



## RESEARCH ARTICLE

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# Linking Biogeochemical and Hydrodynamic Processes to Model Methane Fluxes in Shallow, Tropical Floodplain Lakes

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**Key Points:**

- Methane fluxes from Amazon floodplains lakes simulated with biogeochemical model combined with hydrodynamic model
- Seasonal patterns and magnitudes of simulated and measured fluxes are generally in good agreement
- Methane concentrations and diffusive emissions are sensitive to carbon mineralization and methane production and oxidation

**Supporting Information:**

Supporting Information may be found in the online version of this article.

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**Abstract** Floodplains lakes are abundant in the Amazon basin and are important methane sources to the atmosphere. Existing biogeochemical models require modifications and inclusion of hydrodynamic processes operative in shallow, warm waters to be applied to these aquatic ecosystems. We modified a 1-dimensional process-based, lake biogeochemical model and combined a 3-dimensional hydrodynamic model to suit Amazon floodplains. We evaluated the combined model's performance simulating methane concentrations and fluxes and several related processes in the open lake and an embayment of a well-studied Amazon lake. Parameters for calibration were selected through sensitivity tests using a machine learning-based algorithm, classification, and regression trees. Comparison between simulated and measured fluxes indicate generally good agreement in seasonal patterns and magnitudes. Comparisons of near-surface concentrations varied with no clear patterns. Simulations of methane concentrations at near-surface and near-bottom, and diffusive emissions are most sensitive to carbon mineralization rate,  $Q_{10}$  factors for methanogenesis and oxidation, and methane oxidation potential. Modeled rates of planktonic photosynthesis were generally lower than measurements, though simulated planktonic respiration was often similar to measurements. Simulated rates of methane oxidation were considerably lower, with a few exceptions, than measurements of methane oxidation in oxic water of the lake. Improvements of results of the linked hydrodynamic-biogeochemical model will result from inclusion of advective transport, use of parameter values appropriate for tropical waters, especially for methane oxidation and photosynthesis, and addition of changes in hydrostatic pressure to model of ebullition.

**Plain Language Summary** Methane emissions from lakes are large, highly variable and without adequate measurements, especially in tropical regions. The combination of mechanistic models with results from intensive field data provides one way to improve understanding of the processes and sources of variability. Riverine floodplain lakes, as occur in the Amazon basin, constitute extensive aquatic ecosystems and are important methane sources to the atmosphere. Though tropical lakes typically experience muted seasonal variations in climate, strong diel changes occur, and floodplain lakes have additional biogeochemical and ecological variability caused by changes in water level, connectivity to rivers and optical properties. We modified a one-dimensional process-based, lake biogeochemical model and combined a 3-dimensional hydrodynamic model to be applicable to Amazon floodplains and similar shallow, warm waters. The combined model simulated well methane processes and fluxes based on evaluation using observations in a representative central Amazon floodplain lake with measurements of meteorological variables, water temperatures and ecological conditions, and methane emissions over the seasonal hydrological phases with large differences in water levels.

## 1. Introduction

Estimates of methane emissions from lakes are large with high temporal and spatial variability (Rosentreter et al., 2021). The considerable differences among lakes throughout the globe and a paucity of adequate measurements, especially in tropical regions, lead to uncertainty in empirical estimates and in validation of models of methane fluxes. Key processes producing and consuming methane and factors controlling emissions are known, and have been examined in laboratory and field experiments and through statistical analyses (e.g., Bridgman et al., 2013; DelSontro et al., 2016; Harrison et al., 2021; Knox et al., 2021; Segers, 1998). However, interactions

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among the processes under the wide range of ecological conditions in lakes are not sufficiently understood. The combination of mechanistic models with results from intensive field data provides one way to improve understanding of the processes and sources of variability.

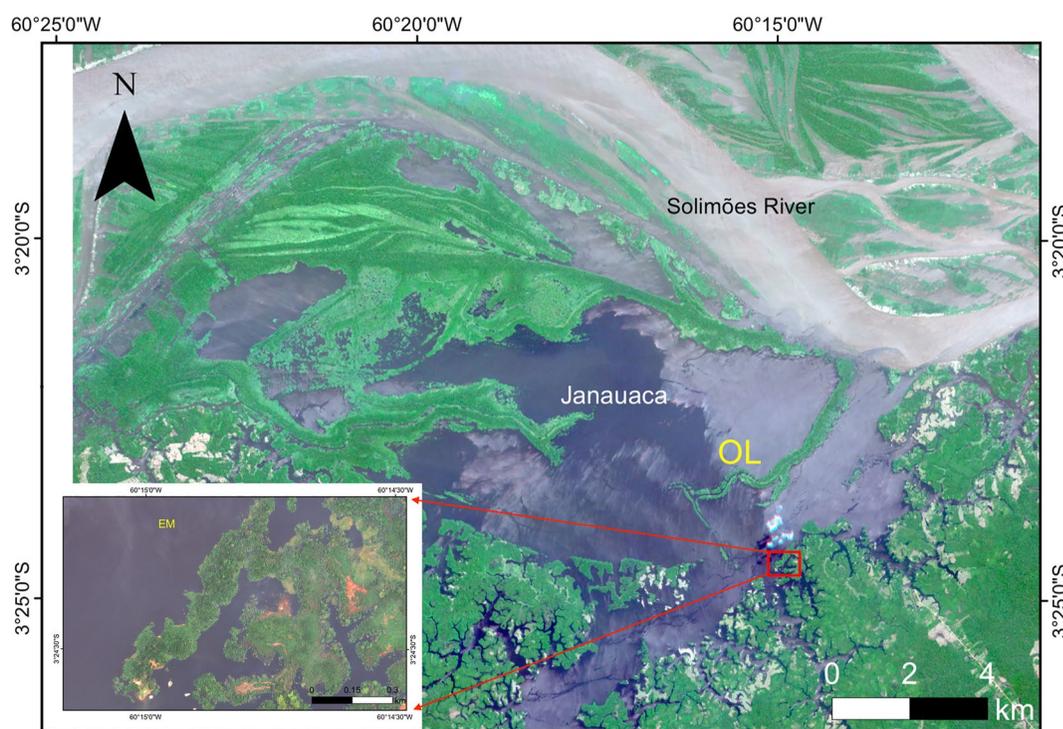
Lakes and associated wetlands cover extensive areas in northern latitudes and in tropical regions (Melton et al., 2013; Messenger et al., 2016; Pekel et al., 2016) and represent major sources of methane to the atmosphere (Kirschke et al., 2013; Peng et al., 2022; Rosentreter et al., 2021; Saunois et al., 2020). Riverine floodplains constitute extensive aquatic ecosystems in the tropics and are characterized by seasonal floods that promote the exchange of nutrients and organisms among habitats and substantial primary production (Junk, 1997). For example, floodplains, lakes, and other wetlands cover approximately 1 million km<sup>2</sup> of the Amazon basin (Hess et al., 2015; Sippel et al., 1991). Due to the large area and abundant carbon supplies, these aquatic habitats are important methane sources to the atmosphere (Barbosa et al., 2020; Basso et al., 2021; Beck et al., 2012; Melack et al., 2004; Pangala et al., 2017). However, large uncertainties persist in estimates of tropical CH<sub>4</sub> emission, largely due to the few studies at appropriate temporal and spatial scales. Most field measurements in the Amazon basin and elsewhere in the tropics do not sufficiently capture diel and seasonal variations and often include diffusive, but not ebullitive, methane fluxes.

While temperate and arctic lakes undergo strong seasonal variations in solar radiation and temperature, tropical lakes typically have muted seasonal variations in climate but undergo diel cycles of stratification and mixing (MacIntyre & Melack, 2009; Talling & Lemoalle, 1998). Floodplain lakes have additional biogeochemical and ecological variability caused by changes in water level, connectivity to rivers and optical properties (Melack et al., 2009, 2021). Despite the importance of floodplains with shallow lakes and variable water levels, existing biogeochemical models of methane fluxes are not designed for these environments.

Most current biogeochemical ecosystem models of methane emissions are focused on wetlands, not lakes, and do not include most mechanisms influencing methane emissions (e.g., Bloom et al., 2017; Nzotungicimpaye et al., 2021; Ringeval et al., 2014). Potter et al. (2014) proposed a model for Amazon floodplains based on the supply of organic carbon as a key factor determining methane production. The model requires estimates of carbon inputs, uses simple statistical relations for physical processes, and was evaluated at one lake. The LAKE model (Stepanenko et al., 2016) includes most key processes, but the methane module has only been tested in a small boreal lake, and several physical processes use formulations not well suited to shallow tropical waters.

The Arctic Lake Biogeochemical Model (ALBM) is a one-dimensional (1-D) process-based, biogeochemical model that simulates the thermal and carbon dynamics of lakes (Tan et al., 2015, 2017). The model has been applied to arctic and boreal lakes on seasonal time scales (Guo et al., 2020; Tan et al., 2015), but the thermal module and several other aspects are not appropriate for conditions in shallow, warm waters. In particular, the daily cycles of stratification and mixing and intense, near-surface stratification, that can enhance gas exchange, are not modeled by ALBM. Shallow, warm lakes often develop strong gradients and large variations in dissolved oxygen, that influence methane production and oxidation, and modeling these conditions over diel cycles is required.

In this study, we modified ALBM and combined it with a 3-dimensional (3-D) hydrodynamic model (AEM3D) suited to tropical floodplain lakes and similar shallow, warm waters. The combined model performances in simulating methane processes and fluxes were evaluated in a representative central Amazon floodplain lake with observations of meteorological variables, water temperatures and limnological conditions, and methane diffusive and ebullitive emissions over the seasonal hydrological phases with large differences in water levels (Barbosa et al., 2020, 2021). Our aim is to build a biogeochemical model that reasonably represents individual processes in Amazon floodplain lakes, and other shallow warm waters, and provides methane fluxes at multiple time scales. To do so, we incorporated algorithms for methane and dissolved oxygen production and consumption and selected and calibrated rate functions and coefficients appropriate for ecological conditions in shallow warm-water lakes. To include physical processes that generate diel variations in mixing we used outputs from a 3-D hydrodynamic model and added improved mechanistic understanding of gas exchange.



**Figure 1.** Janauacá floodplain on southern side of Solimões River in central Amazon basin. OL marks approximate location of sampling site in open water of lake. Red box marks location of embayment with an enlarged image of the embayment (EM) shown in the insert. Planet Scope Rapid-eye image acquired on 15 August 2015 with spatial resolution of 6.5 m resampled to a 5-m grid. Insert is an Apollo WorldView-2 image acquired on 14 August 2014 with 0.7 m resolution.

## 2. Methods

### 2.1. Study Sites and Measurements

Lake Janauacá is a large floodplain lake in the central Amazon basin connected to the Solimões River (3.38°S, 60.25°W; Figure 1). The lake and associated environments represent ecological and hydrological conditions on central Amazon floodplains, as summarized in Melack et al. (2009) and Melack (2016), and therefore, serves well as a site at which to develop and test a methane model. Measurements were made in the main lake and an embayment from August 2014 to September 2016; a subset of these data were used to develop, calibrate and evaluate the model (Table 1, Figure 2). The lake is fringed by flooded forests and floating herbaceous plants during a portion of the year. The wide range of water depths, surface areas and light attenuation and two sites, though typical of floodplain lakes, could be considered examples of different types of lakes.

The seasonal range of chlorophyll-a (Chla) (2.8–50.5  $\mu\text{g L}^{-1}$ ), total phosphorus (1.9–3.8  $\mu\text{mol L}^{-1}$ ) and total nitrogen (21–108  $\mu\text{mol L}^{-1}$ ) in Lake Janauacá indicate mesotrophic conditions during high water and eutrophic conditions during low and rising water (Melack et al., 2021). Dissolved organic carbon is moderately high (2.5–6.6  $\text{mg L}^{-1}$ ), and total suspended solids varied seasonally from up to 115  $\text{mg L}^{-1}$  during low and rising water to 2.4  $\text{mg L}^{-1}$  during high water (Melack et al., 2021).

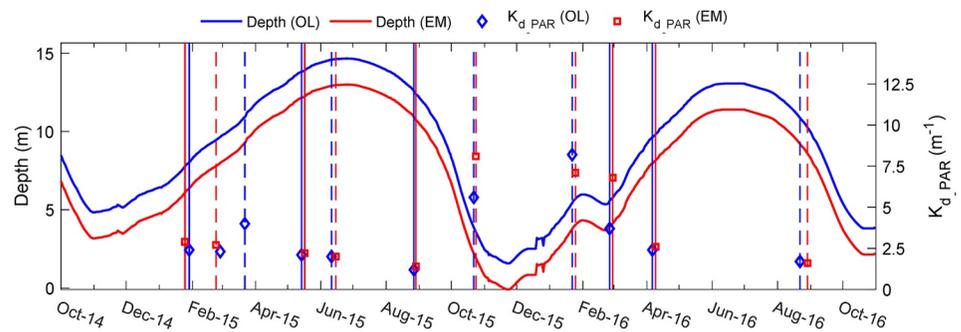
During each field campaign, environmental variables were measured at each site and fringing habitats over 24-hr periods (Barbosa et al., 2020). Water temperatures and dissolved oxygen (DO) concentrations were manually measured every 0.5 m using temperature and oxygen probes and using thermistors and optical DO sensors deployed on moorings at multiple depths. Diffusive methane fluxes were measured with floating chambers and repeated at least three times a day in all habitats. Ebullitive fluxes were obtained using bubble traps. Concentrations of Chla were determined spectrophotometrically using filtered water samples. Detailed methods are described in Barbosa et al. (2020, 2021).

Water levels were recorded daily at stage gauges; a digital elevation model of bathymetry is based on Pinel et al. (2015). Shielded air temperature and relative humidity, solar radiation, wind speed and wind direction,

**Table 1**  
*Site, Measurement Date, Surface Area (km<sup>2</sup>), Maximum Depth (m), and Hydrological Phase: Rising Water, RW; High Water, HW; Falling Water, FW; Low Water, LW*

Calibration		Embayment													
Site		Main lake													
Year	2015	2015	2015	2015	2015	2015	2015	2015	2015	2015	2015	2015	2015	2016	2016
Month	Mar	Jun	Oct	Jan	Aug	Feb	Jun	Oct	Jan	Apr	Aug	Jan	May	Aug	Jan
Area	53.1	53.5	16.7	41.3	53.1	0.15	0.17	0.04	0.09	0.17	0.17	0.17	0.17	0.17	0.09
Depth	7.0	10.7	1.9	3.5	6.8	6.1	11.7	1.0	2.8	11.7	11.0	11.0	9.5	2.9	2.8
Phase	RW	HW	LW	RW	FW	RW	HW	LW	RW	HW	HW	HW	FW	RW	RW
Validation		Embayment													
Site		Main lake													
Year	2015	2015	2015	2015	2015	2015	2015	2015	2015	2015	2015	2015	2015	2015	2016
Month	Jan	May	Aug	Feb	Apr	Jan	May	Aug	Jan	Apr	Aug	Jan	May	Aug	Apr
Area	50.7	53.4	53.4	42.4	52.3	0.12	0.17	0.17	0.12	0.17	0.17	0.17	0.17	0.17	0.16
Depth	6.1	8.6	8.6	3.7	5.7	5.0	11.0	9.5	5.0	11.0	11.0	11.0	9.5	2.9	6.9
Phase	RW	HW	FW	RW	RW	RW	HW	FW	RW	HW	HW	HW	FW	RW	RW

*Note.* Calibration refers to periods used to calibrate the model. Validation refers to periods used to test the model; results for these periods are also referred to as uncalibrated values. Section 2.4 discusses calibration and validation procedures.



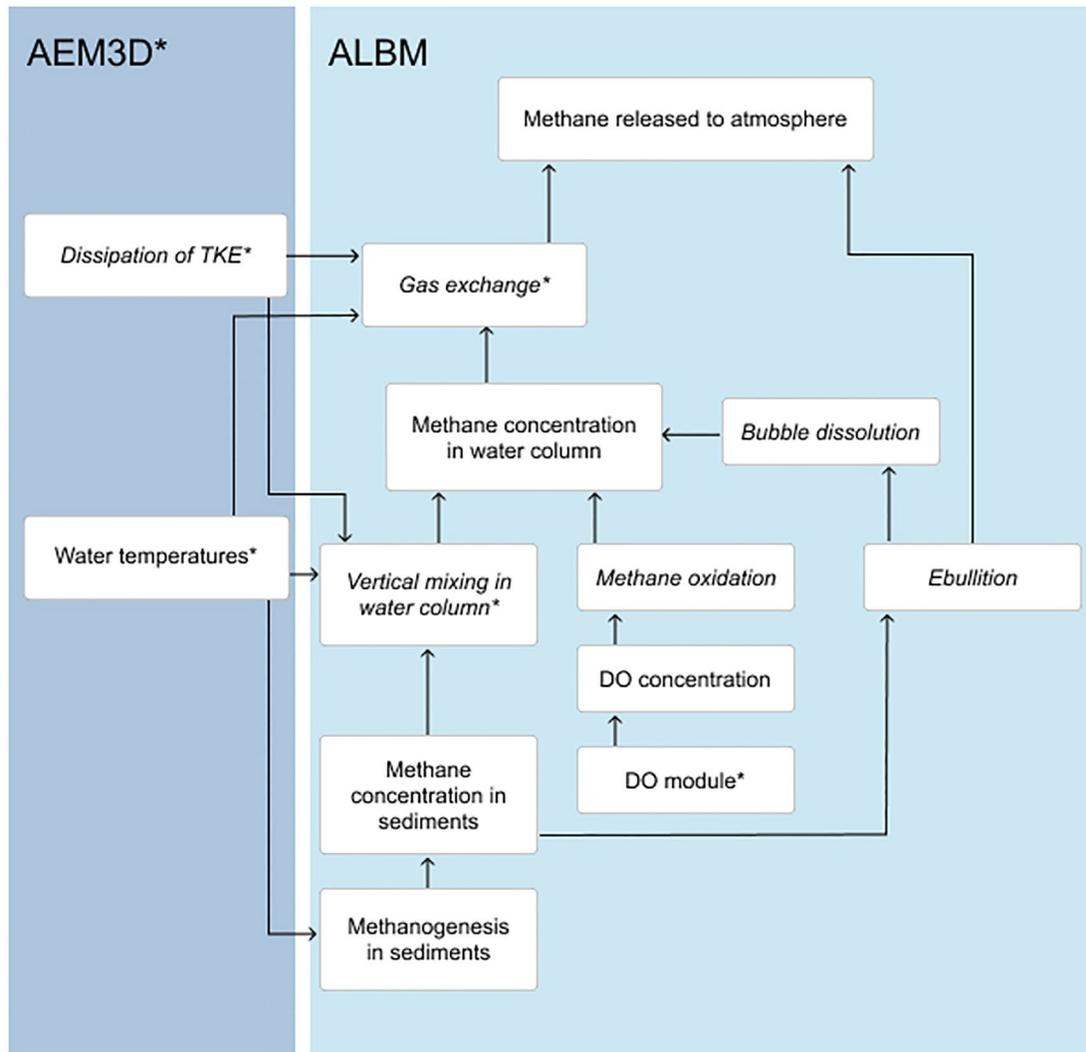
**Figure 2.** Maximum depths in main lake (OL, blue curve) and embayment (EM, red curve) from October 2014 to November 2016. Attenuation coefficient of PAR ( $K_{d\_PAR}$ ) in OL (blue diamonds) and EM (red squares). Blue and red dashed lines mark the periods when AEM3D and ALBM calibration simulations were done, and blue and red solid lines mark the periods of the validation simulations.

sampled per second and averaged to five-minute intervals, were measured near each site at a floating laboratory. Wind speed and direction sensors were also deployed at 2 m above the water surface at each open water site during field campaigns. Underwater light attenuation over the spectral range from 400 to 700 nm (photosynthetically available radiation, PAR) was measured with a submersible sensor; these data were used to calculate the attenuation coefficient ( $K_{d\_PAR}$ ).

## 2.2. Hydrodynamic Model

The hydrodynamic portion of the 3-D Aquatic Ecosystem Model (AEM3D; Hodges & Dallimore, 2019) was used to model thermal structure, mixing and turbulent energy dissipation. AEM3D is derived from the Estuary, Lake and Coastal Ocean Model (Hodges et al., 2000) and uses a z-coordinate Cartesian grid allowing non-uniform spacing in three directions and solves the unsteady Reynolds-averaged Navier-Stokes equation under the Boussinesq approximation. The model adopts a numerical scheme modified from TRIM-3D (Casulli & Cheng, 1992) and simulates temperature with the ULTIMATE-QUICKEST method for scalar transport (Leonard, 1991). Details about the AEM3D numerical schemes are provided by Hodges (2000). The model was run with a 30 s time-step, 100 m  $\times$  100 m  $\times$  0.1 m grid in the main lake and a 20 s time-step, 5 m  $\times$  5 m  $\times$  0.1 m grid in the embayment. It was configured with 150 and 130 Eulerian layers for the main lake and the embayment, respectively; the number of layers is the water depth divided by the vertical resolution and changes with water level. Initial conditions include temperature and salinity profiles. Initial temperature profiles were obtained from temperature measurements at the open water sites at mid-night when the water column was mixed or weakly stratified. Initial salinity profiles were estimated from specific conductivity data. Bulk transfer coefficients for heat and momentum were initialized with values for neutral atmospheric stability, which were updated at each time step taking into account the effects of non-neutral atmospheric stability. Bathymetric, meteorological and water level data, described in Section 2.1, are used as inputs to the model.

Vertical mixing is simulated using the mixed-layer model adopted from a 1-D hydrodynamic model (Imberger & Patterson, 1981; Spigel et al., 1986), in which the rate of turbulent kinetic energy (TKE) dissipated (denoted epsilon,  $\epsilon$ ) is computed as follows: (a) The model calculates the generation of TKE by wind at the surface, drag at bottom and shear in the interior of the water column. (b) The model calculates the energy required to completely mix two adjacent layers at each depth, if stable thermal structure is detected, or TKE generated by convection, if unstable thermal structure is detected. (c) The model conducts full mixing, partial mixing or no mixing depending on the amount of TKE generated compared to the amount of potential energy that needs to be overcome. (d) The amount of TKE to be dissipated is calculated as a function of the simulation timestep, layer thickness and TKE remaining after mixing is conducted, but limited to 100% of the TKE remaining. The TKE dissipation rate is then computed by dividing the amount of TKE dissipated by the simulation time step.



**Figure 3.** Processes and fluxes modeled in ALBM and supplied by AEM3D. Items marked with an asterisk are new features compared to the prior version of ALBM. Items in italics are rates or fluxes, and those not in italics are quantities. Refer to the Methods for equations and explanations of items shown.

### 2.3. Biogeochemical Model

We made several modifications to the Arctic Lake Biogeochemical Model (ALBM, Tan et al., 2015, 2017; Guo et al., 2020) to suit Amazon floodplain lakes (illustrated in Figure 3). The thermal module in ALBM was not used, and hydrodynamic inputs (water temperature and  $\epsilon$ ) were obtained from AEM3D. The Hostetler-based algorithm used in the original ALBM computes eddy diffusivity ( $K_z$ ) as a function of the latitudinal Ekman profile, 2-m wind speed, and the buoyancy frequency induced by the density gradient (Hostetler & Bartlein, 1990), and does not produce correct values in the shallow warm-waters of Amazon floodplain lakes. The Hostetler-based algorithm produces low  $K_z$  with high  $N$  values as it assumes that turbulent mixing is suppressed by stratification. This is not the case in shallow tropical waters where the buoyancy frequency in upper water column during diurnal stratification can reach up to 120 cycles per hour (indicating strong stratification), while active mixing is observed (MacIntyre et al., 2021). In contrast, at deeper depths Hostetler-based algorithm-based eddy diffusivities are too large, mixing dissolved gas too fast, and do not match observations.

The modified ALBM uses vertical profiles of water temperatures provided by AEM3D at five-minute time steps. The water column in AEM3D is gridded with 0.1-m intervals, and ALBM is discretized vertically with the same intervals. The mixing depth is assumed to be the depth at which the water temperature is 0.05°C lower than the temperature at 0.05 m. We used  $\epsilon$  and thermal structure modeled by AEM3D to estimate vertical mixing,  $K_z$ , and

**Table 2**  
Values, Units, and Sources of Parameters in the Formulations of Methane and Oxygen Processes

Fixed-valued parameters			
Parameter symbol	Value	Unit	Source
$K_m$	$1.4 \cdot 10^{-7}$	$m^2 s^{-1}$	Subin et al. (2012)
$T_{p0}$	3.5	$^{\circ}C$	Walter and Heimann (2000), Marotta et al. (2014)
$OQ_{10}$	1.13	–	Guo et al. (2020) <sup>a</sup>
$T_{00}$	30	$^{\circ}C$	Barbosa et al. (2018) <sup>b</sup>
$k_{CH_4}$	$1.41 \cdot 10^4$	$\mu mol m^{-3}$	Segers (1998)
$k_{O_2}$	$7.8 \cdot 10^4$	$\mu mol m^{-3}$	Guo et al. (2020) <sup>a</sup>
$K_2$	$4.2 \cdot 10^{-3}$	$mol m^{-2} s^{-1}$	Megard et al. (1984) <sup>c</sup>
$\theta_r$	1.045	–	Ambrose (1988) <sup>c</sup>
$\theta_p$	1.025	–	Stefan and Fang (1994) <sup>c</sup>
$\theta_s$	1.065	–	Stefan and Fang (1994) <sup>c</sup>
Calibrated parameters			
Parameter symbol	Value range	Unit	Source
$R_c$	$[9.6 \cdot 10^{-3}, 4.8 \cdot 10^{-1}]$	$\mu mol m^{-2} s^{-1}$	Gudasz et al. (2010)
$\alpha_z$	[1,10]	–	Stepanenko et al. (2016)
$PQ_{10}$	[0.9,17]	–	Duc et al. (2010), Inglett et al. (2012); Walter and Heimann (2000) <sup>d</sup>
$\alpha_e$	[0.2,1.0]	–	Baird et al. (2004) <sup>e</sup>
$O_{max}$	$[9.6 \cdot 10^{-4}, 3.73]$	$\mu mol m^{-3} s^{-1}$	Barbosa et al. (2018)
$Ph_{max}$	$[6.39 \cdot 10^{-4}, 3.09 \cdot 10^{-2}]$	$mgO_2(mgChla)^{-1} s^{-1}$	Forsberg et al. (2017)
$R_r$	$[4.94 \cdot 10^{-4}, 4.7 \cdot 10^{-3}]$	$mgO_2(mgChla)^{-1} s^{-1}$	Amaral et al. (2018) <sup>f</sup>
$k_s$	$[1.74 \cdot 10^{-2}, 1.15 \cdot 10^{-1}]$	$mgO_2 m^{-2} s^{-1}$	Stefan and Fang (1994) <sup>c</sup>

Note. Parameters with empirical values are listed with the values and those calibrated are listed with ranges.

<sup>a</sup>Calibrated values from previous study on boreal lake modeling used. <sup>b</sup>Daily mean water temperature of the sampled lake is used. <sup>c</sup>The  $K_2$ ,  $\theta_r$ , and  $\theta_s$  values fitted to experimental data under temperatures  $>10^{\circ}C$  are used. Measured  $k_s$  values for eutrophic lakes with nutrient-rich sediment are used. <sup>d</sup>The  $PQ_{10}$  range obtained from observed values in northern wetlands, subtropical wetlands, and boreal and northern temperate lakes with sediments incubated from 0 to  $35^{\circ}C$ . <sup>e</sup>Bubble formation was found to be activated in two poorly decomposed near-surface bog peats at methane concentrations as low as 20% of the saturation level. <sup>f</sup>Community respiration rates and Chl-a concentrations measured in Lake Janauacá at different times through the year. The Chl-a specific respiration rates are calculated by division.

to distribute the dissolved gases. The gas transfer velocity was modified to a TKE dissipation-based algorithm (MacIntyre et al., 2019). Manually measured DO concentrations at the beginning of the simulation periods were used as initial conditions. A spin-up period of 90 days was used for each hydrological period by repeatedly using representative 24-hr temperatures and turbulence dissipation (from AED3D) and measured dissolved oxygen to numerically stabilize water column methane concentrations before running transient simulations. AEM3D does not require spin-up.

Photosynthesis and metabolism algorithms were simplified by using measured Chla concentrations and Chla-specific process rates. Values of default parameters (Table 2) were adjusted to ranges expected in the Amazon basin. Sediment oxygen demand was added to the model. The revised algorithms and formulations of methane and oxygen processes are introduced below. Parameter values and sources are summarized in Table 2; modeled and physical variables, parameters and coefficients are listed in Table 2 and Appendix A with units.

Methanogenesis in the sediment ( $P$ ) is modeled as

$$P = R_c \cdot PQ_{10}^{\frac{T_s - T_{p0}}{10}} \cdot e^{-\alpha_z z_s} \quad (1)$$

where  $R_c$  is the carbon mineralization rate,  $PQ_{10}$  is a  $Q_{10}$  factor,  $T_s$  is the sediment temperature,  $T_{p0}$  is a reference temperature,  $z_s$  is depth in sediment; production decreases exponentially with sediment depth at rate  $\alpha_z$ . We do not

differentiate the sediment carbon between the fraction utilized for methane production and other processes based on the assumption that the carbon supply does not limit methane production. This is a reasonable assumption based the large carbon inputs from herbaceous plants, litterfall from trees and inflows from river and streams to Amazon floodplain lakes (Melack & Engle, 2010). Sediments in Amazon floodplains generally have moderate to high organic carbon content (Moreira-Turcq et al., 2013; Smith et al., 2003; Sobrinho et al., 2016). Sediment temperature was initialized with the annual mean near-bottom water temperature and then simulated based on heat conduction in water and sediments (Tan et al., 2015).

Methane concentrations ( $C_{CH_4s}$ ) and vertical transfer in the sediment is simulated by

$$\frac{\partial C_{CH_4s}}{\partial t} = \frac{\partial}{\partial z} \left( K_{ms} \frac{\partial C_{CH_4s}}{\partial z} \right) + P - \alpha_{CH_4} E_s \quad (2)$$

where  $K_{ms}$  is molecular diffusivity in sediment,  $\alpha_{CH_4}$  is the percentage of methane in bubbles, and  $E_s$  is ebullition. Bubbles consist of nitrogen and methane, and their formation is activated when sediment methane concentrations reach a saturation level,  $\alpha_s$ , which is calibrated. The initial bubble diameters are assumed to range between 5 and 20 mm with a uniform distribution of surface tension at the water-sediment interface.

Methane is transported through the water column by eddy diffusivity, entrainment, and ebullition. The changes in methane concentrations ( $C_{CH_4w}$ ) in the water column are calculated as

$$\frac{\partial C_{CH_4w}}{\partial t} = \frac{\partial}{\partial z} \left( (K_z + K_m) \frac{\partial C_{CH_4w}}{\partial z} \right) - O + E_{CH_4w} + F_{met} + P \quad (3)$$

where  $K_z$  is eddy diffusivity,  $K_m$  is molecular diffusivity,  $O$  is aerobic methane oxidation,  $E_{CH_4w}$  is the gas exchange with bubbles,  $F_{met}$  is diffusive methane flux at the water-air interface, and  $P$  is methanogenesis in the sediment. Methane exchanges at the sediment-water and water-air interfaces are added to the bottom and top boundaries, respectively. Advection from fringing habitats may also change methane concentrations, as mentioned in the Discussion, but are not included in the 1-D structure of ALBM. Eddy diffusivity is calculated as  $K_z = 0.2\epsilon/N^2$ , where 0.2 is Osborne coefficient,  $\epsilon$  is the TKE dissipation rate, and  $N = \sqrt{-\frac{g}{\rho} \frac{\partial \rho}{\partial z}}$  is the Brunt-Väisälä frequency, and  $\rho$  is water density. Water columns with  $N < 10^{-2} s^{-1}$  are treated as well-mixed, and the gas concentrations are simulated as the volume-weighted mean.

Aerobic methane oxidation is a function of water temperature, and methane and dissolved oxygen concentrations following Segers (1998) and Zhuang et al. (2004):

$$O = O_{max} \cdot OQ_{10}^{\frac{T_w - T_{O0}}{10}} \frac{C_{O_2}}{k_{O_2} + C_{O_2}} \frac{C_{CH_4w}}{k_{CH_4} + C_{CH_4w}} \quad (4)$$

where  $O_{max}$  is methane oxidation potential,  $OQ_{10}$  is a  $Q_{10}$  factor,  $T_w$  is water temperature,  $T_{O0}$  is a reference temperature, and  $k_{O_2}$  and  $k_{CH_4}$  are Michaelis-Menten constants.

The governing equations of bubble transfer in the water column are adapted from ocean models (Liang et al., 2011; Woolf & Thorpe, 1991). The gas concentration in bubbles of certain size at certain depth and time step is calculated by a continuity equation in which the impacts of buoyant rising, gas exchange with ambient water, and bubble expansion are included (Liang et al., 2011). Buoyant rising is driven by the hydrostatic pressure gradient across the water columns and kinematic viscosity, and gas exchange by the pressure difference between in- and outside of the bubble. The size of a single bubble changes during rising depending on the air pressure, hydrostatic pressure, and bubble surface tension. Gases in bubbles are assumed to release instantly to the atmosphere upon reaching the lake surface. Detailed formulations can be found in Tan et al. (2015).

The dissolved oxygen module is based on Stefan and Fang (1994) with modifications to suit the availability of observational data. The changes in concentrations of dissolved oxygen ( $C_{O_2}$ ) in the water column are modeled as

$$\frac{\partial C_{O_2}}{\partial t} = \frac{\partial}{\partial z} \left( (K_z + K_m) \frac{\partial C_{O_2}}{\partial z} \right) + Ph - R - SOD - 2 \cdot O + F_{ox}g \quad (5)$$

**Table 3**  
Calibrated Parameter Values for Main Lake

Parameter	Units	201503	201506	201510	201601	201609
$R_c$	$\mu\text{molm}^{-2}\text{s}^{-1}$	$2.33 \cdot 10^{-2}$	$3.07 \cdot 10^{-2}$	$2.05 \cdot 10^{-2}$	$5.5 \cdot 10^{-2}$	$1.71 \cdot 10^{-2}$
$\alpha_z$	–	4.54	3.0	3.50	4.36	5.64
$PQ10$	–	1.84	2.64	5.99	7.61	1.77
$\alpha_e$	–	0.41	0.45	0.86	0.64	0.63
$O_{max}$	$\mu\text{molm}^{-3}\text{s}^{-1}$	$1.26 \cdot 10^{-2}$	$2.52 \cdot 10^{-3}$	$2.33 \cdot 10^{-2}$	$5.56 \cdot 10^{-3}$	$4.43 \cdot 10^{-2}$
$Ph_{max}$	$\text{mgO}_2(\text{mgChla})^{-1}\text{s}^{-1}$	$1.08 \cdot 10^{-2}$	$7.76 \cdot 10^{-3}$	$3.55 \cdot 10^{-2}$	$7.96 \cdot 10^{-3}$	$1.15 \cdot 10^{-2}$
$R_r$	$\text{mgO}_2(\text{mgChla})^{-1}\text{s}^{-1}$	$2.54 \cdot 10^{-3}$	$4.5 \cdot 10^{-3}$	$1.96 \cdot 10^{-3}$	$3.37 \cdot 10^{-3}$	$4.45 \cdot 10^{-3}$
$k_s$	$\text{mgO}_2\text{m}^{-2}\text{s}^{-1}$	$7.32 \cdot 10^{-2}$	$8.94 \cdot 10^{-2}$	$1.27 \cdot 10^{-2}$	$3.22 \cdot 10^{-2}$	$1.84 \cdot 10^{-2}$

where  $Ph$  is oxygen production by photosynthesis,  $R$  is community respiration,  $SOD$  is sediment oxygen demand,  $O$  is aerobic methane oxidation and  $F_{\text{oxg}}$  is oxygen exchange at the air-water interface. Photosynthetic rate is computed as  $Ph = Ph_{\text{max}} \theta_p^{T_w - 30} f(I, T_w) C_{\text{Chla}}$ , where  $Ph_{\text{max}}$  is the Chla-specific light-saturation rate of photosynthesis,  $\theta_p$  is a temperature coefficient estimated as a function of optimal temperature, standard temperature, and maximum temperature from model input data (Tan et al., 2017),  $f(I, T_w)$  is a light limitation term,  $I$  is the incident photosynthetically active radiation, and  $C_{\text{Chla}}$  is Chla concentration.  $f(I, T_w) = I \left( 1 + 2\sqrt{K_1/K_2} \right) / (I + K_1 + I^2/K_2)$ , where  $K_1$  (approximated as  $0.7 \times 1.1^{T_w - 20}$ ) and  $K_2$  are light inhibition and limitation coefficients. Respiration rate depends on temperature and Chla:  $R = R_r \theta_r^{(T_w - 30)} C_{\text{Chla}}$ , where  $R_r$  is the Chla-specific respiration rate at 30°C, and  $\theta_r$  is a temperature coefficient. The vertical distribution of Chla is assumed uniform, though only involved in photosynthesis within the euphotic zone. The euphotic zone is delimited by the depth where PAR was more than  $1 \mu\text{molm}^{-2} \text{s}^{-1}$ , a value selected because the phytoplankton are circulating in turbid water. SOD is a function of temperature and bathymetry:  $SOD = \frac{k_s \theta_s^{T_w - 20}}{A} \frac{\partial A}{\partial z}$ , where  $k_s$  is the sediment oxygen demand at 20°C,  $\theta_s$  is a temperature coefficient, and  $A$  is sediment area as a function of depth based on the hypsographic curve of depth versus area derived from the lake's bathymetry. As the water level varies seasonally, the appropriate portion of the hypsographic curve is used. If the sediments are overlain by anoxic water, the SOD is zero. Advection between habitats is not included.

Diffusive gas flux at the water-air interface ( $F$ ) is calculated following  $F = k_{600} \cdot (C_w - C_{eq})$ , where  $k_{600}$  is gas transfer velocity normalized to  $\text{CO}_2$  at 20°C,  $C_w$  is near-surface gas concentration, and  $C_{eq}$  is near-surface gas concentration in equilibrium with the atmosphere. Gas transfer velocity is based on MacIntyre et al. (2019):  $k_{600} = c_1 (\epsilon \nu)^{0.25} Sc^{-0.5}$ , where  $c_1 = 0.5$  is a constant coefficient,  $\epsilon$  is the dissipation rate of TKE at water surface,  $\nu$  is kinematic viscosity, and  $Sc$  is the Schmidt number.  $F$  was calculated for both methane and dissolved oxygen.

#### 2.4. Biogeochemical Model Sensitivity Tests, Calibration, and Validation

Parameters for calibration were selected through sensitivity tests using a machine learning-based algorithm, classification and regression trees (CART, Krzywinski & Altman, 2017). The CART method trains a decision tree by recursively partitioning the input data into two subgroups by the value of the explanatory variable at each node. The decision tree can be pruned by adjusting the stopping criteria including the number of iterations and the size of subgroups to achieve the best size of the tree and the lowest misclassification rate. This method has proved adequate and widely used in the inspection of multivariate relationships within large complex data (Choubin et al., 2018; Guo et al., 2020; Rodrigues & de la Riva, 2014). In our study, a tree size of 200 nodes was found optimal using the cross-validation method. For each case, the model was run with a perturbed parameter ensemble (PPE) of size 10,000, and the simulated methane and DO concentrations at lake surface and bottom were used as training data for CART. Data training and sensitivity analysis were done using the  $R$  package “gbm” (Greenwell et al., 2019). Relative influence percentages are based on Friedman (2001).

The model was calibrated separately for each site and water level using a Bayesian approach in which a uniform distribution was prescribed to all parameters, and Monte-Carlo based calibrations were run more than once by sampling from the posterior distribution obtained from the previous round. The periods for calibration were

**Table 4**  
Calibrated Parameter Values for Embayment

Parameter	Units	201502	201506	201510	201601	201609
$R_c$	$\mu\text{molm}^{-2}\text{s}^{-1}$	$4.95 \cdot 10^{-2}$	$4.98 \cdot 10^{-2}$	$3.96 \cdot 10^{-2}$	$5.99 \cdot 10^{-2}$	$2.92 \cdot 10^{-2}$
$\alpha_z$	–	4.93	2.59	3.09	3.0	4.49
$PQ_{10}$	–	2.9	2.57	9.29	6.97	5.48
$\alpha_e$	–	0.53	0.99	0.43	0.42	0.52
$O_{max}$	$\mu\text{molm}^{-3}\text{s}^{-1}$	$6.68 \cdot 10^{-3}$	$2.19 \cdot 10^{-3}$	$1.28 \cdot 10^{-2}$	$6.19 \cdot 10^{-3}$	$1.9 \cdot 10^{-3}$
$Ph_{max}$	$\text{mgO}_2(\text{mgChla})^{-1}\text{s}^{-1}$	$2.2 \cdot 10^{-2}$	$1.51 \cdot 10^{-2}$	$6.89 \cdot 10^{-3}$	$2.54 \cdot 10^{-3}$	$2.33 \cdot 10^{-2}$
$R_r$	$\text{mgO}_2(\text{mgChla})^{-1}\text{s}^{-1}$	$9.39 \cdot 10^{-4}$	$4.63 \cdot 10^{-3}$	$3.93 \cdot 10^{-4}$	$4.11 \cdot 10^{-3}$	$1.37 \cdot 10^{-3}$
$k_s$	$\text{mgO}_2\text{m}^{-2}\text{s}^{-1}$	$3.86 \cdot 10^{-2}$	$6.12 \cdot 10^{-2}$	$5.85 \cdot 10^{-2}$	$1.15 \cdot 10^{-1}$	$3.33 \cdot 10^{-2}$

selected to span the seasonal range of water depths and limnological conditions. The number of the sampling round was case-sensitive and decided by the model performance. The size of the PPE equaled number of parameters multiplied by 1,000 in each round. For methane diffusive fluxes, the simulations were compared to hourly observations while for ebullitive fluxes, daily totals were calculated to compare with the observed daily ebullition collected by bubble traps. Simulated DO concentrations were validated against observations at each observational depth. The optimal parameter values were selected based on the simulation accuracy of both methane fluxes and oxygen concentrations (Tables 3 and 4).

Model validation was done by running simulations for other times using the calibrated parameters. For each site, five additional periods were modeled (Table 1) using calibrated parameters from the period with (a) the same hydrological phase, and (b) the closest lake depth. Simulated methane fluxes and concentration were compared

to the measurements to evaluate the model performance. Root-mean-square errors ( $\text{RMSE} = \sqrt{\frac{\sum_{i=1}^n (S_i - O_i)^2}{n}}$ ) were calculated for methane diffusive fluxes ( $\mu\text{mol m}^{-2} \text{hr}^{-1}$ ) and near-surface methane concentrations ( $\mu\text{mol L}^{-1}$ ).  $S_i$  is simulated value,  $O_i$  is measurement, and  $n$  is the number of measurements during each simulated period. Measured and simulated methane fluxes and concentrations were compared in time-series figures. Measured and modeled thermal structure and DO concentrations were evaluated using time-depth diagrams.

### 3. Results

Results are presented in three complementary sections. First, sensitivities of the simulated concentrations and fluxes to parameters used in the model and their relative importance are presented. Second, the simulated methane concentrations and fluxes are compared to measurements with examples of the four hydrological phases in the main lake and embayment for calibrated and uncalibrated periods. Time-series figures and performance metrics are provided. Third, time-depth diagrams of measured and modeled thermal structure and dissolved oxygen concentrations at high and low water levels are provided. Subsequently, the discussion examines simulations of specific processes to help decipher influences of various factors and the veracity of the simulations.

#### 3.1. Parameter Sensitivities

Parameter sensitivity tests were conducted for high and low water periods in the main lake. The simulated methane concentrations, methane fluxes and DO concentrations are sensitive to 8 parameters and the relative importance (RI) of each parameter is fairly consistent between the two hydrological phases (Table 5). Methane concentrations at near-surface and near-bottom are most sensitive to the carbon mineralization rate ( $R_c$ ),  $Q_{10}$  factors for methanogenesis ( $PQ_{10}$ ) and oxidation ( $OQ_{10}$ ), and methane oxidation potential ( $O_{max}$ ) during both hydrological phases. Diffusive emission is sensitive to the same parameters because it is mainly controlled by near-surface methane concentration. Ebullitive emission is sensitive to methanogenesis-related parameters, and to the decrease of sediment organic carbon with depth and percent saturation of methane concentration, as this initiates bubbling. Near-surface and near-bottom DO concentrations are sensitive to community respiration ( $R_r$ ), sediment oxygen demand, the  $Q_{10}$  factor of methanogenesis, and carbon mineralization rate. Only near-surface DO is sensitive to

**Table 5**

Relative Importance (RI) for Parameters Tested in the Sensitivity Analysis; Diffusive Flux (*dflux*) and Ebullitive Flux (*efflux*)

Parameters	Near-surface CH <sub>4</sub>		Near-bottom CH <sub>4</sub>		dflux		efflux		Surface DO		Bottom DO	
	201506	201510	201506	201510	201506	201510	201506	201510	201506	201510	201506	201510
<i>OQ</i> <sub>10</sub>	2.4	1.8	2.5	1.4	2.3	2.3	0	0	2.1	0.8	0.3	1.0
<i>k</i> <sub>CH<sub>4</sub></sub>	0.8	1.48	14.2	0.4	14.3	1.5	0	0.03	0.3	0	0.04	0
<i>k</i> <sub>O<sub>2</sub></sub>	0.03	0.03	0.05	0.01	0.03	0.02	0	0	0.07	0.01	0	0
<i>Rc</i>	<b>23.8</b>	<b>22.0</b>	<b>23.1</b>	<b>22.5</b>	<b>23.0</b>	<b>21.7</b>	8.8	8.8	14.6	2.2	9.0	1.7
<i>α</i> <sub>z</sub>	0.03	0.1	0.06	0.01	0.06	0.2	<b>20.0</b>	19.5	0.03	0	0.07	0
<i>PQ</i> <sub>10</sub>	<b>56.7</b>	<b>57.3</b>	<b>56.7</b>	<b>60.1</b>	<b>57.2</b>	<b>56.6</b>	<b>24.2</b>	<b>25.9</b>	<b>53.6</b>	7.5	<b>37.4</b>	5.9
<i>α</i> <sub>e</sub>	0.8	14.3	0.7	0.2	0.8	1.1	<b>46.7</b>	<b>45.5</b>	0.05	0.03	0	0
<i>O</i> <sub>max</sub>	14.2	1.0	0.9	0.3	0.9	14.1	0	0	1.8	0.5	0.6	0.8
<i>Ph</i> <sub>max</sub>	0	0	0	0	0	0	0	0.03	0.4	<b>34.4</b>	0.2	2.4
<i>R</i> <sub>r</sub>	0.1	0.4	0.1	0.03	0.2	0.5	0	0	1.6	<b>22.7</b>	2.2	<b>38.9</b>
<i>k</i> <sub>s</sub>	0.4	0.8	0.4	15.0	0.5	0.9	0	0.04	<b>24.9</b>	<b>31.9</b>	<b>49.9</b>	<b>49.2</b>

Note. Values above 20 are bold.

photosynthesis potential ( $Ph_{max}$ ) and is more sensitive to photosynthesis potential at low water than at high water, probably due to the higher chlorophyll concentrations at low water. High-water near-surface DO is sensitive to methanogenesis-related parameters and thus methane concentration, indicating that the longer methane diffusion pathway makes methanotrophy an important sink for both methane and oxygen. For consistency, the parameters important for at least one hydrological phase were selected to be calibrated for all sites and time periods.

### 3.2. Methane Fluxes and Concentrations

*Main lake* - Simulated methane fluxes and concentrations for calibrated (Table 6) and uncalibrated periods (Table S1 in Supporting Information S1) vary in their similarity to measurements. RMSE values for near-surface CH<sub>4</sub> concentrations ranged from 0.5 to 1.5 μmol L<sup>-1</sup> for calibrated periods from 0 to 3.7 μmol L<sup>-1</sup> for uncalibrated periods. RMSE values for CH<sub>4</sub> fluxes ranged from 2.6 to 85 μmol m<sup>-2</sup> hr<sup>-1</sup> for calibrated periods from 1.3 to 68 μmol m<sup>-2</sup> hr<sup>-1</sup> for uncalibrated periods. Time-series of simulated fluxes for calibrated periods show generally good agreement with measurements in Oct 2015 and Jan 2016 but less agreement in Aug 2016 when simulated values are often higher (Figure 4). During uncalibrated periods, simulated fluxes were similar to measurements except for occasional mismatches (Figure S1 in Supporting Information S1).

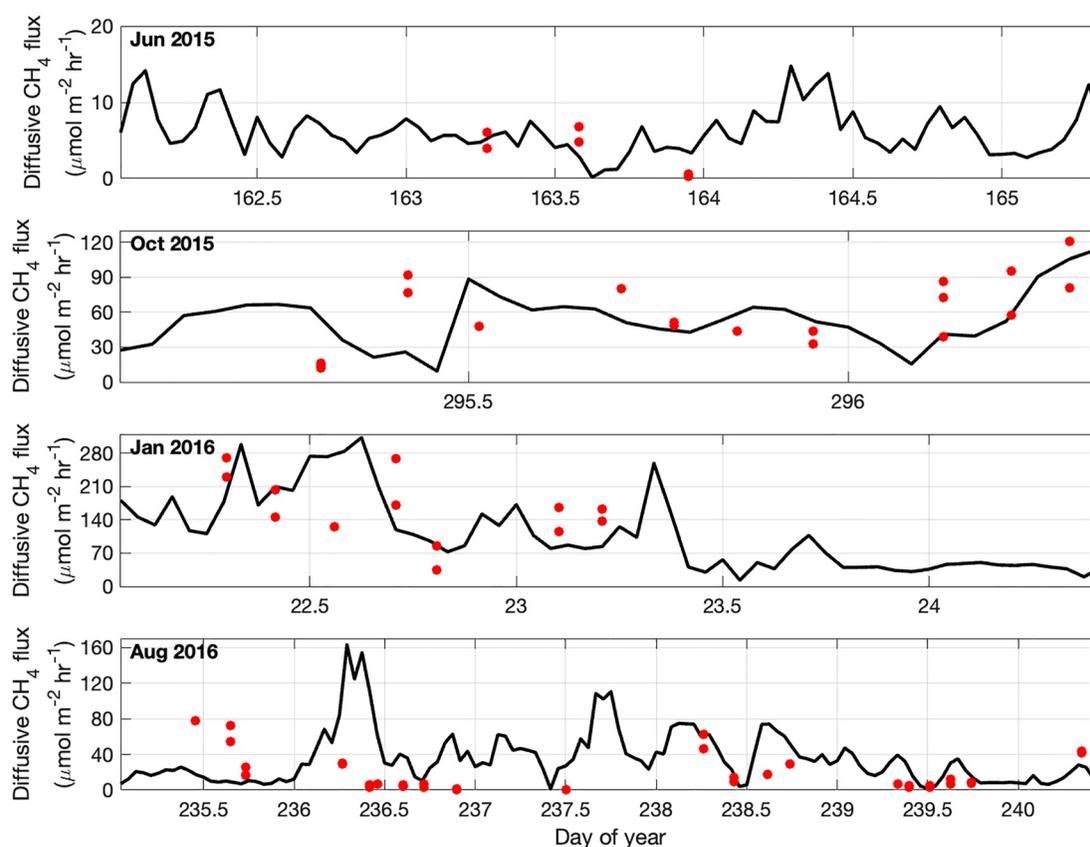
Vertical profiles of simulated CH<sub>4</sub> concentrations during high water in Jun 2015 were similar to measurements near mid-night (22:45 hr), but differed considerably at mid-day and sunrise (Figure S2 in Supporting Information S1). Vertical variations were usually lacking during low water (October 2015 and January 2016) in both measurements (except for a couple of times in October 2015) and simulations (Figure S3 in Supporting Information S1).

**Table 6**

Root-Mean-Square Errors (RMSE) for Simulated Variables During Different Water Levels in Main Lake and Embayment for Calibrated Periods

Site	Main lake				Embayment					
	2015		2016		2015		2015		2016	
Year	2015	2015	2016	2016	2015	2015	2015	2015	2016	2016
Month	Jun	Oct	Jan	Aug	Feb	Jun	Oct	Jan	Aug	
Near-surface CH <sub>4</sub> (μmol L <sup>-1</sup> )	0.5 (3)	0.5 (11)	1.5 (7)	0.8 (20)	0.6 (5)	2.0 (3)	2.2 (7)	2.8 (7)	2.2 (12)	
Diffusive CH <sub>4</sub> flux (μmol m <sup>-2</sup> hr <sup>-1</sup> )	2.6 (6)	33 (22)	85 (14)	45 (37)	23 (12)	28 (8)	246 (18)	242 (15)	190 (24)	

Note. Number in parenthesis is the number of measurements during each simulated period. Mar 2015 not shown because only one measurement overlapped simulated period.

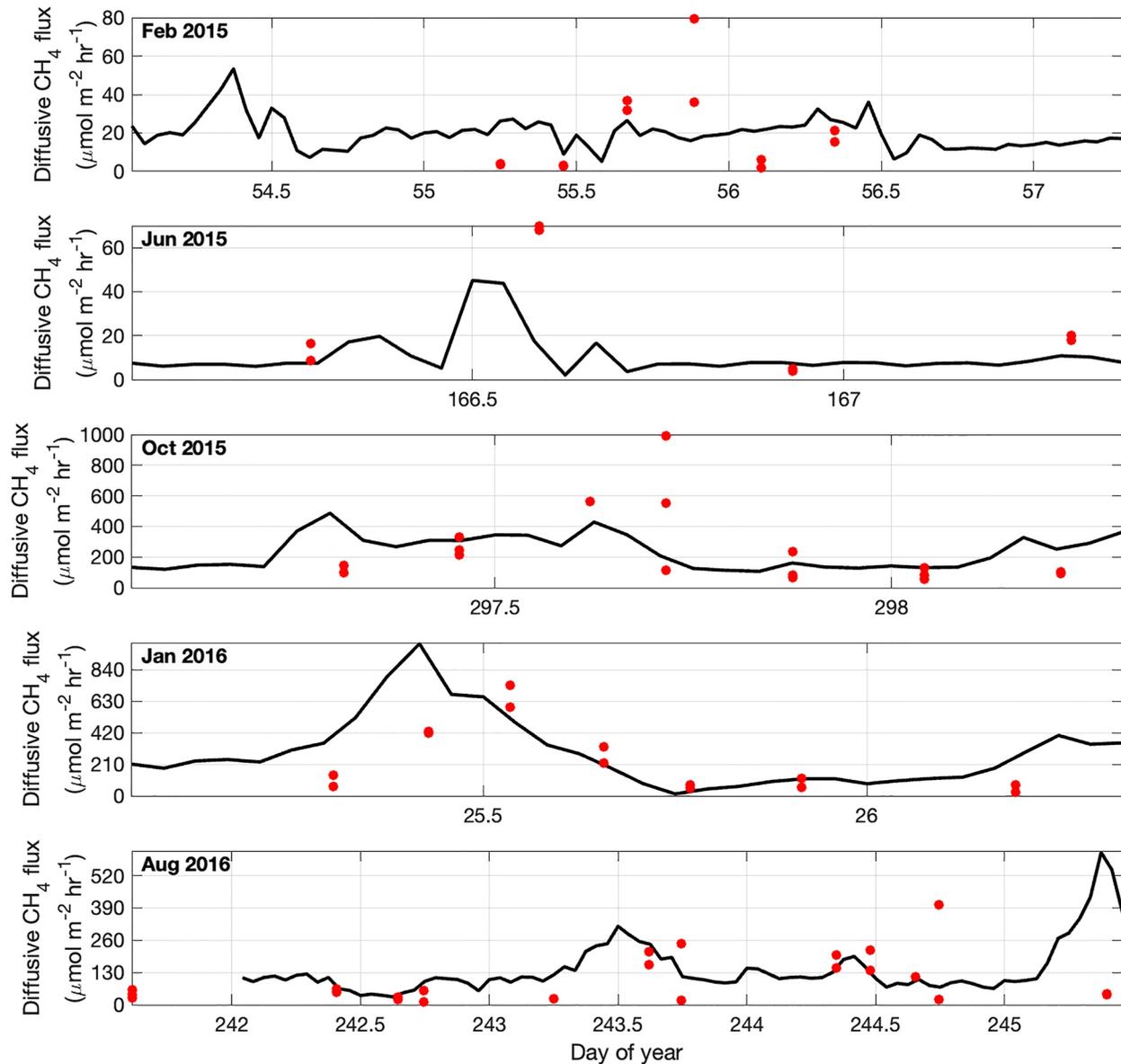


**Figure 4.** Measured (red dots) and simulated (lines) diffusive fluxes in Lake Januacá (main lake) for June 2015 (a), October 2015 (b), January 2016 (c), and August 2016 (d). Note different scales on y-axes. All replicates of measured fluxes are shown and expressed as hourly values. Simulated diffusive fluxes are summed for each hour and the values are assigned to the end of each hour. Mar 2015 not shown because only one measurement overlapped simulated period.

**Table 7**  
Average Daily Diffusive  $CH_4$  Fluxes ( $\mu mol m^{-2} d^{-1}$ ): ALBM (Calibrated and Uncalibrated) and Measurements

Simulation dates	Main lake				Embayment				
	ALBM		Measurements		ALBM		Measurements		
	S days	Flux ( $\mu mol m^{-2} d^{-1}$ )	n	Flux ( $\mu mol m^{-2} d^{-1}$ )	S days	Flux ( $\mu mol m^{-2} d^{-1}$ )	n	Flux ( $\mu mol m^{-2} d^{-1}$ )	
Calibrated	Feb/Mar 2015	1.2	253	4	152	3.3	461	11	482
	Jun 2015	3.3	146	6	90	1.4	250	8	630
	Oct 2015	1.3	1,261	22	1,331	1.3	5,496	8	6,227
	Jan 2016	2.4	2,591	14	3,838	1.4	6,931	13	6,495
	Aug 2016	5.5	825	37	497	3.5	3,380	15	2,388
Uncalibrated	Jan 2015	2.3	182	12	68	2.9	426	16	365
	May 2015	2.4	37	8	22	2.6	318	8	224
	Aug 2015	1.5	184	8	629	3.4	1,239	8	560
	Feb 2016	2.3	2,975	15	1,800	1.3	2,445	15	3,221
	Apr 2016	2.5	368	24	275	1.3	2,038	24	2,431

*Note.* For ALBM simulations, average diffusive  $CH_4$  fluxes computed as the sum of fluxes divided by the length of simulation, and for measurements as the arithmetic mean of the measurements. Both averages are converted to daily values. S days is number of days simulated; n is number of measurements.



**Figure 5.** The same as Figure 4 for Lake Janauacá (embayment) in February 2015 (a), June 2015 (b), October 2015 (c), January 2016 (d), and August 2016 (e).

Time-series of simulated near-surface concentrations were consistently less than measurements in Oct 2015 and consistently higher than measurements in Jan and Aug 2016 (Figure S4 in Supporting Information S1). During uncalibrated periods simulated near-surface concentrations matched measurements well in January 2015 and February and April 2016 but less well in May and August 2015 (Figure S5 in Supporting Information S1).

Average daily diffusive  $\text{CH}_4$  fluxes, calculated from measurements and simulations, have generally consistent seasonal patterns with higher and lower values matching, albeit with conspicuous differences in August 2016 (calibrated) and August 2015 and February 2016 (uncalibrated (Table 7). The few comparisons available for daily ebullitive fluxes indicate negligible fluxes except during low water (Table S2 in Supporting Information S1).

*Embayment*—Simulations of methane fluxes and concentrations for calibrated (Figure 5 and Figures S6–S8 in Supporting Information S1; Tables 6 and 7 and Table S2 in Supporting Information S1) and uncalibrated (Table 7, Tables S1 and S2 in Supporting Information S1; Figures S9 and S10 in Supporting Information S1) periods vary in their similarity to measurements. RMSE values for near-surface  $\text{CH}_4$  concentrations ranged from 0.6 to 2.8  $\mu\text{mol L}^{-1}$  for calibrated periods from 0.1 to 3.9  $\mu\text{mol L}^{-1}$  for uncalibrated periods. RMSE values for  $\text{CH}_4$

fluxes ranged from 23 to 246  $\mu\text{mol m}^{-2} \text{hr}^{-1}$  for calibrated periods from 14 to 88  $\mu\text{mol m}^{-2} \text{hr}^{-1}$  for uncalibrated periods. Time-series of simulated fluxes for calibrated and uncalibrated periods show generally good agreement with measurements except for occasional mismatches (Figure 5 and Figure S9 in Supporting Information S1).

Vertical profiles of simulated  $\text{CH}_4$  concentrations during high water in Jun 2015 were similar to measurements in the upper 2 m, but progressively diverged at deeper depths with simulated values exceeding measurements (Figure S6 in Supporting Information S1). Vertical variations were usually lacking during low water (January 2016) in both measurements (except for a few high values near the bottom) and simulations (Figure S7 in Supporting Information S1). Time-series of simulated near-surface concentrations were consistently more than measurements in August 2016, and comparisons varied in other periods with no patterns (Figures S8 and S10 in Supporting Information S1).

Average daily diffusive  $\text{CH}_4$  fluxes, calculated from measurements and simulations, have generally consistent seasonal patterns with higher and lower values matching, albeit with conspicuous differences in August 2016 (calibrated) and August 2015 and February 2016 (uncalibrated (Table S1 in Supporting Information S1)). The few data available for daily ebullitive fluxes indicate comparable values and seasonal patterns for measurements and simulations except for a mismatch in values in January 2016 (Table S2 in Supporting Information S1).

An overall comparison of measured and simulated fluxes that combines all replicates of measured diffusive fluxes from both sites and the wide range of water levels and associated ecological conditions indicates considerable variability (Figure S11 in Supporting Information S1), as expected by the results illustrated in figures with measurements and simulated methane fluxes. Temporal variability is not expected to be replicated exactly by ALBM, given the inherent variability of methane fluxes and sparseness of field data.

### 3.3. Thermal Structure and Dissolved Oxygen Concentrations

The hydrodynamic model simulated well the diurnal stratification and nocturnal mixing in the open lake and embayment during both high and low water periods (Figures 6 and 7). Time-depth plots of simulated and measured DO values for high and low water periods in main lake (Figure 6) and embayment (Figure 7) indicate general similarities in diel and vertical variations. However, in Oct 2015 in the main lake larger day-night differences were simulated than measured (Figures 6b3 and 6b4). RMSE for simulated near-surface dissolved oxygen concentrations ( $\text{mg L}^{-1}$ ) during calibrated periods ranged from 0.9 to 4.4 (Table 8), and for uncalibrated periods from 0.6 to 6.3 (Table S3 in Supporting Information S1). RMSE values for simulated near-bottom dissolved oxygen concentrations ( $\text{mg L}^{-1}$ ) during calibrated periods ranged from 0.1 to 1.4, except for larger values at low water (October 2015); the especially high value in August 2016 is misleading because most of the water column was anoxic. During uncalibrated periods RMSE values from 0.1 to 2.0  $\text{mg L}^{-1}$ , except for larger values during low water (January 2015 and February 2016) in the main lake (Table S3 in Supporting Information S1).

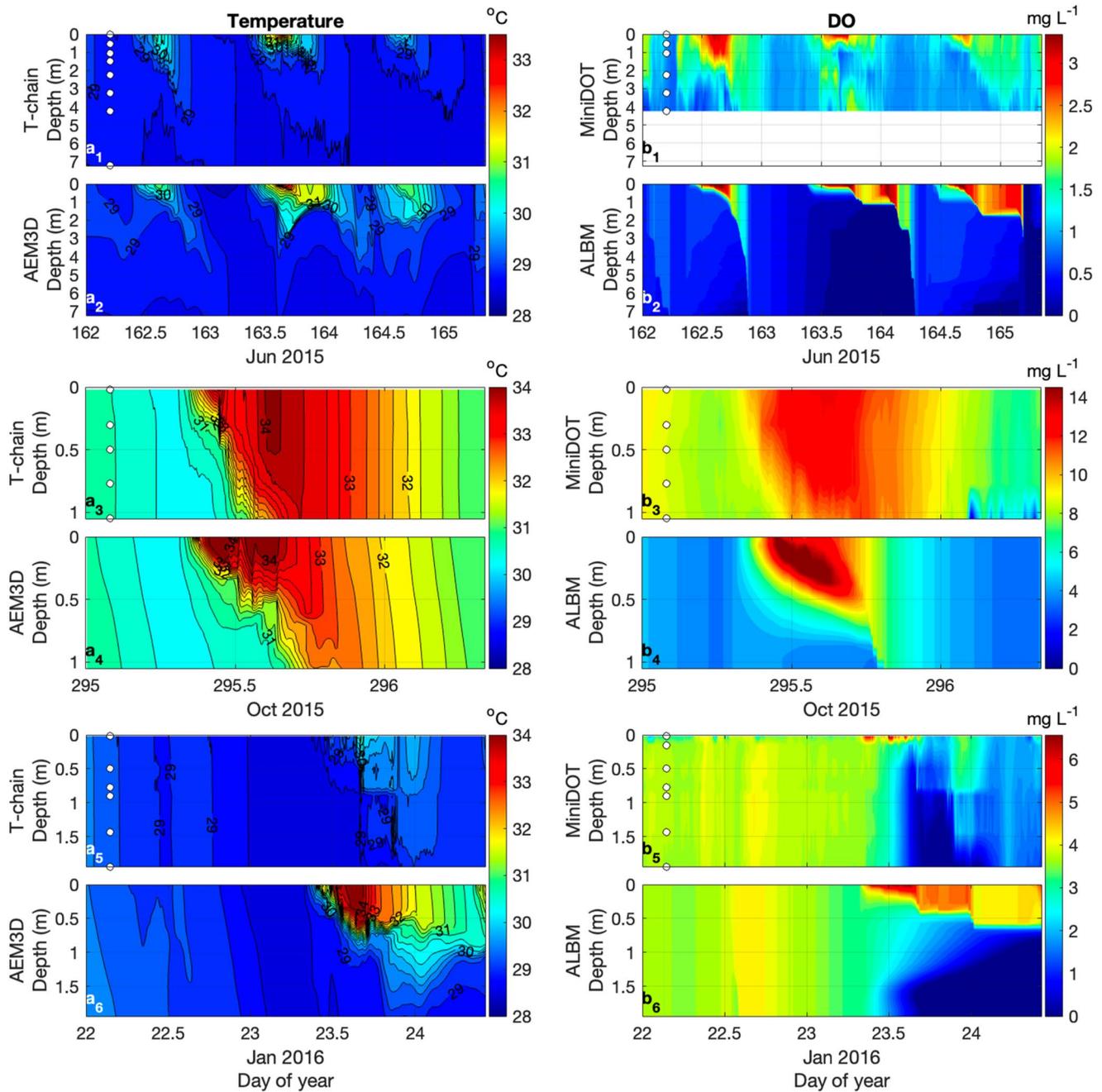
## 4. Discussion

Hipsey et al. (2020) identified several aspects of model performance including comparison of simulated variables with observations, as described in Results, and evaluation of the processes being simulated. Here, we discuss the algorithms used, the basis for revisions of the original ALBM formulations and alternative algorithms for the physical and biogeochemical processes and the inputs needed to apply these algorithms. We compare modeled rates of photosynthesis, respiration and methane oxidation with measurements from Amazon floodplain lakes. We then consider challenges and limitations of modeling methane fluxes including the heuristic value of the model and how the model's result could be used to extend in time and space estimates of methane emissions.

### 4.1. Algorithms and Processes

#### 4.1.1. Hydrodynamic Models and Inputs

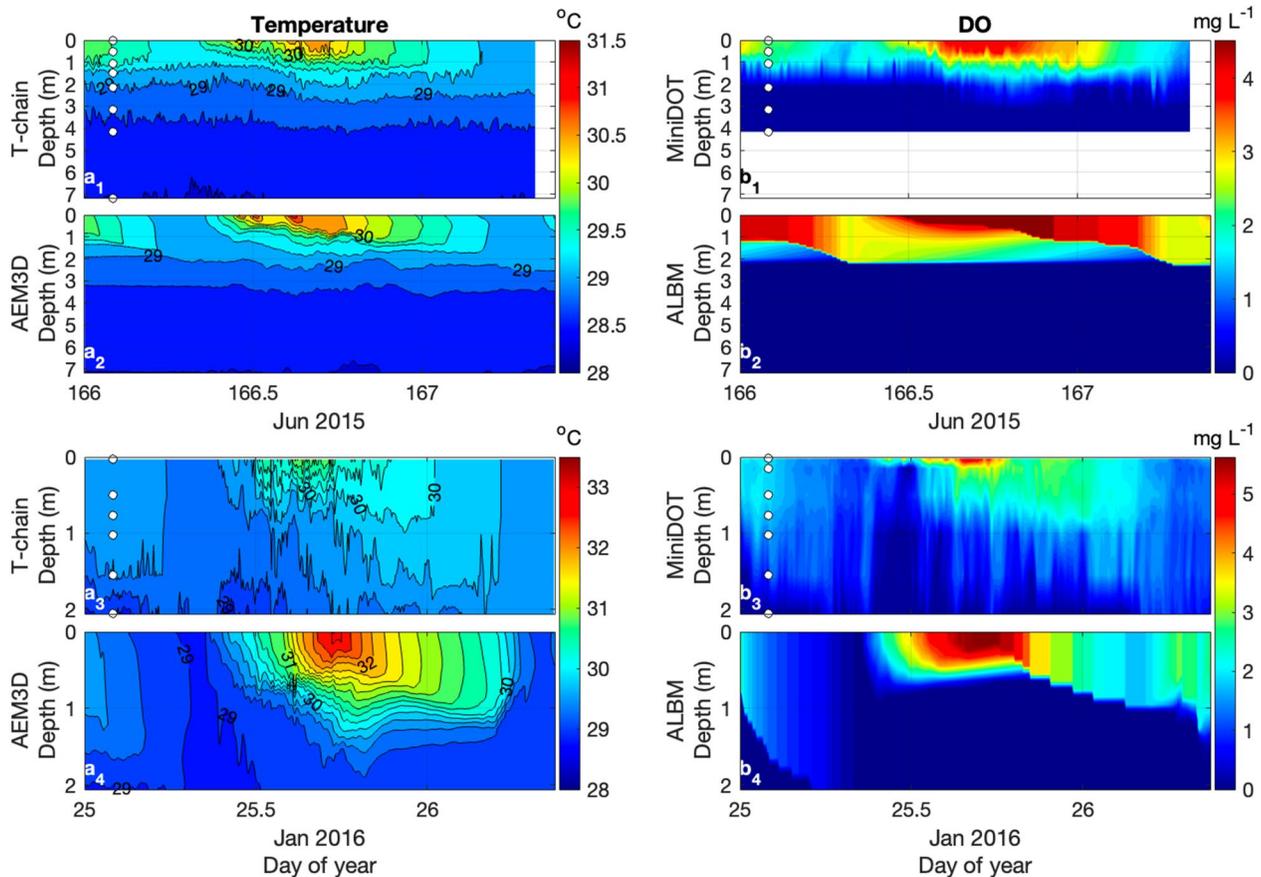
While 3-dimensional hydrodynamic models, such as AEM3D, can characterize most of the relevant physical processes in lakes, these models are computationally demanding. Hence, application of 3-dimensional models to regional analyses over multiple years is not currently practical. One-dimensional hydrodynamic models, such as the "DYnamic REservoir Simulation Model" (DYRESM) and its derivatives (Hipsey et al., 2019; Imberger & Patterson, 1981), also have well characterized parameterizations of physical processes. DYRESM is computationally efficient and has been shown to be accurate with respect to temporal variations in temperature



**Figure 6.** Time-depth plots of measured and simulated temperatures ( $a_1$  to  $a_6$ ) and dissolved oxygen (DO) concentrations ( $b_1$  to  $b_6$ ), respectively, during high water (June 2015) and low water (October 2015 and January 2016) in Lake Janauacá (main lake). White dots indicate depths of thermistors or DO sensors. Both the measured and simulated temperatures were averaged with 5-min bins.

structure in seasonally stratified lakes and reservoirs (Yeates & Imberger, 2003). A recent extension to the Multi-Basin Dynamic REservoir Simulation Model (MB-DYRESM) has been developed to bridge between one-dimensional lake models and computationally expensive, three-dimensional lake models (Zhou et al., 2021).

Given the importance of diel variations in physical processes in shallow, warm water lakes, as well as other types of lakes in some seasons, meteorological data at least hourly intervals are required as inputs. Ideally, meteorological sensors are deployed on or near the lake, but meteorological measurements are sparse for Amazon floodplains and seldom on lakes elsewhere. Alternatives for regionalization may be output of the Weather Research and Forecasting model (e.g., Yang & Dominguez, 2019) or reanalysis results, such as the 3-hourly MERRA-2 data at



**Figure 7.** The same as Figure 6 for high water (June 2015) and low water (January 2016) in Lake Janauacá (embayment). White dots indicate depths of thermistors or DO sensors.

0.5° resolution (<https://gmao.gsfc.nasa.gov/reanalysis/MERRA-2/>), or the ERA5-Land hourly meteorology data at 0.1° (~9 km) resolution (<https://doi.org/10.24381/cds.e2161bac>). Daily data, such as used for climate projections, are not suitable (e.g., Frieler et al., 2017).

The revised version of ALBM uses a formulation of  $K_z$  derived as a TKE-based  $\epsilon$ . As an alternative to estimates of TKE by hydrodynamic models,  $\epsilon$  can be calculated with meteorological data and thermal structure of the lake, as described in MacIntyre et al. (2019).

Hydrodynamic simulations with AEM3D were done as part of an analysis of spatial variations in carbon dioxide in L. Janauacá (Amaral et al., 2021) and illustrate the potential influence of lateral exchanges and advection on dissolved gas concentrations. In the embayment, the presence of floating plants fringing open water led to

**Table 8**  
*Root-Mean-Square Errors for Calibrated Simulations of Near-Surface and Near-Bottom Dissolved Oxygen Concentrations ( $\text{mg L}^{-1}$ ) at Different Water Levels in Lake Janauacá, Main Lake and Embayment Based on 10-Minute Readings of Moored DO Sensors*

Site	Main lake					Embayment				
	2015	2015	2015	2016	2016	2015	2015	2015	2016	2016
Year	2015	2015	2015	2016	2016	2015	2015	2015	2016	2016
Month	Mar	Jun	Oct	Jan	Aug	Feb	Jun	Oct	Jan	Aug
Surface DO ( $\text{mg L}^{-1}$ )	1.3	0.9	3.7	1.4	1.4	1.9	1.6	2.2	1.0	4.4
Near-bottom DO ( $\text{mg L}^{-1}$ )	1.0	0.8	4.8	0.6	1.4	1.2	0.1	2.6	0.4	8.6

*Note.* If lower water column was anoxic, deepest DO sensor was just above oxycline.

differential heating and cooling that resulted in diel changes in the direction and depths of lateral flows. In the open lake, exchange between the littoral and offshore zones occurred at the surface and interior of the lake, and were moderated by wind direction, temperature differences and internal wave motions. A similar approach using methane concentrations in floating plants or flooded forests as transported and dispersed by AEM3D could be done.

#### 4.1.2. Biogeochemical Models of Fluxes and Processes

##### 4.1.2.1. Diffusive Methane Flux

Emission of methane by diffusive flux depends on the concentration gradient near the air-water interface and on the gas transfer velocity that depends on turbulence as a function of heating, cooling and wind speed. The revised version of ALBM uses a formulation of the gas transfer velocity that uses  $\epsilon$ , an improvement especially relevant to warm water conditions (MacIntyre et al., 2019, 2021). Previous versions of ALBM used empirically derived relations with wind speed (Riera et al., 1999) or wind speed and thermal conditions in the lake (Heiskanen et al., 2015) derived with data from northern lakes. These formulations do not represent the enhanced turbulence observed under strong near-surface stratification in tropical lakes and other warm waters.

##### 4.1.2.2. Ebullition

The release of methane via bubbles depends on processes in the sediments and overlying water. Given the importance and wide variation in ebullition reported for Amazon floodplain lakes (Barbosa et al., 2021), the mixed success in simulating these fluxes raises concerns regarding the processes modeled or not included. Once methane concentrations in the pore water reaches saturation, bubbles are initiated. Porosity of the sediments, based on a study of two Amazon lakes by Devol et al. (1984), was included. However, release of bubbles may also be influenced by variations in hydrostatic pressure caused by decreases in atmospheric pressure or water level, by bottom-shear owed to currents or waves, or possibly by disturbances from fish or benthic invertebrates (as summarized in Barbosa et al., 2021). These processes are not represented in the current model. Tang et al. (2010) illustrated effects of variations in water level and atmospheric pressure on ebullition in modifications of a process-based wetland model. Barbosa et al. (2021) show an exponentially increasing rate of ebullition as water levels fall at increasing rates with data for Lake Janauacá.

The rising and dissolution of bubbles through the water column are based on equations developed for oceans, as described by Tan et al. (2015). A suite of physical processes including how hydrostatic pressure influences rise rates, bubble expansion and exchange with water in relation to pressure differences and surface tension, could be added, though doing so requires new parameterizations and assumptions. An alternative approach is provided by McGinnis et al. (2006) and Langenegger et al. (2019).

##### 4.1.2.3. Methane Production

Several factors influence the production of methane, including temperature, supply and metabolic availability of organic matter, redox conditions and microbial activity (Bridgman et al., 2013; Grasset et al., 2021; D'Ambrosio & Harrison, 2022). ALBM used temperatures based on measurements and thermal simulations, and  $Q_{10}$  for relevant processes were obtained from the literature or calibrated. The type and fraction of sediment utilized for methane production in Amazon lakes is not known and was not differentiated by the model. Furthermore, the nature of microbial communities and their influence on methane production are not known for Amazon lakes.

Using chambers deployed over sediments with water slowly circulating within the chamber, Smith-Morrill (1987) measured methane fluxes from sediments under anoxic water in Lake Calado, an Amazon floodplain lake similar to Lake Janauacá, of  $\sim 30\text{--}50 \text{ mmol CH}_4 \text{ m}^{-2} \text{ d}^{-1}$ . This flux is indicative of methanogenesis in the sediments, though not actual rates of methanogenesis. Given the variations of sediments on Amazon floodplains, further studies will likely reveal different methane production rates associated with different sediments (Guyot et al., 2007; Hedges et al., 1986; Martinelli et al., 2003; Moreira-Turcq et al., 2013; Smith et al., 2003). However, as reviewed by D'Ambrosio and Harrison (2022), a wide range of approaches, including sediment incubations, benthic chambers, and models, have been utilized to estimate methane and production and sediment fluxes, all of which have limitations.

##### 4.1.2.4. Methane Oxidation Under oxic Conditions

Simulated rates of methane oxidation varied among seasons and between the main lake and embayment (Table S4 in Supporting Information S1). These results are considerably lower, with a few exceptions, than measurements

of methane oxidation in oxic water of the main lake and embayment in Lake Janauacá during rising, high, falling and low water levels reported by Barbosa et al. (2018). In that study, CH<sub>4</sub> oxidation was measured as the CH<sub>4</sub> concentration decline over time following the procedure proposed by Utsumi et al. (1998). Volumetric CH<sub>4</sub> oxidation rates ranged from 0.4 to 11 mmol CH<sub>4</sub> m<sup>-3</sup> d<sup>-1</sup>, averaging 2.8 mmol CH<sub>4</sub> m<sup>-3</sup> d<sup>-1</sup> in the embayment and from 0.1 to 5 mmol CH<sub>4</sub> m<sup>-3</sup> d<sup>-1</sup>, averaging 1.8 mmol CH<sub>4</sub> m<sup>-3</sup> d<sup>-1</sup> in the main lake. Rates were higher near the oxycline. Depth-integrated rates averaged 9.1 mmol CH<sub>4</sub> m<sup>-2</sup> d<sup>-1</sup> in the embayment and 15.7 mmol CH<sub>4</sub> m<sup>-2</sup> d<sup>-1</sup> in the main lake, which often had a deeper oxic zone.

Methane concentrations, dissolved oxygen and temperature are included in the algorithm used for methane oxidation. The range of values used to bound the calibration of  $O_{max}$  are from Barbosa et al. (2018), and the calibrated values range over an order of magnitude (Tables 3 and 4). The fixed values of the Michaelis-Menten constants ( $k_{O_2}$  and  $k_{CH_4}$ ) are from Seger's (1998) literature review and a calibrated value derived for a study of boreal lakes (Guo et al., 2020); these may need further modification for the conditions in tropical floodplain lakes. For example, methane oxidation rates decreased by 25%–60% as  $k_{O_2}$  varied from 50,000 to 150,000; the fixed value used was 78,000.

Barbosa et al. (2018) found a positive relation between volumetric rates of methane oxidation ( $M_{ox}$ , expressed as mg C m<sup>-3</sup> d<sup>-1</sup>) and initial dissolved CH<sub>4</sub> concentrations ( $[CH_4]$ , expressed as μmol L<sup>-1</sup>). An incorrect equation is shown in Barbosa et al. (2018) for this relation; the correct equation is  $M_{ox} = 65.8 [CH_4] - 1.4$ . Thottathil et al. (2019) developed a model of the kinetics of CH<sub>4</sub> oxidation based on temperature, CH<sub>4</sub> concentrations and non-linear effect of DO concentrations, expressed by an equation in general and with the fitted parameters specific to a set of northern lakes. The applicability of this relation to other types of lakes has yet to be tested.

Further complexity is indicated by the observations of Morana et al. (2020) that methanotrophy was decreased as sunlight increased in tropical African lakes.

#### 4.1.2.5. Processes Influencing DO Concentrations

Methane production and oxidation are influenced by DO concentrations, which result from processes supplying or consuming DO, including algal photosynthesis, methane oxidation, water-column respiration and SOD plus exchange with the atmosphere. Several modifications were made to the algorithms modeling DO changes in ALBM to suit conditions in tropical floodplain lakes. One difference from previous versions of ALBM is the use of chlorophyll-a concentrations and expressing processes per Chla. Instead of modeling growth and losses of small-sized (e.g., cyanobacteria) and large-sized (e.g., diatoms) phytoplankton, measured Chla concentrations are an input, and chlorophyll-specific rates of photosynthesis and community respiration are incorporated into the model and calibrated with field data. In addition, SOD was added given the warm temperatures, shallow water and organic-rich sediments in tropical floodplain lakes.

Simulated rates of photosynthesis varied among seasons and between the main lake and embayment (Table S5 in Supporting Information S1). These results are generally lower than measurements in Lake Janauacá and in several similar lakes. Amaral et al. (2018) reported rates of planktonic photosynthesis in Lake Janauacá from 67 to 2,950 mmol O<sub>2</sub> m<sup>-2</sup> d<sup>-1</sup> spanning the period from September 2015 to May 2016 in the main lake and embayment. Forsberg et al. (2017) reported areal photosynthetic rates of  $95 \pm 65$  (±SD,  $n = 90$ ; range 4.7–361) mmol O<sub>2</sub> m<sup>-2</sup>d<sup>-1</sup> for Amazon floodplain lakes influenced by sediment and nutrient-rich rivers.

Simulated rates of photosynthesis are based on simplified equations and parameter values from several sources.  $Ph_{max}$  values are within the range reported by Forsberg et al. (2017). The light inhibition and limitation coefficients ( $K_I$  and  $K_2$ ) are based on laboratory incubations at a series of temperatures and light levels of phytoplankton and are unlikely to be appropriate for the phytoplankton in Amazon floodplain lakes.

Simulated rates of planktonic respiration varied among seasons and between the main lake and embayment (Table S6 in Supporting Information S1). Some results are similar and others different from measurements in Lake Janauacá reported by Amaral et al. (2018) and for several similar lakes surveyed by Forsberg et al. (2017). For example, Amaral et al. (2018) reported rates of aerobic plankton respiration in Lake Janauacá of 97 mmol O<sub>2</sub> m<sup>-3</sup> d<sup>-1</sup> in the lake and 56 mmol O<sub>2</sub> m<sup>-3</sup> d<sup>-1</sup> in the embayment. For Amazon floodplain lakes influenced by sediment and nutrient-rich rivers Forsberg et al. (2017) reported volumetric respiration rates of  $48 \pm 30$  (±SD,  $n = 97$ ; range 7.5–210) mmol O<sub>2</sub> m<sup>-3</sup>d<sup>-1</sup> and areal rates of  $193 \pm 118$  (±SD,  $n = 95$ ; range 14–525) mmol O<sub>2</sub> m<sup>-2</sup>d<sup>-1</sup>. Additional estimates of water-column respiration reported by Vidal et al. (2015) in five

Amazon floodplain lakes ranged from  $\sim 0.5$  to  $1.5 \text{ mmol O}_2 \text{ m}^{-3} \text{ h}^{-1}$  during high water and from  $0.6$  to  $4.3 \text{ mmol O}_2 \text{ m}^{-3} \text{ h}^{-1}$  during low water; as 24-hr totals, these rates are similar to those by Forsberg et al. (2017) and Amaral et al. (2018).

Sediment oxygen demand depends on the nature of the sediments and whether the overlying water is anoxic or oxic. The sediments of Amazon floodplain lakes sequester some organic carbon and release  $\text{CO}_2$  and  $\text{CH}_4$  to the overlying as a portion of the sedimented carbon is metabolized (Melack & Engle, 2010). As an indication of microbial activity in sediments, a simple model of diagenesis for two small Amazon lakes estimated 6 and  $24 \text{ mmol m}^{-2} \text{ d}^{-1}$  of carbon being oxidized (Devol et al., 1984). Using submerged chambers in an Amazon floodplain lake similar to Lake Janauacá, Smith-Morrill (1987) measured dissolved oxygen uptake during periods when the near-bottom waters were aerobic of  $\sim 50 \text{ mmol m}^{-2} \text{ d}^{-1}$ . For comparison,  $k_s$  values from Stefan and Fang (1994; Table 2), converted to  $\text{mmol m}^{-2} \text{ d}^{-1}$ , are 47 and 310. Simulated SOD values are expressed per  $\text{m}^{-3}$  as an effect on the overlying water, as noted in the Results.

During all simulated periods daily total DO fluxes were from the atmospheric into the water. As examples for the periods illustrated in Figures 6 and 7, fluxes into the embayment were  $53 \text{ mmol m}^{-2} \text{ d}^{-1}$  (Jun 2015) and  $160 \text{ mmol m}^{-2} \text{ d}^{-1}$  (Jan 2016), and fluxes into the main lake were  $166 \text{ mmol m}^{-2} \text{ d}^{-1}$  (Jun 2015) and  $10 \text{ mmol m}^{-2} \text{ d}^{-1}$  (Oct 2015). During low water in October 2015, Chl<sub>a</sub> concentrations were higher ( $58 \mu\text{g L}^{-1}$ ) than other periods, resulting in elevated photosynthesis during day (Table S5 in Supporting Information S1) with periods of DO fluxes from the lake to the atmosphere, reducing the total daily flux into the lake. DO input from the atmosphere is often higher than photosynthetic DO production and is an important term among the terms influencing DO concentrations.

#### 4.1.2.6. Diel Variations

Diel cycles of stratification and mixing influence the fluxes of methane by changing the vertical distribution of dissolved methane and oxygen and gas exchange across the air-water interface. Diel patterns of stratification and mixing are characteristic of shallow tropical waters, and are conspicuous in Lake Janauacá for temperatures, dissolved oxygen and methane (Figures 6 and 7, Figures S2, S3, S6, S7 in Supporting Information S1). Measurements in Lake Janauacá indicate that near-surface  $\text{CH}_4$  concentrations, fluxes and gas exchange velocities were variable over 24-hr periods (Barbosa et al., 2020). Values were higher during the day, but a statistically significant difference between day and night was only found for diffusive fluxes in the embayment. This result is consistent with the day-night differences in wind speed, that were statistically significantly higher during the day. Visual inspection of Figures 4 and 5, Figures S1 and S9 in Supporting Information S1 is suggestive of day-night differences for some periods, and also considerable temporal variability per hour. We did not perform extended simulations to allow a quantitative analysis of day-night proportions.

## 4.2. Challenges and Limitations of Models

### 4.2.1. Structural and Numerical Modeling Issues

As noted by Arhonditsis et al. (2008) and others, because ecological processes can be described by a variety of mathematical relations, and given the uncertainty underlying model structures and data, a single set of parameter values, applicable generally, is not a reasonable expectation, that is, the model equifinality. Instead, evaluation of possible inputs, model structures and parameter values on simulated results is necessary (e.g., Tang & Zhuang, 2008). The sensitivity analyses included demonstrate the relative importance of simulated processes. The ranges of values considered for calibration are based on literature values and, in a few cases, results for Amazon floodplains. Moreover, given the large seasonal variations in environmental conditions, calibrations were done for different hydrological periods, instead of assuming constant values. Although our model simulations reproduce well the observations at our study sites, extrapolating the set of parameters obtained to other Amazon lakes and floodplains remains a challenge. A spatially explicit based model parameterization (e.g., Chen & Zhuang, 2012) might be needed given the heterogeneous Amazonia landscapes. Also, because the calibrated parameters are part of functional relations or rates that are derived from fairly complicated biological measurements, to fully account for the effects of the uncertainties of the observational and experimental data, would require incorporation of insufficiently known quantitative and qualitative uncertainties into the Bayesian calibration.

#### 4.2.2. Methane Fluxes and Related Processes

Seasonal diffusive methane fluxes were simulated well in comparison to field measurements, though short-term temporal variability was represented less well. The veracity of simulated ebullition is less clear given the paucity of comparative field data and the episodic nature of ebullition. Simulated methane oxidation rates were often considerably lower than measured rates which suggests revised coefficients or algorithms are needed. Methanogenesis in sediments is a complex process influenced by biological and chemical conditions with few measurements of in situ rates available for comparison. Hence, the simple parameterization used will depend on further studies for improvement. Three-dimensional results from hydrodynamic modeling, such as advective exchanges with fringing habitats and spatial differences in mixed layer depths and turbulence, could enhance the estimates of methane concentrations and fluxes. Further evaluation of the algorithms used in AEM3D to estimate TKE, and the use of TKE in gas exchange and mixing calculations are recommended.

Several biogeochemical aspects of methane production and consumption are not included in the model. The production of CH<sub>4</sub> via the CO<sub>2</sub> reduction pathway or acetoclastic methanogenesis and associated differences in isotopic fractionation, and the composition of microbial communities active in methane processes are not represented. Methane production in oxic waters has been detected (e.g., Grossart et al., 2011), with several mechanisms supporting the process suggested (Bartosiewicz et al., 2022). However, as is evident in the exchange between Günthel et al. (2021) and Peeters and Hofmann (2021), even in well studied lakes, the magnitude of oxic methane production requires further study that combines analyses of physical and biological processes. Although stable isotope tracer experiments in five tropical African lakes indicated an association of oxic CH<sub>4</sub> production and phytoplankton metabolism, CH<sub>4</sub> emissions to the atmosphere were predominantly supported by CH<sub>4</sub> generated in sediments and physically transported to near-surface waters (Morana et al., 2020). Anaerobic oxidation of methane (AOM) can occur in marine and freshwater sediments and depends on availability of terminal electron acceptors such as sulfate, nitrate, iron, manganese and organic acids (Knittel & Boetius, 2009; Reed et al., 2017; Roland et al., 2021). For example, Martinez-Cruz et al. (2018) measured potential rates of AOM based on incubations of sediment slurries spiked with <sup>13</sup>CH<sub>4</sub> from arctic, temperate and tropical lakes. The importance of AOM in lakes and reservoirs is uncertain and depends on several interacting chemical, physical and microbial processes not well constrained with available data. In sediments of Amazon floodplain lakes, concentrations of potential terminal electron acceptors in lake and pore waters are low (Furch, 1997), though AOM could be occurring.

#### 4.2.3. Regionalization in Time and Space

Key challenges to regionalization of methane fluxes in the Amazon basin are the large seasonal variation in inundated areas and habitats, the wide variety of aquatic ecosystems throughout the Amazon basin, and the variability in methane fluxes in time and space (Melack et al., 2022). Models, such as those discussed here, offer one approach to regionalization of methane fluxes. To do so would entail seasonal and annual simulations that require modification of the hydrodynamic and biogeochemical models to run efficiently for longer times and with different inputs than in the versions presented. Downscaled reanalysis meteorological products can be utilized. Remote sensing estimates of inundation at multiple temporal and spatial scales are now available (Fassoni-Andrade et al., 2021; Fleischmann et al., 2021; Parrens et al., 2019). Incorporation of hydrological and hydraulic models of inundation are also essential, and several such models are available and have been applied successfully to the Amazon basin (Ji et al., 2019; Paiva et al., 2013; Rudorff et al., 2014).

Though several wetland models have been applied to Amazon wetlands, these are not well designed for the conditions on floodplains. For example, the Joint UK Land Environment Simulator (JULES) (Clark et al., 2011), the Lund-Potsdam-Jena model (LPJ-WSL; Zhang et al., 2016), LPX-Bern model (Ringeval et al., 2014), and WetCHARTs (Bloom et al., 2017), do not explicitly include methanogenesis, methane oxidation, mixing through the water, ebullition, or air-water exchange. In these models, grid-average methane fluxes are controlled by soil temperature and carbon availability or heterotrophic respiration. Walter and Heimann (2000), TEM-MDM (Zhuang et al., 2004), JPL-WHyMe (Wania et al., 2010) and CLM4Me (Riley et al., 2011) model diffusive emission as molecular diffusion through soil layers.

Optical and trophic conditions vary considerably among Amazon floodplain lakes (Melack et al., 2009, 2021). Hence, simulations of methane fluxes from lakes throughout the region will require modifying parameter values and inputs from those used for Lake Janauacá. In addition to incorporation of data from field studies, remote sensing offers approaches for estimating chlorophyll, suspended sediment and dissolved organic matter

concentrations, though the optically complex waters add analytical difficulty and uncertainty (Fassoni-Andrade & Paiva, 2019; Novo et al., 2006; Sayers et al., 2015; Silva et al., 2019).

Another difficulty is the variable mosaic of habitats, including open water, flooded forests, and floating herbaceous plants, as inundation changes through the year (Hess et al., 2015; Melack & Hess, 2010). Floodplain bathymetry is an essential aspect of the occurrence and variations in these habitats, and remote sensing techniques can be used to estimate bathymetry (Fassoni-Andrade et al., 2020). A more complete model needs to incorporate temporal changes in habitat areas and water levels and lateral exchanges between interconnected habitats to calculate methane emissions. Furthermore, environmental conditions and processes influencing methane fluxes differ among open water and inundated vegetated areas as shown by fluxes from water surfaces in floating herbaceous plants and flooded forests measured by Barbosa et al. (2020) and from tree trunks by Pangala et al. (2017) and Gauci et al. (2021). However, modeling plant-mediated transport is premature given the lack of a mechanistic understanding of the processes, large diversity of plants and highly variable fluxes, though clearly needed as relevant information becomes available. Additionally, as water levels fall, large areas shift to unflooded land with extensive areas of woody and herbaceous vegetation and exposed sediments. Models of methane uptake or release by soils and possibly via plants under these conditions could be adapted from terrestrial models such as TEM (Liu et al., 2020; Tang et al., 2010; Zhuang et al., 2013). Therefore, a comprehensive model of methane fluxes associated with Amazon floodplains requires further model developments.

## Appendix A: Terms and Names of Modeled and Physical Variables, and Parameters and Coefficients

Terms and names of modeled and physical variables, and parameters and coefficients are listed for fixed values (\*) and # calibrated (#) values. Units are shown as usually reported, not at time-step of simulations.

### Term Name, units

$P$	Methanogenesis in sediment, $\mu\text{mol m}^{-2}\text{s}^{-1}$
$R_c$	#Carbon mineralization rate, $\mu\text{mol m}^{-2}\text{s}^{-1}$
$\alpha_z$	#Coefficient of decrease in $P$ with sediment depth, unitless
$PQ_{10}$	# $Q_{10}$ factor for $P$ , unitless
$T_s$	Sediment temperature, $^{\circ}\text{C}$
$T_{p0}$	*Reference temperature for $P$ , $^{\circ}\text{C}$
$z_s$	Depth in sediment, $m$
$C_{CH_4s}$	Methane concentration in sediment, $\mu\text{mol L}^{-1}$
$K_{ms}$	*Molecular diffusivity in sediment, $\text{m}^2 \text{s}^{-1}$
$\alpha_{CH_4}$	Percentage of methane in bubbles, %
$E_s$	Ebullition, $\text{mmol m}^{-2} \text{d}^{-1}$
$\alpha_e$	#Saturation level of sediment methane concentration, unitless fraction
$C_{CH_4w}$	Methane concentration in water column, $\mu\text{mol L}^{-1}$
$t$	Time, $s$
$K_z$	Eddy diffusivity, $\text{m}^2 \text{s}^{-1}$
$K_m$	*Molecular diffusivity, $\text{m}^2 \text{s}^{-1}$
$E_{CH_4w}$	Gas exchange with bubbles, $\mu\text{mol m}^{-3} \text{s}^{-1}$
$F_{\text{met}}$	Diffusive methane flux at water-air interface, $\mu\text{mol m}^{-2} \text{h}^{-1}$
$z$	Depth in water, $m$
$\epsilon$	Dissipation rate of turbulent kinetic energy, $\text{m}^2 \text{s}^{-3}$
$N$	Brunt-Vaisala frequency, $\text{s}^{-1}$
$\rho$	Density of water, $\text{kg m}^{-3}$
$O$	Aerobic methane oxidation, $\mu\text{mol m}^{-3} \text{s}^{-1}$
$O_{\text{max}}$	#Methane oxidation potential, $\mu\text{mol m}^{-3}\text{s}^{-1}$
$OQ_{10}$	* $Q_{10}$ factor for $O$ , unitless
$T_w$	Water temperature, $^{\circ}\text{C}$
$T_{O0}$	*Reference temperature for $O$ , $^{\circ}\text{C}$
$k_{O_2}$	*Michaelis-Menten constant for $O$ , $\mu\text{mol m}^{-3}$
$k_{CH_4}$	*Michaelis-Menten constant for $O$ , $\mu\text{mol m}^{-3}$

$C_{O_2}$	Concentration of dissolved oxygen in water column, $\text{mg L}^{-1}$
$Ph$	Oxygen production by photosynthesis, $\text{mg L}^{-1}$
$R$	Community respiration, $\text{mg L}^{-1}$
$SOD$	Sediment oxygen demand, $\text{mg m}^{-2} \text{h}^{-1}$
$F_{\text{oxg}}$	Oxygen exchange at air-water interface, $\text{mg m}^{-2} \text{h}^{-1}$
$Ph_{\text{max}}$	#Chla-specific light-saturation rate of photosynthesis, $\text{mg O}_2(\text{mg Chla})^{-1} \text{s}^{-1}$
$\theta_p$	*Temperature coefficient for photosynthesis, unitless
$I$	Incident irradiance, $\mu\text{mol photons m}^{-2} \text{s}^{-1}$
$C_{\text{Chla}}$	Chla concentration, $\text{mg Chla m}^{-3}$
$K_1$	*Light inhibition coefficient, $\text{mol m}^{-2} \text{s}^{-1}$
$K_2$	*Light limitation coefficients, $\text{mol m}^{-2} \text{s}^{-1}$
$R_r$	#Chla-specific respiration rate at $30^\circ\text{C}$ , $\text{mg O}_2(\text{mg Chla})^{-1} \text{s}^{-1}$
$\theta_r$	*Temperature coefficient for respiration, unitless
$k_s$	#Sediment oxygen demand at $20^\circ\text{C}$ , $\text{mg O}_2 \text{m}^{-2} \text{s}^{-1}$
$\theta_s$	*Temperature coefficient for SOD, unitless
$A$	Sediment area, $\text{m}^2$
$F$	Diffusive gas flux at the air-water interface, $\mu\text{mol m}^{-2} \text{h}^{-1}$
$k_{600}$	Gas transfer velocity normalized to $\text{CO}_2$ at $20^\circ\text{C}$ , $\text{cm h}^{-1}$
$C_w$	Near-surface gas concentration, $\mu\text{mol L}^{-1}$
$C_{eq}$	Near-surface concentration in equilibrium with atmosphere, $\mu\text{mol L}^{-1}$
$\nu$	Kinematic viscosity, $\text{m}^2 \text{s}^{-1}$
$Sc$	Schmidt number, unitless

## Data Availability Statement

Measurements and simulated results presented are available from the KNB data repository operated by NCEAS at <https://doi.org/10.5063/F1833QFM> (Guo et al., 2023). The revised ALBM code is available from the Purdue Research Repository at <https://doi.org/10.4231/4WN4-S032> (Guo & Zhuang, 2023).

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