10/U1.5=1.22 is used
The gas exchange models by Cole and Caraco (1998) and MacIntyre et al. (2010) use the wind speed at 10 m as input, whereas the model by Tedford et al. (2014) uses wind speed at 1.5 m. In the calculations, wind speed measurements performed at 1.5 m height (which is, by chance, also the height used in the model by Tedford et al. (2014)) are used, and the conversion between wind speeds at 1.5 and 10 m is performed using the approximation $U_{10}/U_{1.5} = 1.22$. The measurement height used in this study, 1.5 m, is stated later on in the text in section 2.2.2; however, the conversion factor is included in the MyLake C model code and is thus not only

a study-specific value. As the structure of the manuscript has been modified, we have moved the statement to the end of section 2.1.3 and restated the statement in the description of model assessment data in section 2.2.3.

P7 L33: The approximation $U_{10}/U_{1.5} = 1.22$ is used for the wind speed at different heights.

P10 L20–21: [. . .] As in MyLake C, the approximation $U_{10}/U_{1.5} = 1.22$ was used in the calculations.

- in section 2.2.2. When you say the model was calibrated against daily averages of automatic CO2, does this simply mean the parameters in the model were tuned to match observed CO2 concentration? Please be clear about this.

This is exactly what we meant. The calibration procedure is explained in more detail later on in the text, in section 2.2.4. In this section (2.2.2), the measurements used in the calibration procedure are described. The calibration method was statistical, and it would be imprecise to merely state that the model parameters were tuned to match the observed CO_2 concentration, to minimize the root-mean-square error (RMSE) between the simulated and measured concentrations, or to improve the fit between the simulated and calibrated values.

We have clarified the statement as follows:

P9 L5–8: "The model was calibrated against the daily averages of the automatic high-frequency CO_2 concentration measurements: an optimal set of selected model parameters were estimated so that the simulated CO_2 concentration time series matched the corresponding measured CO_2 concentration time series as well as possible. The estimation was performed using a statistical inference algorithm."

- In section 2.2.3 : please provide a rationale for this choice "Missing relative humidities were replaced by a value of 75 % in the calculation of the water-side friction velocity"

Many half-hour values of k_{TE} could not be calculated because of missing data on surface heat fluxes (described in section 2.2.3) or other variables, and the omission of periods with missing relative humidity would have further decreased the number of calculated k_{TE} values. Thus, we chose to approximate the missing values of relative humidity.

Furthermore, relative humidity has a very small effect on the gas transfer velocity calculated with the parameterization by Tedford et al. (2014) (k_{TE}), and it is not included in the other parameterizations. The Air-Sea Toolbox utilized by MyLake includes a formula that calculates air density ρ_a on the basis of air temperature, relative humidity, and air pressure. The variation of air density at different relative humidities compared to the value of 70 % is, at maximum, of the order of 0.1 %. Because k_{TE} is proportional to $\rho_a^{3/8}$, the corresponding variation of the gas transfer velocity is even smaller. However, we chose to include the statement on the relative humidity for completeness.

The mean value of the SMEAR measurements of relative humidity during the period May–October 2013 was 72 %. Platform measurements of relative humidity were relatively well applicable during the period May–August 2013. During May–August, the average values for the SMEAR and platform measurements of relative humidity were 66 % and 68 %, respectively. Thus, the average relative humidity can be assumed to be slightly higher over the lake than at the SMEAR station. Consequently, we find that a value of 75 % is a relatively good as a rough approximation for the average relative humidity at the platform during May–October. We have explained the choice in the text:

P9 L27–32: "In the calculation of the water-side friction velocity, missing relative humidities were replaced by a value of 75 %, which is close to the average of the SMEAR II measurements of relative humidity in May–October 2013, 72 %. The corresponding averages over the period May–August 2013, for which platform measurements were rather well applicable, were 66 % and 68 % for the SMEAR II and platform measurements, respectively. Thus, the relative

humidity can be assumed to have been slightly higher over the lake than at the SMEAR II station."

- In section 2.2.4 : All the summary goodness-of-fit statistics (NS, B*, URMSE'*) can be displayed nicely in a target diagram. See Jolliff et al. 2009 "Summary diagrams for coupled hydrodynamic-ecosystem model skill assessment"

All the statistics are presented in tables in the Supplement. Because the manuscript already contains a rather high amount of figures, we consider that additional target graphs would not provide much additional value to the manuscript.

Referee #2

The manuscript "The Applicability and consequences of the integration of alternative models for CO2 transfer velocity into a process-based lake model" of Petri Kiuru, Anne Ojala, Ivan Mammarella, Jouni Heiskanen, Kukka-Maaria Erkkilä, Heli Miettinen, Timo Vesala, and Timo Huttula is a interessting scientifc report about the performance of different gas exchange models for simulations of CO2 fluxes between lakes and atmosphere. The article represents the high scientific expertise of the finish research community. No doubt, the authors did a grandiose job. In my understanding, the article can be accepted after two minor improvements.

(1) The authors wrote on page 7, line 4 that the lake has a maximum width of only 0.3km. This raises the question whether the footprint of the EC measurements is really representative for the lake-atmosphere exchange. How did the authors approximate the width of the parabolic footprint? And how did the authors consider transversal advection, i.e., advection orthogonally to the mean flow (wind) direction?

The estimation of the flux footprint distribution functions was made using the model by Kormann and Meixner (2001). The average footprint contributing to 80 % of the flux ranges from 100 m up to about 300 m from the measurement platform depending on atmospheric stability conditions as described in Mammarella et al. (2015). However, the simple footprint model may have overestimated the footprint because it does not take into account the additional turbulence generated by the surrounding forest. Neverthless, it is justified to assume that the source area of the measured fluxes was on the lake surface because only the measurements during the periods when the wind was blowing along the lake were used in the analysis.

The wind is channeled along the lake for most of the time. When the wind is blowing along the lake, the footprints are within the lake fetch. Transversal wind directions were filtered out in the data used in the study. Typically, 15 % of the flux data are excluded from the analysis, when the wind is not blowing along the lake (the excluded wind directions are 350°–130° and 180°–320°). However, in calm nights some air can be transversally advected even if the wind is along the lake. In principle, the standard quality checking (described in detail in Mammarella et al. (2015)) removes the data contaminated by advection. Although the advection may still affect the concentrations and temperatures, the covariances with wind, that is, the eddy fluxes, are somewhat immune to advective effects.

We have added discussion on the aforementioned issues in section 2.2.3.

P9 L33–P10 L4: "The estimation of the flux footprint distribution functions was made using the model by Kormann and Meixner (2001). The average footprint contributing to 80 % of the fluxes varies from 100 m up to about 300 m from the measurement platform depending on atmospheric stability conditions as described in Mammarella et al. (2015). Only wind directions along the lake (130°–180°and 320°–350°) were included to ensure that heat fluxes from the surrounding land were excluded. Furthermore, possible remaining effects of transversal

advection during calm nights were removed through EC quality screening."

(2) The authors discuss in section "4.2 Comparison to CO2 flux measurement" potential reasons for discrepancies between EC flux measurements and simulations results. Especially, they mentioned measurement errors and the spatial variability of governing parameters as major reasons. In my understanding, the authors are completely right with this statement. However, I would like to encourage the authors to provide quantitative support for this statement through a short error analysis.

Estimates of the random uncertainty of EC fluxes on Lake Kuivajärvi for the years 2010 and 2011 have been studied in detail in Mammarella et al. (2015). On average, the estimated total relative random error was around 10 % for both sensible and latent heat fluxes. The estimated relative CO_2 flux random error was approximately double as large as that of energy fluxes, 20 % of measured fluxes, which is a typical value for EC CO_2 flux reported also in other types of ecosystems.

We have included some quantitative error analysis, related to both the underestimation of surface heat fluxes and the random measurement error, in the text:

P19 L26–31: "[...] The differences may be in part attributed to an underestimation of surface heat fluxes by the EC method, which was seen, for example, in a study on energy balance over a small boreal lake by Nordbo et al. (2011) and also in Mammarella et al. (2015). The sum of the measured EC heat fluxes in Lake Kuivajärvi was on average 83 % and 79 % of available energy in 2010 and 2011, respectively, in Mammarella et al. (2015). In addition, the total relative random error of the EC measurements is generally around 10 % for both sensible heat flux and latent heat flux as estimated in Mammarella et al. (2015). [...]"

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List of major changes made to the manuscript

- A more detailed description of the applied gas transfer velocity parameterizations

  - A new, separate section (2.1.1) for presenting different ways of parameterization of gas exchange

  - A separate section (2.1.2) for presenting the applied models for the gas transfer velocity and their prior usage

- More detailed descriptions of the footprint of the EC fluxes (in section 2.2.3) and the error of EC heat flux measurements (in section 4.2)

- A new section (4.4) on modeling advice (recommendations on the selection of a gas exchange model on the basis of our intercomparison study).

- Conclusions: Highlighting the impact that the choice of more accurate gas exchange parametrizations has on global efflux from lakes

- A new table (Table 1) for the parameters used in the applied parameterizations of the gas transfer velocity

- Figures 3 and 5: Inclusion of cross plots that also contain some summary statistics along with each subplot for the gas transfer velocity (Figure 3) and for the CO_2 flux (Figure 5)

Applicability and consequences of the integration of alternative models for CO_2 transfer velocity into a process-based lake model

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Abstract. Freshwater lakes are important in carbon cycling especially in the boreal zone, where many lakes are supersaturated with the greenhouse gas carbon dioxide (CO_2) and emit it to the atmosphere, thus ventilating carbon originally fixed by the terrestrial system. The exchange of CO_2 between water and the atmosphere is commonly estimated using simple wind-based parameterizations or models of gas transfer velocity (k). More complex surface renewal models, however, have been shown to yield more correct estimates of k in comparison with direct CO_2 flux measurements. We incorporated four gas exchange models with different complexity into a vertical process-based physicobiochemical lake model MyLake C and assessed the performance and applicability of the alternative lake model versions to simulate air–water CO_2 fluxes over a small boreal lake. None of the incorporated gas exchange models significantly outperformed the other models in the simulations in comparison to the measured near-surface CO_2 concentrations or respective air–water CO_2 fluxes calculated directly with the gas exchange models using measurement data as input. The use of more complex gas exchange models in the simulation, on the contrary, led to difficulties in obtaining sufficient gain of CO_2 in the water column and thus resulted in lower CO_2 fluxes and water column CO_2 concentrations compared to the respective measurement-based values. Inclusion of sophisticated and more correct models for air–water CO_2 exchange in process-based lake models is crucial in efforts to properly assess lacustrine carbon budgets through model simulations both in single lakes and on a larger scale. However, finding higher estimates for both the internal and the external sources of inorganic carbon in boreal lakes is important if the improved knowledge of the magnitude of CO_2 evasion from lakes is included in future studies on lake carbon budgets.

1 Introduction

The majority of inland waters, especially in the boreal zone, are found to be supersaturated with carbon dioxide (CO_2) with concentrations that can exceed the equilibrium concentration by several times and are therefore net sources of carbon to the atmosphere (Cole et al., 1994; Algesten et al., 2014). The contribution of lakes to the global carbon budget is recognized to be substantial in comparison to the role of marine and terrestrial ecosystems as global carbon sinks, but global quantitative estimates show significant variation (Cole et al., 2007; Battin et al., 2009; Tranvik et al., 2009). Atmospheric CO_2 exchange between lakes and the atmosphere is one of the key processes needed to be determined in constructing carbon budgets of lakes and in evaluating the role of lakes in global carbon cycling.

The exchange of weakly soluble gases, like CO_2 and oxygen, across the air–water interface is often modeled as a boundary-layer process in which the gas flux is proportional to the gas concentration gradient at the interface. The proportionality factor k is known as the gas transfer velocity. In many long-used models for the gas transfer velocity, or gas exchange models, k is parameterized by wind speed alone (Wanninkhof 1992, Cole and Caraco 1998). However, direct measurements of air–water CO_2 exchange using the eddy covariance (EC) method (Jonsson et al., 2008; MacIntyre et al., 2010; Heiskanen et al., 2014) have resulted in higher estimates of k compared to wind-based gas exchange models. For weakly soluble gases, k depends mainly upon turbulence in near-surface water (Banerjee, 2007), which is not generated merely by wind. Near-surface turbulence is initiated predominantly by wind shear and negative buoyancy flux related to thermal convection induced by surface heat loss (Imberger, 1985). Buoyancy flux is relatively more important in small, wind-sheltered lakes, and parameterizations of the gas transfer velocity that are based solely on wind speed may not be applicable under such conditions (Read et al., 2012). Turbulence-driven gas exchange models have been shown to be well in accordance with in situ measurements of k (e.g., Zappa et al., 2007; Vachon et al., 2010).

In surface renewal models, k is calculated as a function of the turbulent kinetic energy dissipation rate ε, which provides an indication of the intensity of near-surface turbulence (MacIntyre et al., 1995). Kinetic energy dissipation can be due to viscous and thermal processes, and ε is thus dependent on wind shear and convective heat flux (Lombardo and Gregg, 1989). Wind shear is characterized by the wind-induced water-side friction velocity. The water-side friction velocity can be estimated from the atmospheric friction velocity, which can be measured directly (Mammarella et al., 2015) or calculated by bulk formulas using meteorological variables (Fairall et al., 1996). Heat-induced turbulence is generated if the surface heat flux is ~~negative, that is,~~ directed out of the lake. If measurements of the components of surface heat flux are not available, they can also be estimated using bulk formulas (Fairall et al., 1996).

Global estimates of carbon emissions from lakes often use conservative estimates of CO_2 fluxes or models that yield potentially underestimated values for k leading to low estimates of CO_2 fluxes (e.g., Cole et al., 2007; Raymond et al., 2013). Thus, revised estimates of lacustrine CO_2 emissions will require higher terrestrial ecosystem production to close the global carbon balance (Battin et al., 2009). Many studies concerning modeling of lake carbon balance (e.g., Bade et al., 2004; McDonald et al., 2013) or determination of lake carbon budgets (e.g., Sobek et al., 2006; Stets et al., 2009; Chmiel et al., 2016) also use simple wind-based models for k. Potential subsequent underestimates in carbon efflux may have consequences for the inter-

pretation of carbon budgets in single lakes (Dugan et al., 2016). A higher efflux may result in a re-evaluation of the amount of net ecosystem production in lakes or it can mean that external carbon sources are inadequately accounted for in lake carbon budgets.

The efflux of CO_2 from a lake is sustained mainly by in-lake CO_2 production through bacterial or photochemical degra-
5   dation of organic matter in water column or in sediment. Widely across the boreal zone, the importance of the degradation of allochthonous organic matter as an inorganic carbon source in lakes is conspicuous (Jonsson et al., 2001; Sobek et al., 2003). Also the direct loading of terrestrially produced dissolved inorganic carbon (DIC) through surface water and groundwater inflows may lead to high CO_2 concentrations in some lakes (Maberly et al., 2013; Weyhenmeyer et al., 2015; Einarsdóttir et al., 2017).

10   In this study, we evaluated the performance of different gas exchange models in the simulation of air–water CO_2 flux in a boreal lake with a process-based lake model and the adaptability of the lake model application to different CO_2 losses via efflux. We also calculated CO_2 budgets for the epilimnion of the lake during summer stratification on the basis of the simulation results and assessed the relative importance of different biogeochemical processes on the epilimnetic CO_2 conditions. We incorporated four alternative gas exchange models into a vertical process-based physicobiogeochemical lake model for the
15   simulation of year-round profiles of water temperature and CO_2 concentrations with a daily time step. We then applied the lake model to a humic boreal lake located in southern Finland for the period 2013–2014, calibrating each of the resultant alternative lake model versions against high-frequency water column CO_2 concentration measurements. We compared the simulated gas transfer velocities and air–water CO_2 fluxes with those calculated with the gas exchange models on the basis of measurement data. The aims of our study are (i) to assess the applicability of gas exchange models of different complexity to a process-based
20   lake model with a daily time step and (ii) to assess the implications of higher CO_2 efflux estimates for the lake carbon budget.

2   Materials and methods

2.1   Modeling approach

In this study, we assessed the applicability of four different models for the gas transfer velocity, referred to as gas exchange models, to a process-based physicobiogeochemical lake model MyLake C. The four gas exchange models were selected
25   because their performance in estimating air-water CO_2 fluxes in a small boreal lake has been extensively assessed in previous studies by Heiskanen et al. (2014), Mammarella et al. (2015), and Erkkilä et al. (2018) by comparing the calculated fluxes with direct CO_2 flux measurements. The models include (1) the widely applied experimental wind-based regression formula by Cole and Caraco (1998), (2) a boundary-layer model developed by Heiskanen et al. (2014), (3) a surface renewal model by Tedford et al. (2014), and (4) a regression model by MacIntyre et al. (2010).

30   #### 2.1.1   Parameterization of air–water gas exchange

The flux of CO_2 between water and the atmosphere, F_{CO2}, can be parameterized as the product of the CO_2 concentration difference between the surface water and the atmosphere and the gas transfer velocity k (Cole and Caraco, 1998):

$$F_{CO2} = \alpha k (C_w - C_{eq}),\tag{1}$$

where C_w is the CO_2 concentration in the surface water below the air–water interface, C_{eq} is the equilibrium concentration of CO_2, that is, the water column CO_2 concentration in the state of equilibrium with the overlying atmosphere, and α is the chemical enhancement factor applicable for reactive gases, such as CO_2. Gas fluxes from water to the atmosphere are thus defined to be positive. If a lake is nonalkaline, α can be assumed to be 1 (Cole and Caraco, 1998). The equilibrium concentration is calculated by Henry's law as

$$C_{eq} = K_H \chi p_a,\tag{2}$$

where K_H is the temperature-dependent aqueous-phase solubility (also known as the Henry's law constant) of CO_2 at surface water temperature, χ is the mole fraction of the gas in the atmosphere, and p_a is the atmospheric pressure.

The gas transfer velocity k can be simply parameterized by wind speed alone, or more complex models can be applied to describe the air–water gas exchange process or the near-surface turbulence that governs the gas exchange. In each of the four gas exchange models assessed in this study, the parameterization of k is made using a different combination of parameters. The parameters of each model and their units are listed in Table 1. With the exception of the simple wind-based model by Cole and Caraco (1998), near-surface turbulence is driven in the models by both wind shear and thermal convection promoted by heat loss from the surface.

Convection-driven turbulence occurs when surface heat flux is directed out of the lake, that is, when the buoyancy flux is negative (MacIntyre et al., 2010). The buoyancy flux β is defined as (Imberger, 1985)

$$\beta = \frac{g\alpha_w Q_{eff}}{\rho_w c_{pw}},\tag{3}$$

where g is the gravitational acceleration, α_w is the thermal expansion coefficient of water, Q_{eff} is the effective heat flux, ρ_w is the density of water, and c_{pw} is the specific heat capacity of water. The effective heat flux is defined as

$$Q_{eff} = Q_S + Q_{SW}(0) + Q_{SW}(z_{AML}) - \frac{2}{z_{AML}} \int_0^{z_{AML}} Q_{SW}(z)\mathrm{d}z,\tag{4}$$

where $Q_S = Q_H + Q_L + Q_{LW}$ is the net surface heat flux, Q_H is sensible heat flux, Q_L is latent heat flux, Q_{LW} is net longwave radiation, Q_{SW} is shortwave radiation, and z_{AML} is the depth of the actively mixing layer (AML) (Imberger, 1985). All heat fluxes from the atmosphere into the lake are defined positive. The last three terms in the equation represent the fraction of shortwave radiation that is trapped within the AML, denoted as $Q_{SW,AML}$. The attenuation of shortwave radiation at depth z in the water column can be calculated using the Beer–Lambert law

$$Q_{SW}(z) = Q_{SW}(0)\mathrm{e}^{-K_L z},\tag{5}$$

4

where K_L is the total attenuation coefficient of shortwave radiation. The AML is defined as the near-surface layer in which the water column temperature is within a certain range, usually $0.02\,°C$, of the temperature at the air–water interface (MacIntyre et al., 2001). The buoyancy flux is positive when the near-surface water is heating and negative under cooling conditions.

In the boundary-layer model developed by Heiskanen et al. (2014), near-surface turbulence is parameterized through wind-induced and convection-induced water-side velocity scales, which are characterized by the wind-induced water friction velocity at a reference depth, u_{*ref}, and the penetrative convection velocity w_*, respectively. The penetrative convection velocity is calculated as (Imberger, 1985)

$$w_* = (-\beta z_{AML})^{1/3}. \tag{6}$$

The gas transfer velocity can also be parameterized by the total turbulent kinetic energy dissipation rate ε (MacIntyre et al., 1995). The rate can be measured directly or estimated from other measurable quantities with similarity scaling (Tedford et al., 2014). In the parameterization of ε by Tedford et al. (2014), both wind-induced stress and heat-induced convection generate turbulence near the lake surface during cooling, but wind is the only factor responsible for the turbulence during heating. The total turbulent kinetic energy dissipation rate is determined in terms of shear production $\varepsilon_s = u_{*w}^3/\kappa z'$, where u_{*w} is the wind-induced water-side friction velocity, $\kappa = 0.4$ is the von Kármán constant, and z' is a reference depth, and convective turbulence production ε_c equaling the buoyancy flux β, as

$$\varepsilon_{TE} = \begin{cases} 0.56\varepsilon_s + 0.77|\varepsilon_c| & \text{if } \beta < 0, \\ 0.6\varepsilon_s & \text{if } \beta \geq 0, \end{cases} \tag{7}$$

The wind-induced water friction velocity u_{*w} can be calculated from the atmospheric friction velocity $u_{*a} = (\tau/\rho_a)^{0.5}$, where τ is the wind shear stress and ρ_a is the density of air, as in MacIntyre et al. (1995)

$$u_{*w} = u_{*a}\left(\frac{\rho_a}{\rho_w}\right)^{0.5}. \tag{8}$$

2.1.2 Gas exchange models

The widely applied experimental wind-based regression formula for k by Cole and Caraco (1998) gives the gas transfer velocity in units of $cm\ h^{-1}$ as

$$k_{CC} = (2.07 + 0.215U_{10}^{1.7})\left(\frac{Sc}{600}\right)^{-0.5}, \tag{9}$$

where U_{10} ($m\ s^{-1}$) is the wind speed at 10 m and Sc is the temperature-dependent Schmidt number of CO_2.

In the boundary layer model by Heiskanen et al. (2014), the wind-induced water friction velocity is approximated to be a linear function of the wind speed at 1.5 m height, $U_{1.5}$:

$$u_{*ref} = C_1 U_{1.5}, \tag{10}$$

where C_1 is an empirical dimensionless constant, and the equation for k_{HE} (m s^{-1}) is

$$k_{\text{HE}} = ((C_1 U_{1.5})^2 + (C_2 w_*)^2)^{0.5} Sc^{-0.5}, \tag{11}$$

where $C_1 = 1.5 \times 10^{-4}$ and $C_2 = 0.07$ is another experimental dimensionless constant. The model by Heiskanen et al. (2014) is used in the vertical process-based Arctic Lake Biogeochemistry Model (ALBM) (Tan et al., 2017), which simulates inorganic and organic carbon cycling in permafrost lakes. The model by Heiskanen et al. (2014) is also included in the LakeMetabolizer package (Winslow et al., 2016), in which several lake metabolism models can be combined with models for computing the gas transfer velocity.

In the simple wind-based regression model by MacIntyre et al. (2010), the gas transfer velocity k_{MI} (cm h^{-1}) is calculated separately for heating and cooling conditions as

$$k_{\text{MI}} = \begin{cases} (2.04 U_{10} + 2.0)\left(\frac{Sc}{600}\right)^{-0.5} & \text{if } \beta < 0, \\ (1.74 U_{10} - 0.15)\left(\frac{Sc}{600}\right)^{-0.5} & \text{if } \beta \geq 0. \end{cases} \tag{12}$$

In the surface renewal model of air–water gas exchange, k is parameterized by the total turbulent kinetic energy dissipation rate as $k = c(\nu \varepsilon)^{0.25} Sc^{-0.5}$, where c is an empirical dimensionless constant and ν is the kinematic viscosity of water (MacIntyre et al., 1995). Tedford et al. (2014) integrated the parameterization of the total turbulent kinetic energy dissipation rate, ε_{TE}, into the surface renewal model to yield a model for the gas transfer velocity in units of m s^{-1}:

$$k_{\text{TE}} = c(\nu \varepsilon_{\text{TE}})^{0.25} Sc^{-0.5}. \tag{13}$$

The models by Cole and Caraco (1998), Heiskanen et al. (2014), and Tedford et al. (2014) are included in a gas exchange model intercomparison study by Dugan et al. (2016).

2.1.3 Lake model MyLake C

We used an application of a one-dimensional process-based lake model MyLake C (Kiuru et al., 2018) for the simulation of the vertical distributions of water column temperature and CO_2 concentration and air–water CO_2 flux in the study lake. In addition, we integrated three alternative models for the gas transfer velocity into the lake model. MyLake C simulates inorganic and organic carbon cycling in a lake, taking into account terrestrial carbon loading, air–water exchange of CO_2, and changes in water column pH. However, groundwater exchange and changes in water level due to rainfall or evaporation are excluded. The model operates on a daily time step, and the vertical grid length can be defined by the user. The model is based on a lake model MyLake v.1.2 (Saloranta and Andersen, 2007), which simulates lake thermal structure, seasonal ice and snow cover, and phosphorus-phytoplankton dynamics. In the model, vertical heat and mass diffusion are calculated with a diffusion equation using a vertical turbulent diffusion coefficient derived from the buoyancy frequency and parameterized by lake surface area by default. Settling of particulate substances is also taken into account in the equation. In addition, convective and wind-induced water column mixing processes are included. As an exception to the daily time step, heat exchange between the water column

and the atmosphere is calculated separately for daytime and nighttime. MyLake v.1.2 and its various extensions have been used in studies on stratification and lake ice cover (e.g., Saloranta et al., 2009; Dibike et al., 2012; Gebre et al., 2014), total phosphorus concentration and phytoplankton biomass (e.g., Romarheim et al., 2015; Couture et al., 2018), dissolved organic carbon (DOC) concentration (Holmberg et al., 2014; de Wit et al., 2018), and dissolved oxygen (DO) conditions (Couture et al., 2015).

MyLake C has been designed to include only the most substantial physical, chemical, and biological processes related to carbon cycling in a well-balanced and robust way. CO_2 is produced in the lake through organic carbon degradation both within the water column and in the sediment and through phytoplankton respiration. Inorganic carbon production is coupled to DO consumption, and vice versa. A division is made between readily degradable, phytoplankton-originated autochthonous particulate organic carbon (POC) and more refractory allochthonous POC. The model includes also the sedimentation, the resuspension and the permanent burial of POC. Correspondingly, DOC is classified into three compound classes with different bacterial degradabilities. A separate submodule (Holmberg et al., 2014) calculates the conversion of DOC into an inorganic form via bacterial and photochemical degradation. The meteorological model forcing includes daily global radiation, cloud cover fraction, atmospheric temperature, relative humidity, atmospheric pressure, wind speed at $10\,\mathrm{m}$ height, and precipitation. Hydrological forcing data include daily inflow volumes, inflow temperatures, inflow pH, and the inflow concentrations of modeled substances, including DOC, POC, and DIC. Complete data requirements are presented and model structure and applied equations are described in detail in Kiuru et al. (2018).

MyLake uses the Air-Sea Toolbox (Air-Sea, 1999) based on the parameterizations and algorithms in Fairall et al. (1996) for calculation of surface wind stress and the components of surface heat flux. The sensible heat flux Q_{H}, the latent heat flux Q_{L}, and the wind shear stress τ are obtained from aerodynamic bulk formulas of the form

$$Q_{\mathrm{H}} = \rho_{\mathrm{a}} c_{pa} C_{\mathrm{h}} U (T_{\mathrm{a}} - T_{\mathrm{s}}) \tag{14}$$

$$Q_{\mathrm{L}} = \rho_{\mathrm{a}} L_{\mathrm{e}} C_{\mathrm{l}} U (q_{\mathrm{a}} - q_{\mathrm{s}}) \tag{15}$$

$$\tau = \rho_{\mathrm{a}} C_{\mathrm{d}} U^2, \tag{16}$$

where ρ_{a} is the air density, c_{pa} is the specific heat capacity of air, C_{h} and C_{l} are the transfer coefficients of sensible and latent heat, respectively, C_{d} is the drag coefficient, U is wind speed, T_{a} is air temperature, T_{s} is water surface temperature, L_{e} is the latent heat of evaporation of water, q_{a} is the specific humidity, and q_{s} is the saturation specific humidity at the water surface temperature. No wind sheltering effect on U is applied in the calculation of surface wind stress and surface heat flux components.

The flux of air–water CO_2 between water and the atmosphere, flux F_{CO2}, given in units of $\mathrm{mg\,m^{-2}\,d^{-1}}$ in MyLake C, is calculated as the product of the concentration gradient between the surface water and the atmosphere and the gas transfer velocity k () as

$$F_{\mathrm{CO2}} = \alpha k (C_{\mathrm{w}} - C_{\mathrm{eq}}),$$

where ~~C_w () is the concentration in the topmost model grid layer representing the water surface, C_{eq} ()is the equilibrium concentration of , that is, the water column concentration in the state of equilibrium with the overlying atmosphere, and α is the~~ with Eq. (1) using the model for k by Cole and Caraco (1998) (Eq. (9)). The chemical enhancement factor ~~applicable for reactive gases, such as . Fluxes from water to the atmosphere are thus defined to be positive. If a lake is nonalkaline, α can assumed to be~~ is set to 1~~(Cole and Caraco, 1998)~~, which is also the default value in the model. ~~The equilibrium concentration is calculated by Henry's law as~~

$$\underline{C_{eq} = K_H \chi p_a,}$$

~~where K_H is the Henry's law constant for the gas at surface water temperature, χ is the mole fraction of the gas in the atmosphere, and p_a is the atmospheric pressure. The~~ , and the temperature dependence of the ~~solibility of~~ aqueous-phase solubility K_H is calculated according to Weiss (1974).

2.1.4 ~~Gas exchange models~~

~~In MyLake C, the calculation of k is performed using the widely applied experimental wind-based regression formula by Cole and Caraco (1998), which gives the gas transfer velocity in units of as~~

$$\underline{k_{CC} = (2.07 + 0.215 U_{10}^{1.7}) \left(\frac{Sc}{600} \right)^{-0.5},}$$

~~where U_{10} ()is the wind speed at 10 and Sc is the temperature-dependent Schmidt number determined for surface water conditions using the polynomial fit in Wanninkhof (1992). The approximation $U_{10}/U_{1.5} = 1.22$, where $U_{1.5}$ is the wind speed measured at 1.5 , is used in the calculations.~~ In this study, we incorporated the models for k by ~~MacIntyre et al. (2010), Heiskanen et al. (2014) , and Tedford et al. (2014)~~ Heiskanen et al. (2014) (Eq. (11)), MacIntyre et al. (2010) (Eq. (12)), and Tedford et al. (2014) (Eq. (13)) into MyLake C as alternatives to the default model by Cole and Caraco (1998).

~~In a surface renewal model by Tedford et al. (2014), the gas transfer velocity k_{TE} () is parameterized by the total turbulent kinetic energy dissipation rate ε_{TE} as~~

$$\underline{k_{TE} = c(\nu \varepsilon_{TE})^{0.25} Sc^{-0.5}.}$$

~~where c is a dimensionless constant and ν is the kinematic viscosity of water. In the model, both wind-induced stress and heat-induced convection generate turbulence near the lake surface during cooling, but wind is the only factor responsible for the turbulence during heating. The total turbulent kinetic energy dissipation rate is determined in terms of shear production $\varepsilon_s = u_{*w}^3 / \kappa z'$, where u_{*w} is the wind-induced water-side friction velocity, $\kappa = 0.4$ is the von Kármán constant, and z' is a reference depth, and convective turbulence production ε_c equaling the buoyancy flux β, as~~

$$\underline{\varepsilon_{TE} = \begin{cases} 0.56\varepsilon_s + 0.77|\varepsilon_c| & \text{if } \beta < 0, \\ 0.6\varepsilon_s & \text{if } \beta \geq 0, \end{cases}}$$

In this study, the constants ~~The constants~~ The constants in the model by Tedford et al. (2014) are defined as $c = 0.5$ and $z' = 0.15$ m as in Erkkilä et al. (2018). ~~The wind-induced water friction velocity u_{*w} is calculated from the atmospheric friction velocity $u_{*a} = (\tau/\rho_a)^{0.5}$ as in MacIntyre et al. (1995)~~

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

5 ~~where ρ_w is the density of water.~~

~~The buoyancy flux is defined as in Imberger (1985)~~

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

~~where g is the gravitational acceleration, α_w is the thermal expansion coefficient of water, Q_{eff} is the effective heat flux, and c_{pw} is the specific heat capacity of water. The effective heat flux is defined as~~

10
$$Q_{\text{eff}} = Q_S + Q_{\text{SW}}(0) + Q_{\text{SW}}(z_{\text{AML}}) - \frac{2}{z_{\text{AML}}}\int_0^{z_{\text{AML}}} Q_{\text{SW}}(z)\,\mathrm{d}z,$$

~~where $Q_S = Q_H + Q_L + Q_{\text{LW}}$ is the net surface heat flux, Q_{LW} is net longwave radiation, Q_{SW} is shortwave radiation, and z_{AML} is the depth of the actively mixing layer (AML). The last three terms in the equation represent the fraction of shortwave radiation that is trapped within the AML, denoted as $Q_{\text{SW,AML}}$. The attenuation of shortwave radiation at depth z in the water column is calculated using the Beer–Lambert law~~

15 $$Q_{\text{SW}}(z) = Q_{\text{SW}}(0)\mathrm{e}^{-K_L z},$$

~~where K_L is the total attenuation coefficient of shortwave radiation. The AML is defined as the near-surface~~ In MyLake C, the actively mixing layer includes the model grid layers in which the water column temperature is within 0.02 °C of the temperature ~~at the air–water interface (MacIntyre et al., 2001). All heat fluxes from the atmosphere into the lake are defined positive. Thus, the buoyancy flux is positive when the near-surface water is heating and negative under cooling conditions~~.

20 ~~In a boundary-layer model developed by Heiskanen et al. (2014), near-surface turbulence is parameterized through wind-induced and convection-induced water-side velocity scales, and the equation for k_{HE} () is~~

$$k_{\text{HE}} = ((C_1 U_{1.5})^2 + (C_2 w_*)^2)^{0.5} Sc^{-0.5},$$

~~where $U_{1.5}$ is~~ of the topmost grid layer. The temperature dependence of Sc for CO_2 is determined for surface water conditions using the polynomial fit in Wanninkhof (1992). The approximation $U_{10}/U_{1.5} = 1.22$ is used for the wind speed at ~~1.5 height,~~ ~~$w_* = (-\beta z_{\text{AML}})^{1/3}$ is the penetrative convection velocity, and $C_1 = 1.5 \times 10^{-4}$ and $C_2 = 0.07$ are experimental dimensionless constants~~ different heights.

The fourth model applied in our study was a wind-based regression by MacIntyre et al. (2010), in which the gas transfer velocity k_{MI} () is calculated separately for heating and cooling conditions as

$$k_{MI} = \begin{cases} (2.04U_{10} + 2.0)\left(\frac{Sc}{600}\right)^{-0.5} & \text{if } \beta < 0, \\ (1.74U_{10} - 0.15)\left(\frac{Sc}{600}\right)^{-0.5} & \text{if } \beta \geq 0. \end{cases}$$

2.2 Model application

We used the MyLake C application to Lake Kuivajärvi presented in Kiuru et al. (2018) as the basis of the study. The model setup, including model forcing data and the initial in-lake conditions, is nearly identical to that described in Kiuru et al. (2018). The minor differences are pointed out in Sect. 2.2.2.

2.2.1 Study lake

Lake Kuivajärvi is an oblong, mesotrophic, and humic lake located in southern Finland (61° 50' N, 24° 16' E) at the vicinity of the SMEAR II station (Station for Measuring Ecosystem–Atmosphere Relations; Hari and Kulmala (2005)). The length of the lake is 2.6 km, the maximum width is 0.3 km, and the surface area is 0.63 km². The north-south-oriented lake has two distinct basins. The maximum depth of the deeper southern basin is 13.2 m (Heiskanen et al., 2014), which is more than double the mean depth 6.3 m. A measurement platform (Lake-SMEAR) is situated close to the deepest region of the lake. The approximate retention time of the lake is 0.65 years. Lake Kuivajärvi is surrounded by managed mixed coniferous forest together with small open wetland areas (Miettinen et al., 2015). The majority of the catchment area (9.4 km²) of the lake is flat. The main inlet stream with a mean pH of 6.5 (Dinsmore et al., 2013) drains four upstream lakes, which are smaller in area than Lake Kuivajärvi. The lake is dimictic: the spring turnover usually occurs rapidly right after ice-off in late April or early May, and the summer stratification period lasts until the autumn turnover in September or October. The duration of the ice-covered period and the concomitant inverse stratification is usually 5–6 months (Heiskanen et al., 2015). The turnover periods are hot moments for the release of CO_2 accumulated in the hypolimnion of the lake during stratification (Miettinen et al., 2015). Because of high terrestrial inputs of organic matter, a median concentration of DOC in the surface water is 12–14 mg L^{-1} (Miettinen et al., 2015) and water clarity is rather low, a median light attenuation coefficient K_L being around 0.6 m^{-1} (Heiskanen et al., 2015).

2.2.2 Model forcing and calibration data

The meteorological forcing data and hydrological loading data used in the model application are described in detail in Kiuru et al. (2018). The daily averages of wind speed at 1.5 m and incoming shortwave radiation together with in-lake temperature and CO_2 concentration were obtained from automatic platform measurements (Heiskanen et al., 2014; Mammarella et al., 2015), and the remaining meteorological forcing data were obtained from the SMEAR II station or from weather stations (Finnish Meteorological Institute) in Hyytiälä located less than 1 km from the lake (precipitation) and in Tikkakoski located approximately 95 km to the north-east from the lake (cloud cover fraction). Differing from Kiuru et al. (2018), the CO_2 mixing

ratio in the atmosphere was assumed to be 395 ppm on the basis of the rather fragmentary time series of the high-frequency in situ measurements of the CO_2 mixing ratio, the method of which is described in Erkkilä et al. (2018).

The construction of the time series for lake inflow was based on continuous measurements of the discharges at the main inlet and at the outlet of Lake Kuivajärvi in 2013–2014 (Dinsmore et al., 2013). Because the total measured outflow volumes were approximately double the main inlet discharge volumes on an annual scale, the daily inflow volumes were corrected by a factor of 2 in order to include the potential contributions of smaller inlet streams and groundwater to lake inflow. At the main inlet, water temperature was measured approximately two times a month in 2013 and continuously in 2014 and CO_2 concentration was measured two times a month in 2013 but mostly at intervals of 2–3 d around the period of ice-off in April and May using the procedure described in Miettinen et al. (2015). Daily time series were generated by linear interpolation.

The model was calibrated against the daily averages of the automatic high-frequency CO_2 concentration measurements: an optimal set of selected model parameters were estimated so that the simulated CO_2 concentration time series matched the corresponding measured CO_2 concentration time series as well as possible. The estimation was performed using a statistical inference algorithm. In addition, the automatic water column temperature measurements were used in model performance validation. The CO_2 concentrations were measured at 0.2, 1.5, 2.5, and 7.0 m, and the temperature measurements were performed at 0.2 m, at 0.5 m intervals from 0.5 to 5.0 m, and at 6, 7, 8, 10 and 12 m using the measurement systems described in Heiskanen et al. (2014) and Mammarella et al. (2015).

2.2.3 Model assessment data

We used additional meteorological measurements in assessing the performance of the alternative models for k incorporated into MyLake C during the period May–October 2013. An EC system located on the measurement platform measures the turbulent fluxes of momentum, heat, and water vapor (H_2O) over the lake (Mammarella et al., 2015). The EC flux measurement system includes an ultrasonic anemometer (USA-1, Metek GmbH, Elmshorn, Germany) and a closed-path infrared gas analyzer (LI-7200, LICOR Inc., Nebraska, USA) for measuring CO_2 and H_2O mixing ratios at 1.8 m height above the lake surface. Air temperature and relative humidity were measured with a Rotronic MP102H/HC2-S3 (Rotronic Instrument Corp., NY) and radiation components with a CNR1 net radiometer (Kipp & Zonen, Delft, Netherlands). Automatic platform measurements of net surface longwave radiation and EC measurements of sensible heat flux, H_2O flux, and momentum flux were used in the determination of net surface heat flux and atmospheric friction velocity. During EC data post-processing, latent heat flux was calculated from the H_2O flux, and the atmospheric friction velocity was derived from the momentum flux. All EC measurement data were given as half-hour block averages. The EC measurements are explained in more detail in Erkkilä et al. (2018), and the description of EC data post-processing is found in Mammarella et al. (2015) and Mammarella et al. (2016). Contrary to the model forcing data, the air temperatures that were used in the measurement-based determination of the gas transfer velocities were obtained from the platform measurements instead of the SMEAR II station when platform measurements were available. In addition, the rather intermittent platform measurement data on relative humidity were used. Missing In the calculation of the water-side friction velocity, missing relative humidities were replaced by a value of 75 % in the calculation of the water-side friction velocity. , which is close to the average of the SMEAR II measurements of relative humidity in May–October 2013,

72 %. The corresponding averages over the period May–August 2013, for which platform measurements were rather well applicable, were 66 % and 68 % for the SMEAR II and platform measurements, respectively. Thus, the relative humidity can be assumed to have been slightly higher over the lake than at the SMEAR II station.

~~There was a gap in the heat flux data on 14–27 June because of EC system malfunction, and some of the existing data~~ ~~were discarded through the application of EC quality screening criteria presented in Erkkilä et al. (2018). In addition, only~~ The estimation of the flux footprint distribution functions was made using the model by Kormann and Meixner (2001). The average footprint contributing to 80 % of the fluxes varies from 100 m up to about 300 m from the measurement platform depending on atmospheric stability conditions as described in Mammarella et al. (2015). Only wind directions along the lake (130°–180°and 320°–350°) were included ~~so~~ in the calculations to ensure that heat fluxes from the surrounding land were excluded. Furthermore, possible remaining effects of transversal advection during calm nights were removed through EC quality screening. In addition to the exclusion of some of the EC measurement data through the application of the quality screening criteria presented in Erkkilä et al. (2018), there was a gap in the heat flux data on 14–27 June because of EC system malfunction. The monthly data coverage was 43–69 % and 32–70 % of the original data for sensible and latent heat fluxes, respectively. We constructed gap-filled half-hour time series for sensible and latent heat fluxes using linear fits between the measured sensible heat flux and wind speed multiplied by the air–surface water temperature difference and between the measured latent heat flux and wind speed multiplied by the vapor pressure difference, according to Mammarella et al. (2015). Only the vapor pressures calculated from the measured relative humidities were used in the latter fit. The fitting was performed independently for each month.

We compared the simulated gas transfer velocities for CO_2 and the simulated air–water CO_2 fluxes to those determined directly from measurements using the corresponding gas exchange models. The latter are hereinafter referred as to calculated gas transfer velocities and calculated CO_2 fluxes. The calculated CO_2 transfer velocities for each of the four gas exchange models were obtained using the daily averages of required measured variables. The calculated air–water CO_2 fluxes were further obtained as the product of the calculated CO_2 transfer velocities and the daily averages of the measured air–water CO_2 concentration gradient. The conditions were thus compatible with the daily time step applied in MyLake C. The atmospheric equilibrium concentrations of CO_2 were calculated from the measured atmospheric CO_2 mixing ratios. The daily averages of the depth of the AML were estimated from the daily averaged temperature profiles as the depth at which water column temperature was within 0.25 °C of the temperature at 0.2 m as in Erkkilä et al. (2018). As in MyLake C, the approximation $U_{10}/U_{1.5} = 1.22$ was used in the calculations. Following Mammarella et al. (2015), a value of 2 m^{-1} was used for the total attenuation coefficient of shortwave radiation K_L in the calculation of Q_{eff}.

2.2.4 Model calibration and validation

We estimated the MyLake C parameters utilizing a Markov chain Monte Carlo-based Bayesian inference algorithm following the procedures in the original calibration of the Lake Kuivajärvi application presented in Kiuru et al. (2018). Each of the four new versions of the MyLake C Lake Kuivajärvi application, using the models for k by Cole and Caraco (1998) (both the MyLake C version and the respective gas exchange model being hereinafter referred to as CC), Heiskanen et al. (2014) (HE),

MacIntyre et al. (2010) (MI), and Tedford et al. (2014) (TE), was calibrated individually. The simulations with the MyLake C versions using different gas exchange models are hereinafter collectively referred to as GEMs. The model grid length was 0.5 m. The model was run from 8 January 2013 to 31 December 2014. The calibration period extended from 8 January to 31 December 2013, and the measurements in 2014 were used for model validation.

5   The calibrations were performed against the daily averages of the automatic water column CO_2 concentration measurements at the depths of 0.2, 2.5, and 7 m. We chose to apply the automatic measurements instead of the corresponding manual measurements used in the model calibration in Kiuru et al. (2018) because the calculation of daily CO_2 fluxes was based on the automatic measurements at 0.2 m in this study and the simulation results were thus comparable with the calculated CO_2 fluxes. Even though the near-surface CO_2 concentration was the most significant factor considering air–water CO_2 exchange,
10 deeper depths were included so that model behavior would remain reasonable also at deeper levels.

    The calibrated model parameters were selected on the basis of the original calibration. However, because the new calibrations were not performed against water column DO concentrations, the parameters related to interactions between DO and CO_2 were excluded from the parameter set. The DIC inflow concentration scaling factor $C_{DI,IN}$, applied during open water seasons, was introduced as a new calibration parameter. The other parameters included in the calibration were the vertical
15 turbulent diffusion parameter a_k, the wind sheltering coefficient W_{str}, the DOC-related specific attenuation coefficient of photosynthetically active radiation β_{DOC}, the maximal phytoplankton growth rate at 20 °C μ'_{20}, the phytoplankton death rate at 20 °C m_{20}, the degradation rates of labile DOC $k_{DOC,1}$ and semilabile DOC $k_{DOC,2}$, the fragmentation rates of autochthonous POC $k_{POC,1}$ and allochthonous POC $k_{POC,2}$, and the sedimentary POC degradation rate $k_{POC,sed}$. The parameters obtained in the original calibration, or the default parameters, were used as the means of the prior parameter distributions.

20   One parameter chain with 3000 iterations was produced in each calibration. The starting points were set to 50th percentiles of the prior distributions. The first half of each resultant chain was discarded as a burn-in period, and the final parameters chains included 1500 parameter sets. The medians of the final posterior distributions (Figs. S1–S4) were chosen as the calibrated parameters. They are presented, together with the default parameters, in Table 2. After the calibrations, additional goodness-of-fit metrics were calculated. The Nash–Sutcliffe efficiency (NS) gives a relative evaluation assessment, determining the
25 relative magnitude of the residual variance compared to the variance of measurement data (Moriasi et al., 2007). The value of the normalized bias (B^*) describes a systematic overestimation ($B^* > 0$) or underestimation ($B^* < 0$) of a state variable in the simulation, whereas the normalized unbiased root-mean-square difference ($RMSD'^*$) shows if the standard deviation of the simulated values is higher ($RMSD'^* > 0$) or smaller ($RMSD'^* < 0$) than that of the measurements (Los and Blaas, 2010).

2.2.5   Calculation of CO_2 budgets

30 After the calibrations, we calculated CO_2 budgets for the epilimnion of the lake during the periods of continuous summer stratification in 2013 and 2014 for each GEM. The epilimnion was defined as the layer in which water temperature was within 1 °C of surface temperature. The stratified period was defined to begin on the day of the formation of the thermocline after ice-off and to finish when the depth of the epilimnion (z_{epi}) reached the value of 7 m in the simulations. The exchange of CO_2 between the epilimnion and the atmosphere is balanced in MyLake C by (1) net external loading of CO_2, (2) net epilimnetic

CO_2 production, and (3) the release of CO_2 from deeper layers to the epilimnion. The net external loading equals the amount of terrestrially produced CO_2 entering the lake via stream inflow subtracted by the amount of CO_2 in lake outflow. The release of CO_2 from the metalimnion or the hypolimnion occurs through deepening of the epilimnion due to wind-induced mixing or thermal convection. If the epilimnetic volume becomes smaller, a portion of CO_2 is again confined below the epilimnion and the amount of CO_2 in the remaining epilimnion is reduced.

3   Results

3.1   Model calibration

Even though the differences between the formulations of the gas exchange models incorporated into MyLake C are rather notable, the resultant CO_2 concentrations did not differ substantially between the GEMs, that is, between the simulations with the MyLake C versions using different gas exchange models (Fig. 1). However, an optimal simulation result can be attained through many different combinations of processes related to in-lake carbon dynamics and fluvial and atmospheric exchange in MyLake C, which is seen in the variation between the parameter values obtained from the different calibrations (Table 2). The calibrations were performed only against CO_2 concentrations, and the aim of the calibration was not to try to reproduce the actual in-lake carbon cycling but rather to compare different possible ways to generate an optimal water column CO_2 concentration. The performance metrics for CO_2 concentration shown in the Supplement (Table S1) indicate that all GEMs yielded too low CO_2 concentrations ($B^* < 0$) at all depths during the calibration and validation periods with only few exceptions. However, the CO_2 concentration measurements performed during the ice-covered periods were largely not applicable at 0.2 m because of the lake ice cover and sometimes inapplicable also at deeper levels because of system malfunction.

The average near-surface (0–0.5 m) CO_2 concentrations over the open water seasons were notably higher in CC (44.3 mmol m^{-3} and 40.3 mmol m^{-3} in the calibration year 2013 and in the validation year 2014, respectively) than in the other GEMs (HE: 34.2 mmol m^{-3} and 31.6 mmol m^{-3}; MI: 31.5 mmol m^{-3} and 29.4 mmol m^{-3}; TE: 36.9 mmol m^{-3} and 34.1 mmol m^{-3}). Only the days with applicable corresponding water column CO_2 concentration measurement data were included in the averaging. By contrast, the open water season averages of the measured near-surface (0.2 m) CO_2 concentrations were 45.2 mmol m^{-3} in 2013 and 37.2 mmol m^{-3} in 2014. Thus, CC yielded a higher near-surface CO_2 concentration compared to the measurements in 2014 when only the ice-free season, the period of air–water CO_2 exchange, is considered. The simulated open water seasons were determined from the simulated ice-off and ice-on dates. Because CO_2 flux differs from zero starting from the day after ice-off in MyLake C, the simulated open water seasons applied in the study were 3 May–25 November 2013 and 16 April–22 November 2014. In 2013, the observed open water season lasted from 1 May to 27 November. In 2014, the observed ice-off date was 12 April.

The simulated CO_2 transfer velocities and air–water CO_2 fluxes are presented in Fig. S5. The yearly average values of k were lowest in CC and rather similar between the other GEMs (CC: 2.81 cm s^{-1} and 2.76 cm s^{-1} for the calibration period and the validation period, respectively; HE: 5.44 cm s^{-1} and 5.33 cm s^{-1}; MI: 5.87 cm s^{-1} and 5.82 cm s^{-1}; TE: 4.73 cm s^{-1} and

4.66 cm s^{-1}). The differences in the simulated fluxes between GEMs were dissimilar to those in k because of the differences in the simulated near-surface CO_2 concentrations. The smallest k values in CC were compensated by the highest near-surface CO_2 concentrations. By contrast, a high daily CO_2 efflux due to a high k in MI reduced the simulated near-surface CO_2 concentration compared to the other GEMs during the whole simulation period. Overall, the differences in yearly air–water

5   CO_2 fluxes between GEMs were smaller than those in the values of k (CC: 0.22 µmol m^{-2} s^{-1} and 0.20 µmol m^{-2} s^{-1} for the calibration period and the validation period, respectively; HE: 0.28 µmol m^{-2} s^{-1} and 0.26 µmol m^{-2} s^{-1}; MI: 0.25 µmol m^{-2} s^{-1} and 0.24 µmol m^{-2} s^{-1}; TE: 0.28 µmol m^{-2} s^{-1} and 0.27 µmol m^{-2} s^{-1}).

The CO_2 efflux during the first few days after ice-off was higher in GEMs with a high k, which increased the water column pH in comparison to CC. The differences remained rather constant during most of the open water seasons. The near-surface pH

10   was on average 0.20–0.26 and 0.18–0.25 units higher in the other GEMs than in CC during the open water seasons of 2013 and 2014, respectively. As a result, the average fractions of CO_2 of DIC in the near-surface layer were, respectively, 6–8 and 5–6 percentage units higher in CC than in other GEMs, which also contributed to the higher near-surface CO_2 concentration in CC than in other GEMs. In addition, the open water season average near-surface pH was 0.22 units higher in 2014 than 2013 in all GEMs. Accumulation of bicarbonate in the water column in the course of the simulations may have resulted in an excessively

15   high pH and thus a relatively lower CO_2 concentration in 2014 compared to 2013.

The differences in simulated temperatures between GEMs, primarily due to different attenuation of shortwave radiation in the water column, were rather small especially at 0.2 m and at 2.5 m (Fig. S6). High epilimnetic concentrations of both Chl a and DOC, resulting from a low phytoplankton death rate and a high allochthonous POC fragmentation rate, respectively, in MI resulted in the strongest attenuation of shortwave radiation and thus the highest near-surface temperature because of a

20   thinner and warmer epilimnion than in other GEMs. The open water season average near-surface temperatures were 0.28–0.47 °C and 0.65–0.86 °C lower than the corresponding measured averages in the calibration and validation periods, respectively, being highest in MI and lowest in TE. The differences were greatest in November before ice-on. The simulated near-surface temperatures tended to be somewhat too low in spring and early summer during both periods and somewhat too high in the late summer and autumn of the calibration year.

25   Heat transfer to the depth of 7 m right after the onset of the summer stratified period was insufficient in the calibration year in all GEMs, and small values of a_k also reduced heat transfer through the epilimnion during summer stratification. As a result, water column temperature remained too low at the depth of 7 m, which was located in the hypolimnion for most of the summer, during the stratified period in the simulations. However, the performance of the simulation of CO_2 concentration was successful also at the depth of 7 m. The summertime mixed layer thickness was rather similar between GEMs during the calibration year

30   but more variable during the validation year. Simulated thermocline deepening matched the measurements during the late summer of the calibration year but was too early in the validation year. The deepening was slowest in HE because a somewhat stronger temperature gradient in the metalimnion, which was due to the smallest a_k, resisted wind-induced thermocline erosion during summer.

3.2 Effective heat flux

The effective heat fluxes at the air–water interface simulated with each GEM on 3 May to 31 October 2013 and the corresponding values calculated on the basis of heat flux and radiation measurements are presented in Fig. 2a. The largest differences between the magnitudes and the directions of simulated and measured Q_{eff} were seen in early May. The simulated Q_{eff} was directed out of the lake throughout the study period except for few occasions in early May and in October, whereas measurement-based calculations yielded more frequent occurrences of a positive daily Q_{eff}. Also, a negative Q_{eff} was often overestimated by the simulations because of overly high negative sensible and latent heat fluxes and net longwave radiation (Fig. S7). The performance of the simulation of the components of surface heat flux was rather poor (Table S2). Overall, the Q_{eff} simulation performance was not very good ($R^2 = 0.39$–0.41, RMSE = 48.2–49.2 W m^{-2}, NS = 0.11–0.14, $B^* = -0.47\ldots -0.46$, $n = 164$). The differences in the simulated Q_{eff}'s between GEMs, resulting mainly from different surface temperatures, were quite small.

The extent of shortwave radiative heating of the AML, $Q_{\mathrm{SW,AML}}$, is dependent on z_{AML}. The simulated z_{AML} was greater than the measured daily average with few exceptions at the beginning and near the end of the study period (Fig. 2b), which increased the simulated $Q_{\mathrm{SW,AML}}$ and decreased a negative Q_{eff}. The simulation with a daily time step generated clear temperature variation in the epilimnion only on days with a high amount of surface heating in early summer and midsummer, which resulted in an overly deep AML during most of the period. In addition, the model with a sequential description of thermal processes did not catch simultaneous wind mixing and surface heat exchange processes that resulted in a deeper observational AML in spring and late autumn. However, day-to-day variation in the discrepancy of $Q_{\mathrm{SW,AML}}$ was high throughout the study period. Also, the simulations highly underestimated the atmospheric friction velocity ($R^2 = 0.35$, RMSE = 0.11 m s^{-1}, NS = -3.2, $B^* = -1.89$, $n = 166$) (Fig. S8), the simulated $u_{*\mathrm{a}}$ being on average only 46 % of the measured daily average. The simulated daily drag coefficient C_{d} at 1.5 m was affected by atmospheric stability conditions. The median C_{d} varied from 1.589×10^{-3} to 1.593×10^{-3} between the GEMs.

3.3 CO$_2$ exchange

The differences between simulated gas transfer velocities for CO$_2$ and the respective calculated values during the study period 3 May–31 October 2013 were rather small in the cases of gas exchange models based solely on wind speed, CC and MI, but the discrepancies were higher in HE and TE, which include also the effect of thermal convection on gas exchange (Fig. 3, Table S3). The simulations with CC and MI often yielded slightly higher values of k than the respective calculations because the simulated surface temperature was higher than the measured daily average (Fig. S6) and thus the temperature-dependent Schmidt number correction of k was different. Also, the occurrences of a simulated negative β in early May in MI yielded higher k_{MI}'s compared to the respective calculated values obtained from the observed positive β. The simulated k_{HE} was often higher than the calculated counterpart because of a high negative Q_{eff} or a deep AML in the simulations (Fig. 2), which resulted in a high penetrative convection velocity. In HE, the effects of wind-induced shear and thermal convection on k are set to be roughly of the same order of magnitude and the wind-induced shear velocity is calculated from wind speed, whereas CO$_2$ flux

is driven principally by wind shear, which is calculated directly from u_{*a}, in TE. Because the simulated u_{*a} was consistently significantly lower than the corresponding daily measured average, the simulated k_{TE} was on average 40 % lower than the calculated value.

The simulated near-surface CO_2 concentrations were significantly too low during most of the study period in all GEMs except for CC, which yielded too high concentrations in autumn (Fig. 4, Table S3). The higher the simulated k and daily CO_2 efflux, the greater was the resulting decrease in near-surface CO_2 concentration. The decline of near-surface CO_2 concentration after ice-off was too rapid in all GEMs, especially in MI, the GEM with the highest k. Simulated near-surface CO_2 concentration declined close to the atmospheric equilibrium concentration in all GEMs also in late summer because of insufficient gain of CO_2 in a shallow epilimnion developed under warm and calm conditions. The low simulated air–water CO_2 concentration gradients in May resulted in an underestimated air–water CO_2 flux from the water column compared to the respective calculated fluxes (Fig. 5, Table S3). The simulated flux was notably lower than the calculated flux in TE during the whole study period because of a small k_{TE}. On the contrary, CC notably overestimated the corresponding calculated CO_2 flux in August and September because of a high simulated near-surface CO_2 concentration. Also, the simulated CO_2 flux was slightly higher than the calculated flux in HE in August and September because of high epilimnetic net CO_2 production. The total simulated CO_2 flux during May–October matched the calculated flux in CC but was notably lower in HE and MI and less than half of the calculated flux in TE (Table 3). The underestimated near-surface CO_2 concentrations were somewhat compensated for by the higher simulated k_{HE} and k_{MI} compared to the calculated counterparts, which decreased the difference between the simulated and calculated fluxes in HE and MI.

The applied gas exchange models yielded notably different calculated monthly CO_2 effluxes (Table 3). The CO_2 fluxes were calculated using the measured air–water CO_2 concentration gradients, and thus the differences between the calculated fluxes were only due to different values of k. Monthly fluxes calculated with MI were nearly or even more than double of those calculated with the other wind-based model CC. Days with a positive β, resulting in a lower k_{MI}, occurred mainly in May and October, and thus the difference between the CO_2 fluxes calculated with MI and CC was slightly smaller in those months. The models that include the effect of thermal convection, HE and TE, yielded notably higher CO_2 fluxes than the simplest model, CC. Nevertheless, the CO_2 fluxes calculated with MI were slightly higher than those calculated with HE. The CO_2 fluxes calculated with TE were clearly the highest in all months, which was, however, not the case in the simulations.

The calculated daily values of k and CO_2 flux were dependent on the calculation interval. If the daily k had been calculated as the daily average of calculated half-hour values of k instead of using the daily averages of the input variables, the results would have been different. The daily averages of calculated half-hour k_{MI} (RMSE = 0.70 cm h^{-1}, $B^* = -0.16$) and k_{TE} (RMSE = 0.22 cm h^{-1}, $B^* = -0.04$) were lower than the respective values calculated using daily averages of input variables, whereas the opposite was the case for k_{HE} (RMSE = 0.48 cm h^{-1}, $B^* = 0.20$) and k_{CC} (RMSE = 0.16 cm h^{-1}, $B^* = 0.15$). On the contrary, the calculation of a daily CO_2 flux as the average of half-hour fluxes yielded a slightly higher CO_2 flux in all GEMs (HE: RMSE = 0.066 µmol m^{-2} s^{-1}, $B^* = 0.13$; CC: RMSE = 0.034 µmol m^{-2} s^{-1}, $B^* = 0.11$; MI: RMSE = 0.10 µmol m^{-2} s^{-1}, $B^* = 3.4 \times 10^{-4}$; TE: RMSE = 0.11 µmol m^{-2} s^{-1}, $B^* = 0.05$).

The differences resulting from the different methods of the calculation of a daily k can partly be explained by the behavior of the driving variables of the models. Using the daily averages of the input variables in the calculation may have smoothened out the effects of the spells of stronger negative buoyancy flux or a deeper AML that increase the half-hour k_{HE} and the effects of the occasions of positive buoyancy flux that decrease the half-hour k_{MI}. Daily averaging of wind speed may have cut out the rapid increase of k_{CC} under stronger-wind conditions during the course of day due to the greater-than-linear dependence of k_{CC} on wind speed. By contrast, because the dependence of k_{TE} on $u_{*\mathrm{a}}$ is less than linear and the impact of thermal convection on k_{TE} is minor, the effect of the diel variation of $u_{*\mathrm{a}}$ and thus the relative difference between the methods of the calculation of k_{TE} was rather small.

3.4 Lake CO_2 budgets

The simulated CO_2 budgets for the epilimnion of the lake during the periods of continuous summer stratification in 2013 and 2014 differed between GEMs as a response to different CO_2 effluxes (Table 4). The simulations were not able to reproduce the short-lived episodes of a very shallow epilimnion on days with high solar radiation and low wind speeds in late August and early September 2013, but at other times the simulated z_{epi} matched rather well the depths estimated from the measured daily temperature profiles (Fig. 6). The epilimnion formed 11 d earlier and extended to 7 m 16–22 d later in 2013 than in 2014. The in-lake CO_2 concentrations were higher at the onset of stratification in 2013 than in 2014 because of less effective water column ventilation during the shorter spring mixing period. As a result, the amount of CO_2 in the epilimnion decreased during the stratified period in 2013, whereas it increased slightly in 2014.

A higher net in-lake CO_2 production or a higher terrestrial CO_2 load was required to compensate for the higher CO_2 efflux in GEMs that yielded higher values of k (Table 4). Phytoplankton concentration, regulated in MyLake C by the growth and death rates μ' and m, respectively, impacts CO_2 dynamics both directly through the amount of carbon fixation and indirectly through changes in epilimnetic thermal structure due to attenuation of solar radiation. A high μ' resulted in faster phytoplankton growth in spring and thus in an earlier occurrence of the spring bloom, and a small m resulted in a higher phytoplankton biomass during midsummer and late summer. HE and MI yielded the highest maximum near-surface Chl a concentrations, approximately 15 mg m^{-3} in 2013 and close to 20 mg m^{-3} in 2014. In CC and TE, Chl a concentrations were greater than 10 mg m^{-3} during the growth peaks but less than 5 mg m^{-3} at other times because of the high values of m. The open water season average near-surface Chl a concentration was highest in HE (9.6 and 9.3 mg m^{-3} in 2013 and 2014, respectively), followed by MI (7.5 and 6.1 mg m^{-3}), CC (3.9 and 4.0 mg m^{-3}), and TE (2.3 and 2.1 mg m^{-3}).

However, a high phytoplankton biomass did not imply high CO_2 consumption because of phosphorus limitation of phytoplankton growth in the model and the resultant reduction of photosynthetic CO_2 consumption under high Chl a and low bioavailable phosphorus concentrations in the simulations. Instead, CO_2 fixation occurred at a steady rate and the total CO_2 consumption over the whole growing season was relatively higher under a low Chl a concentration due to a high m. The highest average phytoplankton biomass in HE resulted in the highest CO_2 fixation; however, also total net CO_2 production was highest in HE because of high $k_{\mathrm{POC,1}}$ and $k_{\mathrm{DOC,1}}$. Small values of $k_{\mathrm{POC,1}}$ and $k_{\mathrm{DOC,2}}$ resulted in a relatively low net CO_2

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production despite low CO_2 fixation and a high $k_{POC,sed}$ in TE. Net CO_2 production was lowest in CC because of rather high total CO_2 fixation during the long growing season and the rather small $k_{POC,1}$ and $k_{DOC,1}$.

A considerable increase in the inflow DIC concentration by way of the scaling factor was essential in order to significantly increase the terrestrial CO_2 input to the lake in GEMs with a high CO_2 efflux. The measured inflow CO_2 concentration was 200–250 $mmol\,m^{-3}$ until ice-off, less than 80 $mmol\,m^{-3}$ during May, and mainly between 50 and 100 $mmol\,m^{-3}$ during the summer and autumn. Thus, the default inflow CO_2 concentration was only approximately double the simulated near-surface CO_2 concentrations during most of the open water season, and the effect of external CO_2 loading on in-lake CO_2 concentration was inevitably rather small especially during the low-discharge period in late summer and autumn. The values of $C_{DI,IN}$ determined the order of the amounts of the net external CO_2 load to the lake in the GEMs (TE: 42000 and 45000 kg CO_2 over the years 2013 and 2014, respectively; MI: 27500 and 31400 kg CO_2; HE: 26500 and 30600 kg CO_2; CC: 22200 and 25800 kg CO_2).

However, the total net external CO_2 loads to the lake over the stratification periods were slightly higher than the net external CO_2 loads to the epilimnion in Table 4 because stream inflow was directed into the metalimnion on days when the inflow temperature was lower than the epilimnetic temperature. The epilimnetic loads were 90–92 % and 98–99 % of the total loads in 2013 and 2014, respectively, the proportions being highest in CC and lowest in MI. The amount of CO_2 outflow was relatively large in CC because of the high epilimnetic CO_2 concentration; thus, the net external CO_2 load was relatively lower in CC than in other GEMs compared to the differences in $C_{DI,IN}$. In addition, because inflow pH was unaltered in the scaling of inflow DIC concentration, some of the increased CO_2 load was eventually evaded to the atmosphere in the simulations but the bicarbonate fraction of DIC remained in the water column, which resulted in a slight increase in in-lake pH and a decline in the CO_2 fraction of DIC especially in GEMs with a high k. Nevertheless, the impact of different amounts of bicarbonate loading on the in-lake pH was minor compared to the impact of different springtime CO_2 effluxes between GEMs.

4 Discussion

4.1 Differences between calculated and simulated CO_2 fluxes

There was less variation between the air–water CO_2 fluxes simulated with different GEMs, that is, simulated with the MyLake C versions using different gas exchange models, than between the CO_2 fluxes calculated with the corresponding different gas exchange models on the basis on measured surface heat fluxes and air–water CO_2 concentration gradients (Table 3). This was caused both by differences between the simulated and calculated values of k and by insufficient epilimnetic CO_2 production in the simulations. An increased terrestrial CO_2 loading or an increased in-lake CO_2 production was needed to balance the higher CO_2 loss from the epilimnion through efflux in GEMs with a higher k compared to the simple wind-based CC (Table 4). Still, the simulations yielded too low near-surface CO_2 concentrations (Fig. 4, Table S3), which contributed to the underestimation of CO_2 fluxes (Fig. 5). Calibrating the model only against the near-surface CO_2 concentration and thus using even higher values for organic carbon fractionation and degradation parameters would have improved the performance of the simulation

of epilimnetic CO_2 concentration; however, it would have resulted in uncontrollable and probably excessively high CO_2 concentrations in deeper layers, which is disadvantageous in a year-round, vertically layered lake model.

The day-to-day performance of the simulation of epilimnetic CO_2 concentration was also partly determined by the simulated thermal stratification and epilimnetic volume. The simulations generally yielded too low a near-surface CO_2 concentration when the simulated z_{epi} was in accordance with the observed depth and performed more adequately only during periods when the simulated z_{epi} was too high (Figs. 4 and 6). The measurements showed an increase in the near-surface CO_2 concentration when the epilimnion became thicker, and vice versa, during the stratified period in 2013. Thermocline tilting-induced upwelling and convection-induced entrainment transported more CO_2-rich water into the epilimnion on windy and cool days (Heiskanen et al., 2014). Conversely, high solar radiation input combined with calm conditions results in the warming of near-surface water and the formation of a thin epilimnion with a lower CO_2 concentration. High solar radiation also enhances photosynthesis and thus increases the uptake of CO_2 (Provenzale et al., 2018). An overly deep simulated epilimnion resulted in enhanced CO_2 release from deeper layers and a higher total net CO_2 production in a larger epilimnetic volume, which were able to compensate for the CO_2 efflux in the simulations.

The accuracy of the determination of a daily Q_{eff} and the applicability of the concept of a daily AML are issues that may cause uncertainties when the gas exchange models are used either to calculate or to simulate daily estimates of k. The calculated half-hour Q_{eff} was generally directed into the lake on some occasions at daytime because of solar heating of the AML and always directed out of the lake at nighttime, and z_{AML} often increased during nighttime and decreased under radiative heating of near-surface water at daytime. Boundary layer models and surface renewal models have been developed to describe short-term dynamics of turbulence in a shallow AML, and thus they may not perform equally well in calculations with a daily time step.

The wind-based CC yielded the lowest and the surface renewal model TE the highest calculated air–water CO_2 fluxes, which is in line with the comparisons of different gas exchange models using data from Lake Kuivajärvi by Mammarella et al. (2015) and Erkkilä et al. (2018); however, the differences in simulated CO_2 fluxes between CC and other GEMs were notably smaller than the corresponding differences in the two experimental studies. The performance of TE is strongly dependent on the magnitude of u_{*a} because wind shear is highly dominant over thermal convection as the generator of turbulence in the model. Because the simulations yielded significantly lower u_{*a} compared to the values obtained through EC measurements (Fig. S8), the CO_2 flux obtained with TE was much lower than the corresponding calculated flux. Also Erkkilä et al. (2018) found that u_{*a} calculated from wind speed was lower than the measured u_{*a} in Lake Kuivajärvi. Bulk models for surface stress may yield low values for u_{*a} over a lake especially when parameterized for open sea conditions with low surface roughness (Wang et al., 2015), which is the case in MyLake C. Lake size may also affect the relative differences between gas transfer velocities obtained with different gas exchange models. Dugan et al. (2016) applied different gas exchange models to the calculation of DO exchange in temperate lakes of various sizes. Simple, wind-based models yielded clearly lower values of k than more complex models in lakes similar to Lake Kuivajärvi in size, whereas the differences between the model types were smaller in larger lakes with generally higher wind speeds and a higher relative importance of wind-induced mixing compared to convection. In

addition, ecosystem-specific empirical regression models may not be suitable for lakes with dissimilar characteristics (Vachon and Prairie, 2013).

4.2 Comparison to EC CO_2 flux measurements

Estimates of air–water CO_2 fluxes obtained with the gas exchange models applied in our study have been compared with 30-min block-averaged EC CO_2 flux measurements over Lake Kuivajärvi (Heiskanen et al., 2014; Mammarella et al., 2015; Erkkilä et al., 2018). Heiskanen et al. (2014) compared the half-hour k's calculated with HE, CC, and MI with those obtained through EC measurements of CO_2 flux in August–November 2011. In the study, the average values of k_{HE} and k_{MI} were approximately 70 % of the corresponding measurement-based values, but the average k_{CC} was only about half of the average k_{HE} and k_{MI}. Erkkilä et al. (2018) compared the daily medians of EC CO_2 flux during a two-week period in October 2014 with the daily median CO_2 fluxes calculated with CC, HE, and TE. The CO_2 fluxes obtained with HE and TE were 60 % of the EC CO_2 fluxes and approximately double the CO_2 fluxes obtained with CC. Overall, TE yielded the best correspondence with the EC fluxes. TE outperformed CC also in the comparison of half-hour CO_2 fluxes during the open water periods of 2010 and 2011 in Mammarella et al. (2015). In our study, the best agreement with simulated and calculated CO_2 fluxes was found in CC, whereas TE yielded the lowest simulated fluxes in comparison to the corresponding calculated fluxes. Thus, none of the GEM outputs can be considered compatible with EC CO_2 fluxes, provided that the conclusions from the half-hour comparisons in the above-mentioned studies can be extended to a daily scale.

The simulation results for the daily air–water CO_2 fluxes cannot be directly compared with EC data because the data coverage of EC flux measurements is often low. For example, the data coverages for CO_2 flux were 27 % and 37 % in Erkkilä et al. (2018) and Mammarella et al. (2015), respectively. Quality screening excludes much of the measurement data, and short-time system malfunction may cause significant data loss during long study periods. Daily average or median EC CO_2 flux may not be representative for the whole day because of the temporal bias of the measurements. EC flux measurements often tend to be inapplicable especially at nighttime because of flux nonstationarity during light winds and cooling (Heiskanen et al., 2014) or advection of CO_2 from the surrounding forest (Erkkilä et al., 2018). EC CO_2 fluxes over boreal lakes are often enhanced at night by water-side convection (Podgrajsek et al., 2015) or because of a higher air–water CO_2 concentration gradient due to the absence of photosynthesis as a CO_2 sink (Erkkilä et al., 2018).

Both the calculated and the simulated values of k were determined by means of the platform data. They were thus suitable for comparison with each other but, however, may not represent the average conditions over the lake and hence may not yield correct estimates of whole-lake CO_2 fluxes. Wind speed, u_{*a}, Q_H, and Q_L were measured at a single point on the platform, and the source area of the EC measurements of u_{*a}, Q_H, and Q_L ranges from 100 to 300 m along the wind direction over the lake (Mammarella et al., 2015). Thus, the values may not be representative for the whole lake. Wind speed and the resulting u_{*a} over lakes surrounded by forests are lower in sheltered near-shore areas than in the central zones of the lakes (Markfort et al., 2010). Sheltering affects the spatial variation of wind speed especially in small lakes, such as Lake Kuivajärvi. Because Q_H and Q_L are dependent on wind speed over the lake, they may also be higher at the center of the lake than in near-shore areas. Also, the estimation of u_{*a}, Q_H, and Q_L in the simulations was based on wind speed and other forcing data obtained from the

single-point measurements, and the simulated values may have been overestimates of the spatial averages. However, despite the same measurement location, some disparities existed between the simulated and measured Q_H and Q_L. The differences may be in part attributed to an underestimation of surface heat fluxes by the EC method, which was seen, for example, in a study on energy balance over a small boreal lake by Nordbo et al. (2011) and also in Mammarella et al. (2015). The sum of the measured EC heat fluxes in Lake Kuivajärvi was on average 83 % and 79 % of available energy in 2010 and 2011, respectively, in Mammarella et al. (2015). In addition, the total relative random error of the EC measurements is generally around 10 % for both sensible heat flux and latent heat flux as estimated in Mammarella et al. (2015). Considerable spatial variability may also occur in near-surface water CO_2 concentration in small, shallow boreal lakes (Natchimuthu et al., 2017), which may result in further discrepancies in the estimates on whole-lake CO_2 flux obtained on the basis of gas exchange models or by using a vertical, horizontally integrated lake model.

4.3 Factors influencing the epilimnetic CO_2 budget

The model parameter sets obtained through calibration of the MyLake C applications using different incorporated gas exchange models were notably different from each other, thus emphasizing different processes related to carbon cycling within the water column or to carbon exchange with the surrounding terrestrial ecosystem or the atmosphere. However, considering the main objective of the study, the simulation of near-surface CO_2 concentration and air–water CO_2 flux, the different outcomes of the calibration processes can be considered equally applicable as they give insight on the diversity of biogeochemical processes that impact lacustrine CO_2 dynamics.

Phytoplankton is an significant factor in the lake CO_2 budget and the main driver of the diurnal variation of CO_2 concentration in Lake Kuivajärvi (Provenzale et al., 2018). In MyLake C, inorganic carbon is fixed by phytoplankton and carbon is stored in autochthonous organic matter within the water column or in bottom sediments until it is mineralized by bacteria. A relatively large portion of epilimnetic phytoplankton and dead autochthonous particulate organic matter sank from the epilimnion into deeper layers in MI because of the small values of m and $k_{POC,1}$. Production of CO_2 via degradation of phytoplankton-originated organic matter, as well as the release of bioavailable phosphorus in the epilimnion through mineralization of autochthonous organic matter, was also slow in MI because of a small $k_{DOC,1}$. As a result, the net production of CO_2 in the epilimnion was rather low in MI (Table 4) despite the relatively high simulated phytoplankton biomass. Overall, differences in total net CO_2 consumption by phytoplankton during the stratified period between GEMs were rather small despite the large variation in the simulated phytoplankton biomasses because of the phosphorus limitation of photosynthesis in GEMs with a high phytoplankton biomass and because of the variation in the length of the active growing season between GEMs.

The simulated Chl a concentrations were rather constant over the growing season with the exceptions of the substantial spring growth peaks in CC and TE. No data exist on Chl a concentration in Lake Kuivajärvi in 2013, but the Chl a concentration at 0–3 m was at its highest, 30–50 $mg\ m^{-3}$, in mid-July and decreased to a level of less than 2 $mg\ m^{-3}$ in late autumn in years 2011–2012 (Heiskanen et al., 2015). The epilimnetic Chl a concentration is usually 3–5 $mg\ m^{-3}$ during the growing season with diatom-induced peaks under cool conditions in spring and autumn (Provenzale et al., 2018). Thus, the GEMs with low near-surface Chl a concentrations, CC and TE, may have yielded better estimates of the overall phytoplankton biomass than

HE and MI. The net consumption of CO_2 by phytoplankton was, however, not only related to the amount of phytoplankton biomass. Nevertheless, none of the GEMs captured the supposed monthly variation of epilimnetic CO_2 concentration caused by the seasonal succession of phytoplankton.

A conspicuously high $C_{DI,IN}$ was needed to balance the high CO_2 efflux in the GEMs with a high k (Table 2). The restriction
of the scaling of the inflow DIC concentration to the open water season was a rough way to increase the gain of epilimnetic CO_2, and the summertime inflow CO_2 concentrations may have been unnaturally high especially in TE. However, the use of $C_{DI,IN}$ can be thought as the inclusion of the input of CO_2 through groundwater seepage to the lake. In budget calculations, groundwater DIC load can be generally estimated by applying groundwater DIC flow as a percentage of stream DIC load (Chmiel et al., 2016). The amount of inflowing groundwater and its properties in Lake Kuivajärvi are unknown. However, in
addition to inflow through minor inlet streams and surface runoff especially during snowmelt in spring, groundwater seepage may contribute somewhat to the total lake inflow volume because the measured total outflow volume over the year 2013 was approximately double the inflowing volume via the main inlet stream. The CO_2 concentration in groundwater in southern Finland is around 700–900 $\mathrm{mmol\ m^{-3}}$ (Lahermo et al., 1990), which is about tenfold higher than the estimated average inflow CO_2 concentration in Lake Kuivajärvi over the stratified period in 2013, 86 $\mathrm{mmol\ m^{-3}}$, and well in line with the yearly average
of groundwater CO_2 concentration near a boreal stream determined by Leith et al. (2015). Thus, also groundwater-derived CO_2 transport to the lake may affect the water column CO_2 concentration.

The effect of CO_2 inputs through minor inlets or groundwater may be supported by the fact that the simulated near-surface CO_2 concentration decreased too fast in all GEMs after ice-off in May 2013, that is, during a period when the snowmelt-induced flow in minor inlet streams may be substantial and when groundwater level is generally relatively high (Fig. 4). The simulated
epilimnetic CO_2 sinks were rather small at that time because net CO_2 consumption by phytoplankton was low in cool water and because CO_2 efflux was relatively low because of a low air–water CO_2 concentration gradient. Labile, autochthonous DOC was absent in the epilimnion in the simulations, and the degradation of allochthonous DOC was slow under the relatively cold conditions in May. Despite the measured inflow CO_2 concentration being approximately twice the simulated epilimnetic CO_2 concentration and the scaled inflow CO_2 concentrations and terrestrial CO_2 loads being even higher, the decline of epilimnetic
CO_2 concentration was rapid in all GEMs. The high abundance of diatoms in Lake Kuivajärvi in spring may have resulted in a supply of easily degradable organic matter, but net primary production also consumed CO_2. Thus, substantial CO_2 loadings through surface runoff, minor inlet streams, or groundwater seepage could have been plausible additional sources of epilimnetic CO_2 in May, provided that the additional surface inflow was rich in CO_2. The impact of groundwater seepage is supported by a study on the carbon budget of a small boreal lake by Chmiel et al. (2016), in which the discrepancy between the estimates of
gain and loss of inorganic carbon was explained by a possible underestimation of the impact of groundwater inflow.

4.4 Implications for lake modeling

None of the four MyLake C versions with different gas exchange models surpassed the other ones in the study because of the complex interplay between the near-surface water CO_2 concentration and air-water CO_2 flux in the simulations. A higher CO_2 efflux would have required a higher gain of CO_2 in the lake through in-lake CO_2 production or external loading of

inorganic carbon, but the MyLake C versions with gas exchange models yielding a high k were not capable of increasing the CO_2 gain sufficiently. Hence, it is not a trivial task to judge which of the four gas exchange models is most suitable for integration into MyLake C or other coupled physical-biogeochemical lake models. However, several experimental studies (e.g., Jonsson et al., 2008; MacIntyre et al., 2010; Heiskanen et al., 2014) have shown that traditional, wind-based models often

5   yield low CO_2 fluxes when compared to estimates based on direct measurements. Thus, it is recommended to strive to use the more sophisticated and probably more correct gas exchange models provided that the biogeochemical lake model can be made adaptable to higher CO_2 losses and that the parameters included in the more complex, turbulence-based models can be correctly simulated. This also means that further improvements related to the description of in-lake carbon processes in lake models and to the modeling or other means of estimation of external inorganic and organic carbon loading are still needed. Despite the

10   challenges in using complex process-based models in the assessment of carbon cycling in lakes, modeling is an effective means to quantify underlying processes related to lacustrine CO_2 emissions and to study the development of lake ecosystems under changing conditions.

5   Conclusions

We studied the applicability of four gas exchange models with different complexity incorporated into a vertical physicobiogeo-

15   chemical lake model MyLake C to the simulation of air–water CO_2 exchange and water column CO_2 concentration in a humic boreal lake. The gas transfer velocities simulated using the simplest, wind-based gas exchange model by Cole and Caraco (1998), or CC, were best in accordance with the corresponding values calculated on the basis of direct in-lake measurements, whereas simulations with the other gas exchange models either overestimated (the models by Heiskanen et al. (2014) and MacIntyre et al. (2010)) or underestimated (the model by Tedford et al. (2014)) the respective calculated gas transfer velocities

20   because of discrepancies in the simulation of wind stress or daily effective surface heat flux.

None of the applied gas exchange models resulted in a highly improved simulation performance regarding water column CO_2 concentration or air–water CO_2 flux. On the contrary, the more complex gas exchange models, which include both wind-induced stress and heat-induced convection as the drivers of CO_2 exchange, yielded higher gas transfer velocities and thus higher CO_2 fluxes in the simulations, which resulted in difficulties in obtaining sufficient gain of CO_2 in the water column to

25   balance the loss to the atmosphere. In addition, the model with a daily time step was not always able to simulate the changes in near-surface CO_2 concentration and air–water CO_2 flux resulting from short-term physical processes, such as nighttime cooling or simultaneous surface heating and wind mixing. As a result, all the incorporated gas exchange models except for CC yielded notably too low summertime epilimnetic CO_2 concentrations in the simulations, which was also reflected by a significant underestimation of CO_2 fluxes compared to the corresponding fluxes calculated from the calculated gas transfer

30   velocities and measured air–water CO_2 concentration gradients. The daily CO_2 fluxes simulated with CC were closest to the corresponding calculated fluxes. The long and widely used CC was, however, shown to produce too low CO_2 flux estimates and its use was discouraged in an empirical gas exchange model intercomparison study by Erkkilä et al. (2018), whereas the more complex models yielded presumably more correct CO_2 fluxes. Nevertheless, it has to be noted that the comparison between

the gas exchange models is more complex in our modeling study than in Erkkilä et al. (2018) because of the interplay between the simulated CO_2 flux and water column CO_2 concentration.

The present model application was not highly adaptable to increased CO_2 effluxes. The extent of in-lake production of CO_2 is largely related to model structure, process descriptions, and the estimation of parameter values, whereas the amount of external CO_2 inputs ~~are~~ is governed by the quality of hydrological forcing data. ~~Thus, both further lake model development and improved estimates of external loading are~~ Therefore, research on processes contributing to carbon cycling in boreal freshwaters and on the roles of different internal and external sources of CO_2, such as groundwater, in lakes is sorely needed in order to enhance the predictive performance of model simulations. ~~However, despite the challenges in using complex process-based models in the assessment of carbon cycling in lakes, modeling is an effective means to quantify underlying processes related to lacustrine emissions and to study the development of lake ecosystems under changing conditions.~~

The issues raised in our study concerning lacustrine carbon budgets can also be generalized to a larger scale. ~~If the~~ The application of advanced gas exchange models ~~results in higher~~ has been shown to lead to increased estimates of CO_2 emissions from boreal inland waters~~, a higher~~. Thus, higher estimates of net terrestrial ecosystem production and ~~an increased~~ carbon flux from land to inland waters ~~is~~ are required to close the regional carbon budget. ~~Therefore, research on processes contributing to carbon cycling in boreal freshwaters and on the roles of different internal and external sources of , such as groundwater, in lakes is sorely needed~~ Also, the use of advanced, possibly more correct gas exchange models in the assessment of global gas efflux from freshwaters may result in higher estimates of the impact of freshwater ecosystems on global carbon cycling.

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Table 1. Parameters used in the parameterizations of the gas transfer velocity in the gas exchange models by Cole and Caraco (1998), Heiskanen et al. (2014), MacIntyre et al. (2010), and Tedford et al. (2014)).

Gas exchange model	Parameter	Unit
Cole and Caraco (1998)	Wind speed at 10 m (U_{10})	$\mathrm{m\ s^{-1}}$
Heiskanen et al. (2014)	Wind-induced water friction velocity ($u_{*\mathrm{ref}}$)	$\mathrm{m\ s^{-1}}$
	Penetrative convection velocity (w_*)	$\mathrm{m\ s^{-1}}$
MacIntyre et al. (2010)	Wind speed at 10 m (U_{10})	$\mathrm{m\ s^{-1}}$
	Buoyancy flux (β)	$\mathrm{m^2\ s^{-3}}$
Tedford et al. (2014)	Total turbulent kinetic energy dissipation rate (ε)	$\mathrm{m^2\ s^{-3}}$

Table 2. Calibrated model parameters for the different versions of MyLake C application to Lake Kuivajärvi with different incorporated gas exchange models (HE: Heiskanen et al. (2014), CC: Cole and Caraco (1998), MI: MacIntyre et al. (2010), TE: Tedford et al. (2014)). The default parameter values were used as the means of the prior parameter distributions.

|	Default	HE	CC	MI	TE	Unit
a_k	3.92	0.27	0.45	0.39	1.18	$\times 10^{-3}$
β_DOC	2.85	2.94	3.47	3.22	2.75	$\times 10^{-5}\ \mathrm{m^2\ mg^{-2}}$
$C_\mathrm{DI,IN}$	1.00	1.86	1.55	1.91	3.05	-
$k_\mathrm{DOC,1}$	0.80	5.71	1.11	0.46	9.01	$\times 10^{-1}\ \mathrm{d^{-1}}$
$k_\mathrm{DOC,2}$	1.01	1.40	2.41	3.35	1.07	$\times 10^{-2}\ \mathrm{d^{-1}}$
$k_\mathrm{POC,1}$	0.94	4.54	0.91	1.78	0.60	$\times 10^{-1}\ \mathrm{d^{-1}}$
$k_\mathrm{POC,2}$	0.90	2.91	5.01	15.9	4.49	$\times 10^{-2}\ \mathrm{d^{-1}}$
$k_\mathrm{POC,sed}$	2.53	4.11	2.43	2.84	3.72	$\times 10^{-4}\ \mathrm{d^{-1}}$
m_{20}	0.21	0.11	0.24	0.090	0.31	$\mathrm{d^{-1}}$
μ'_{20}	2.37	2.96	5.95	1.62	3.84	$\mathrm{d^{-1}}$
W_str	0.29	0.33	0.35	0.35	0.24	-

Table 3. Total and monthly averages of simulated and calculated CO_2 fluxes (µmol m^{-2} s^{-1}) in May–October 2013 obtained with different gas exchange models. Only the days with available measurement data are included in the averaging of the simulated fluxes. Monthly values for June are excluded because measurement data were available only for 7 days.

|	May–October		May		July	
	Calc.	Sim.	Calc.	Sim.	Calc.	Sim.
Heiskanen	0.38	0.31	0.79	0.41	0.37	0.34
Cole & Caraco	0.23	0.24	0.53	0.33	0.20	0.26
MacIntyre	0.45	0.29	0.97	0.52	0.44	0.26
Tedford	0.71	0.30	1.90	0.43	0.56	0.33
	August		September		October	
	Calc.	Sim.	Calc.	Sim.	Calc.	Sim.
Heiskanen	0.27	0.30	0.31	0.35	0.24	0.16
Cole	0.15	0.22	0.16	0.27	0.13	0.17
MacIntyre	0.33	0.22	0.35	0.32	0.25	0.16
Tedford	0.41	0.26	0.45	0.34	0.43	0.17

Table 4. Simulated CO_2 budgets (kg CO_2) for the epilimnion of Lake Kuivajärvi during summer stratification in 2013 and 2014 using different gas exchange models incorporated into MyLake C.

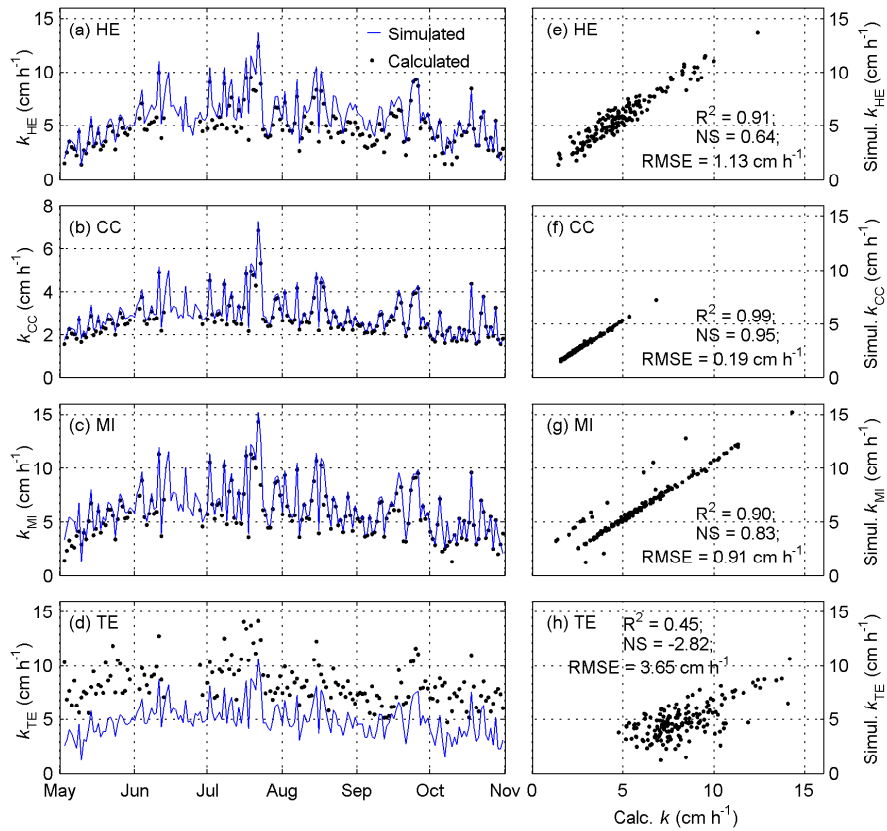|	Heiskanen	Cole & Caraco	MacIntyre	Tedford
2013				
Net production	52300	38700	40400	44800
Change due to efflux[a]	−89900	−72300	−74500	−89200
Net external loading	10800	8600	11000	18500
Change due to epilimnion deepening	16100	15100	15800	18800
Change in epilimnetic storage	−10700	−9900	−7200	−7100
Duration (d)	134	134	134	134
2014				
Net production	38300	24900	25400	28700
Change due to efflux[a]	−63600	−42700	−46600	−57100
Net external loading	8300	6300	8100	12200
Change due to epilimnion deepening	17500	13100	14100	17400
Change in epilimnetic storage	500	1600	1000	1200
Duration (d)	107	101	101	101

[a] The change in water column CO_2 content due to CO_2 efflux was approximately 1 % lower than the amount of CO_2 evaded because of consequent equilibrium reactions in the carbonate system.
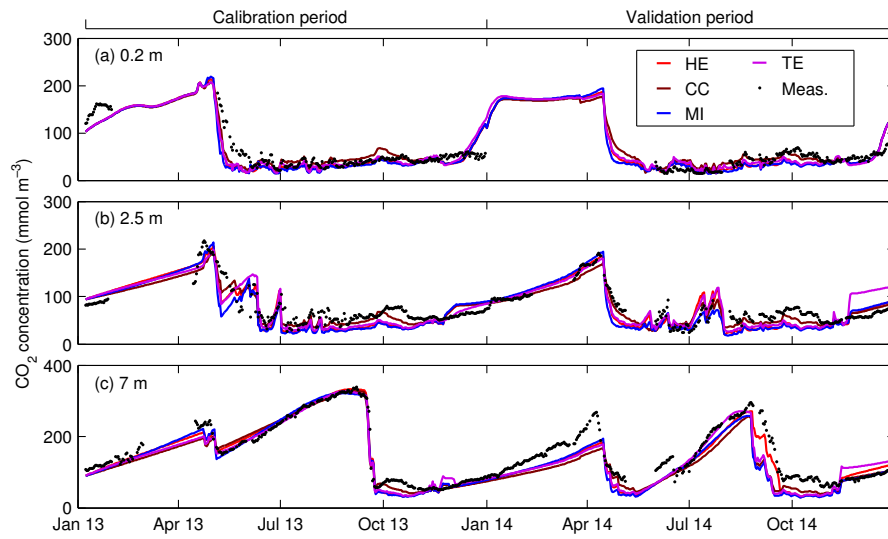
Figure 1. Simulation results for CO_2 concentration with each GEM (mmol m^{-3}) versus the daily averages of automatic high-frequency CO_2 concentration measurements at the depths of (a) 0.2 m, (b) 2.5 m, and (c) 7.0 m in Lake Kuivajärvi during the calibration year 2013 and the validation year 2014.
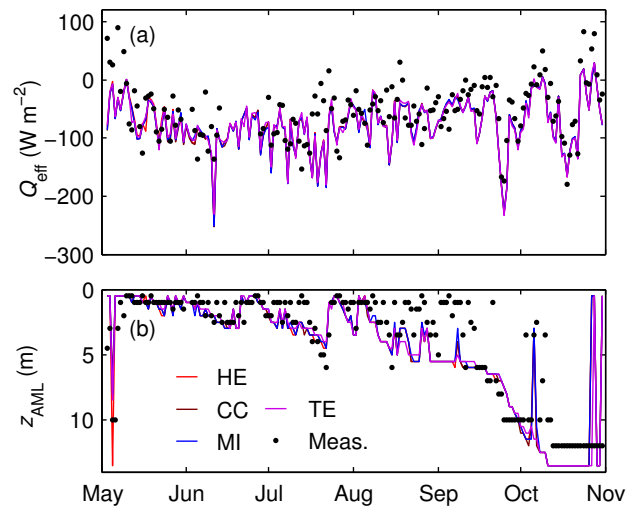
Figure 2. (a) Daily effective surface heat fluxes (W m^{-2}) simulated with each GEM and calculated on the basis of heat flux measurements and (b) simulated and empirically determined depths of the daily actively mixing layer (m) in Lake Kuivajärvi in May–October 2013.
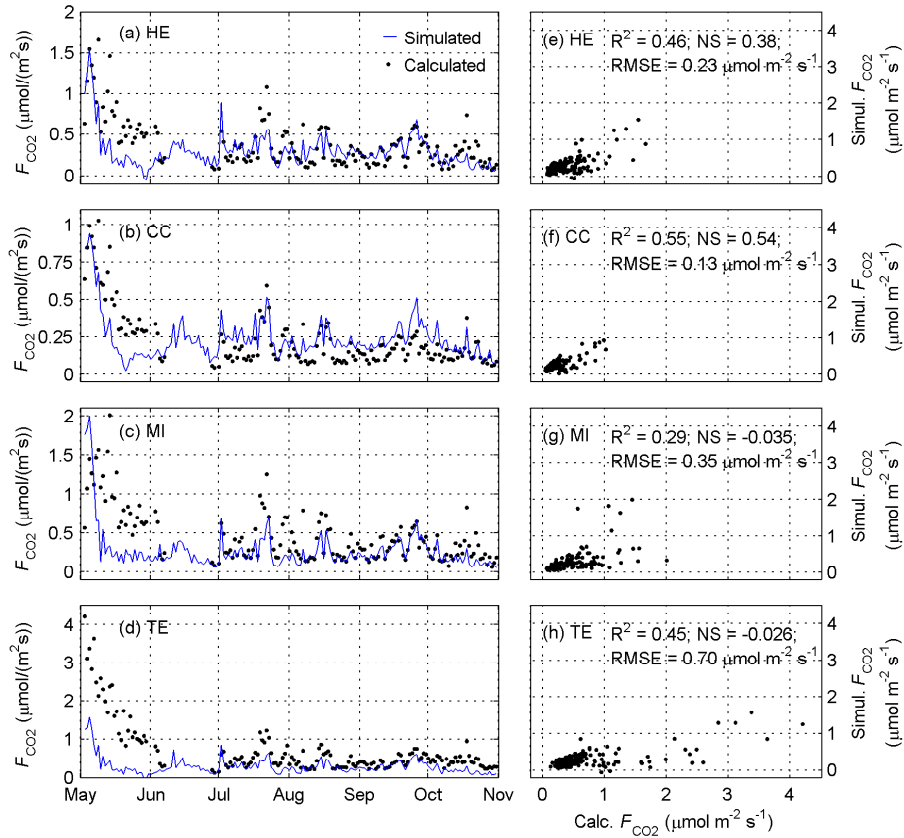
Figure 3. Simulated and calculated gas transfer velocities for CO_2 (cm h^{-1}) in Lake Kuivajärvi on 3 May–31 October 2013 obtained with the gas exchange models by (a, e) Heiskanen et al. (2014), (b, f) Cole and Caraco (1998), (c, g) MacIntyre et al. (2010), and (d, h) Tedford et al. (2014).
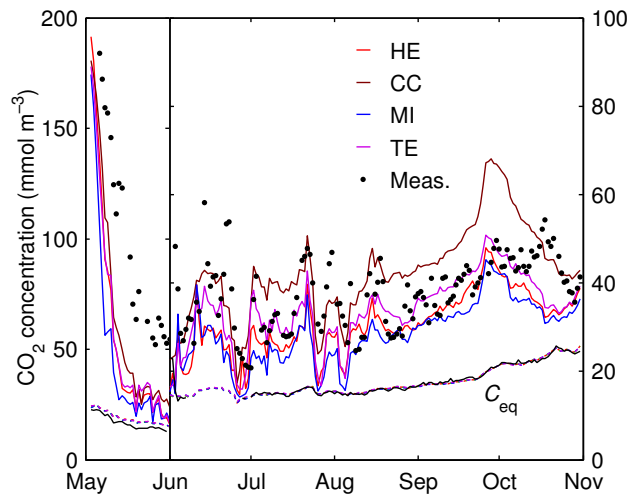
Figure 4. Simulated CO_2 concentrations ($mmol\ m^{-3}$) in the surface layer (0–0.5 m) obtained with each GEM and the daily averages of the automatic measurements at 0.2 m in Lake Kuivajärvi in May–October 2013. Also shown are the atmospheric equilibrium concentrations of CO_2 (C_{eq}) obtained from the simulations (dotted colored lines) and calculated from the measured atmospheric CO_2 concentration and surface water temperature (solid black line). Note the different vertical scales in May and in June–October.

Figure 5. Simulated and calculated air–water CO_2 fluxes (μmol m^{-2} s^{-1}) in Lake Kuivajärvi on 3 May–31 October 2013 obtained with the gas exchange models by (a, e) Heiskanen et al. (2014), (b, f) Cole and Caraco (1998), (c, g) MacIntyre et al. (2010), and (d, h) Tedford et al. (2014).
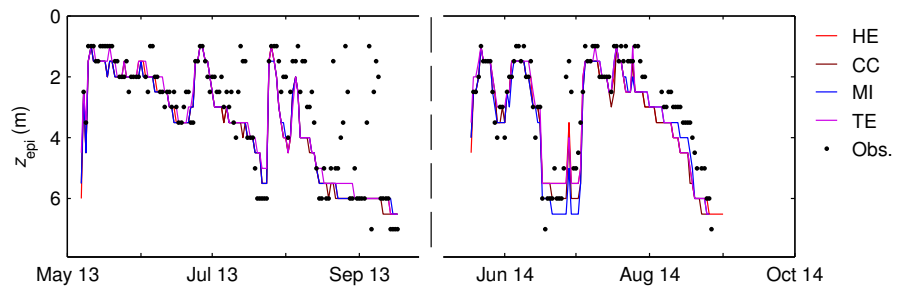
Figure 6. Simulated and observed depths of the epilimnion (m) in Lake Kuivajärvi during the continuous summer stratification in 2013 and 2014. The simulations were performed using each of the gas exchange models incorporated into MyLake C.