

Hybrid Lake Model (HyLake) v1.0: unifying deep learning and physical principles for simulating lake-atmosphere interactions

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Abstract. Lake-atmosphere interactions, which significantly modulate the impacts of climate change on water and heat exchange on land-air water and heat exchange, playing a critical role in Earth systems dynamics. However, modeling key indicators of these interactions, i.e., lake surface temperature (LST), latent heat (LE) and sensible heat (HE) fluxes, remains challenges. This stems from oversimplified physics in traditional process-based models and the limited interpretability of purely data driven "black-box" structure. Hybrid models that unifying physical principles with sparse observations offer a promising solution for simultaneously predicting lake-atmosphere interactions.

This study presents the Hybrid Lake Model v1.0 (HyLake v1.0), which integrates a Bayesian Optimized Bidirectional Long Short-Term Memory-based (BO-BLSTM-based) surrogate trained on data from Meiliangwan (MLW) site in Lake Taihu to approximate LST dynamics. LE and HE are subsequently derived using surface energy balance equations. We intercompare HyLake v1.0 against the Freshwater Lake (FLake) model and hybrid lake models using different surrogates (Baseline and TaihuScene) across multiple Lake Taihu sites. Forcing datasets include eddy flux covariance observations and ECMWF Reanalysis v5 (ERA5) datasets.

Results demonstrate HyLake v1.0's capability to predict lake-atmosphere interactions with satisfactory performance. At MLW, HyLake v1.0 outperformed the best among all models, achieving R and RMSE of 0.99 and 1.08 °C for LST, R and RMSE of 0.94 and 24.65 W/m² for LE and R and RMSE of 0.93 and 7.15 W/m² for HE, respectively. To assess model generalization and transferability in ungauged lake sites, HyLake v1.0 exhibited superior performance across all lake sites compared to FLake and TaihuScene, with MAEs of 0.85 °C (LST), 21.56 W/m² (LE) and 6.63 W/m² (HE). When forced by ERA5 datasets, HyLake v1.0 outperformed benchmarks for 14 of 15 variables (including LST, LE, and HE across 5 lake sites), yielding MAEs of 0.90 °C (LST), 35.02 W/m² (LE) and 7.97 W/m² (HE). It indicates strong capacity for application with unlearned forcing datasets. HyLake v1.0 exhibits excellent skill in estimating lake-atmosphere interactions for untrained lake sites, supporting its potential for extending the application to other ungauged lakes. This advancement promotes hybrid modeling techniques in Earth system science, enhancing understanding of land-atmosphere interaction dynamics.

1 Introduction

Lakes are a critical component of [Earth](#) system and serve as sensitive indicators of climate-land surface [interactions](#) (O'Reilly et al., 2015; W. J. Wang et al., 2024). [Lake](#) surface temperature (LST) plays a key [role](#) in lake-atmosphere systems, which also regulates the hydro-biogeochemical processes (e.g., evaporation rate, ice cover, mixing regime, and thermal storage) (Tong et al., 2023; Culpepper et al., 2024; Woolway et al., 2020). It has been observed that LST has risen globally at a rate of 0.34 °C per decade, driving shifts in biodiversity and altering ecosystem services within aquatic environments, with far-reaching consequences for [global](#) climate (W. J. Wang et al., 2024; Woolway et al., 2020). These trends highlight the severe threats posed by climate change to global lake ecosystems in recent decades (Carpenter et al., 2011; Woolway et al., 2020).

Accurately predicting LST under pronounced climate change benefits from positioning the cascade of physical and biogeochemical [changes in lakes](#), such as algal blooms, lake heatwave and cold spells (O'Reilly et al., 2015; X. W. Wang et al., 2024a; X. W. Wang et al., 2024b; Woolway et al., 2024). A variety of lake [thermodynamics](#) models has been developed to predict LST, including statistical models, process-based models, and machine learning (ML) models. Process-based lake [thermodynamics](#) models, such as the Freshwater Lake model (FLake) ([Mironov et al., 2010](#)), the General Lake Model (GLM) ([Hipsey et al., 2019](#)), and [the lake thermodynamics model in Weather Research & Forecasting Model \(WRF-Lake\) \(Gu et al., 2015\)](#), are built on relationships between climate variables and LST, often employing simplified assumptions based on empirical physical principles (Mironov et al., 2010; Piccolroaz et al., 2024; L. J. Xu et al., 2016). However, these models are limited in their capacity to incorporate data-driven information and require extensive datasets for calibration and parameterization, which specifically pose significant challenges in data-scarce regions (Shen et al., 2023). In contrast, statistical models, such as the Air2Water model, are often applied in well-mixed lakes and rely on mathematical relationships between forcing variables and LST without incorporating mechanistic linkages (Piccolroaz et al., 2020; W. J. Wang et al., 2024). While these models are simpler and require fewer forcing data, they are constrained by the size of high-quality observational data, limiting their applicability across different lakes (Huang et al., 2021). ML models, considered a subset of statistical models, offer greater complexity and automation by leveraging large datasets (Piccolroaz et al., 2024; Wikle & Zammit-Mangion, 2023). ML models, such as Artificial Neural Networks (ANNs) and Long Short-Term Memory (LSTM) networks, have demonstrated superior performance in reconstructing LST compared to purely process-based models across global lakes (Almeida et al., 2022; Willard et al., 2022). These models excel at capturing complex relationships from datasets, however, their reliance on large training datasets, high computational costs, and the opaque "black-box" structure of their predictions present significant challenges. Specifically, their lack of transferability and explainability often make them less preferable (Korbmacher & Tordeux, 2022; Piccolroaz et al., 2024). [These](#) limitations in predicting lake-atmosphere interactions highlight the need for hybrid approaches [combining](#) the strengths of process-based and data-driven [models](#).

Hybrid models combine the physical principles of process-based models with the data-driven models, offering a multi-output structure that enhances both explainability and transferability while maintaining the flexibility and accuracy of data-driven models (Kurz et al., 2022; Piccolroaz et al., 2024). For example, Read et al. (2019) developed a hybrid deep-learning-based

framework that integrates an energy balance-guided loss function from GLM with a Recurrent Neural Network (RNN) to reconstruct LST. This hybrid approach, which embedded the physical principles into deep-learning-based models, outperforms process-based models when transferred to unmonitored lakes (Willard et al., 2021). Nevertheless, such models face challenges related to computational expense, explainability and transferability in ungauged lakes and periods (Raissi et al., 2019; Willard et al., 2023). Alternatively, hybrid models can incorporate ML-based surrogates into process-based backbones, where surrogates replace processes with insufficient physical understanding, enabling multiple outputs to be predicted simultaneously. These models, widely used in hydrological models, combine physical principles with ML-based surrogates, offering improved interpretability, generalizability, and transferability capabilities in ungauged regions (Shen et al., 2023). Specifically, Feng et al. (2022) embedded neural networks into the Hydrologiska Byråns Vattenbalansavdelning (HBV) hydrological model to predict multiple physical outputs, achieving performance comparable to purely data-driven models. Similarly, L. J. Zhong et al. (2024) developed a distributed framework integrating ML and traditional river routing models to predict streamflow. These hybrid approaches outperform traditional process-based models and require relatively less training data by involving the integration of physical constraints, thereby providing a powerful tool for uncovering previously unrecognized physical relationships (Shen et al., 2023). Lake-atmosphere interactions represent a tightly coupled system (B. B. Wang et al., 2019), where process-based models traditionally approximate the interdependence between LST, latent heat (LE) and sensible heat (HE) fluxes. The increasing LST influences these fluxes, while the emitted heat fluxes act as boundary conditions that in turn affect LST (Woolway et al., 2015). Thus, the development of novel hybrid lake models is promising in offering improved approximations and advance our understanding of lake-atmosphere interactions.

Lakes exhibit considerable regional variability, making it challenging to conduct long-term and large-scale observations (Zhang et al., 2019). Traditional lake models seem challenging to be generalized in ungauged lake or even regions in a large lake. Lake Taihu, the third largest freshwater lake in China, which indicates a significant regional difference in its biological characteristics (Table 1), has experienced severe deterioration in water quality, thereby significantly threatening drinking water security (Zhang et al., 2020; Yan et al., 2024). These issues have prompted extensive field investigations and data collection in Lake Taihu, providing rich observational data for lake-atmosphere modeling. Specifically, the Lake Taihu Eddy Flux Network has supported long-term observations of microclimate, radiation, and energy fluxes, offering a valuable dataset for the development of hybrid lake models (Zhang et al., 2020). To improve novel hybrid modeling techniques and enhance the understanding of lake-atmosphere interactions, the objectives of this study are to (1) develop a novel hybrid lake model HyLake v1.0 by embedding LSTM-based surrogate into process-based model; (2) validate the performance of HyLake v1.0 in LST, LE, and HE based on observations from Taihu Lake Eddy Flux Network; and (3) evaluate the transferability of HyLake v1.0 in ungauged lake sites with different biological characteristics using ECMWF Reanalysis v5 (ERA5) forcing datasets. The results will provide reliable evidence for improving lake-atmosphere interactions modeling by unifying physical principles and deep learning in ungauged regions.

2 Materials and Methodology

2.1 Study area and datasets

Lake Taihu (30.12–32.22°N, 119.03–121.91°E), located in the Yangtze Delta, is the third-largest freshwater lake in China, covering an area of 2,400 km² with an average depth of 1.9 m, with a rapid increasing rate of ~0.37 °C/decade in LST (Yan et al., 2024; Zhang et al., 2020; Zhang et al., 2018). As a typical urban lake, Lake Taihu is situated in one of the most densely populated regions of China. It has experienced significant eutrophication, characterized by recurrent algae blooms that threaten local drinking water security (Yan et al., 2024). Given the pressing need to understand the challenges surrounding water quality improvement and hydro-biogeochemical processes in Lake Taihu, this study employs the lake models to assess these issues across 5 distinct sites from the Taihu Lake Eddy Flux Network (Zhang et al., 2020): Meiliangwan (MLW), Dapukou (DPK), Bifenggang (BFG), Xiaoleishan (XLS), and Pingtaishan (PTS) (Figure 1, Table 1). These sites span varying biological characteristics and eutrophication gradients, offering a comprehensive view on lake ecological diversity (Zhang et al., 2020), providing a solid data base for evaluating the generalizability and transferability of lake models. Specifically, MLW (31.4197°N, 120.2139°E) as the first lake site in Lake Taihu Eddy Flux Network, located at the northern shore of the lake in MLW Bay, has a biological characteristic of eutrophication. BFG (31.1685°N, 120.3972°E) is located in the eastern shore of Lake Taihu, features a submerged macrophyte community and relatively clean water. PTS (31.2323°N, 120.1086°E), situated centrally in the lake, has experienced significant algae blooms and lacks aquatic vegetation. DPK (31.2661°N, 119.9312°E), located on the western shore of Lake Taihu, is marked by severe eutrophication and deeper water; while XLS (30.9972°N, 120.1344°E), located on the southern shore of Lake Taihu, is a vegetation-free, clean water site (Zhang et al., 2020).

The datasets included two parts: (1) hydrometeorological variables observed from the Taihu Lake Eddy Flux Network to force and validate the models, and (2) meteorological variables from ERA5 datasets to fill the gaps of observations and force the models. Within the network, each site is equipped with an eddy covariance system that continuously monitors LE and HE using sonic anemometers and thermometers (Model CSAT3A; Campbell Scientific, Logan, UT, USA) positioned 3.5 to 9.4 m above the lake surface. Hydrometeorological variables, including air humidity and temperature (Model HMP45D/HMP155A; Vaisala, Helsinki, Finland), wind speed (Model 03002; R.M. Young Co., Traverse City, MI, USA), and net radiation components (Model CNR4; Kipp & Zonen, Delft, the Netherlands), are also measured. These meteorological variables were used to force lake models while LE, HE and LST from observations were used to validate the results of each numerical experiment, on top of which, the inferred radiative LST, were collected at 30-minute intervals that are publicly accessible via Harvard DataVerse (Lee, 2004; Zhang et al., 2020; <https://doi.org/10.7910/DVN/HEWCWM>). The dataset spans from 2012 to 2015 and contains several data gaps across these lake sites. Specifically, 475 time steps (~1.36%) of observed surface pressure were found missing at the DPK site during 2012 and 2015; 7,959 time steps (~22.71%) of all observed variables were missing at the XLS site; 12,539 time steps (~35.78%) of all observed variables were missing at the PTS site. Observations at the MLW and BFG sites were complete during the entire study periods. In the evaluation of all observations-forced experiments, the data gaps of observed variables in these lake sites were directly filled by ERA5 datasets at the corresponding time steps to

predict lake-atmosphere interactions. In this study, observed meteorological variables from the MLW site, an eutrophic lake site that presents the trophic status of Lake Taihu (Table 1, Wang et al., 2019), are used to train the Long Short-Term Memory (LSTM)-based surrogates (Sect. 2.2), while data from the remaining sites serve to evaluate the generalization of HyLake v1.0 and train the LSTM-based surrogates. To further address the generalization and transferability of HyLake v1.0 across different forcing datasets, this study utilized 8 meteorological variables that obtained from hourly ERA5 datasets from 2012 to 2015, with a spatial resolution of 0.25° at a single level to force HyLake v1.0. These datasets, available from the Climate Data Store (Hersbach et al., 2020; <https://cds.climate.copernicus.eu>), include variables such as air temperature, dew point temperature, surface pressure, wind speed, and surface net longwave and shortwave radiation, which has similar probability distribution to observations across Lake Taihu (Figure S1). The ERA5 datasets are also individually used to force FLake and TaihuScene for comparison and predict lake-atmosphere interactions in Lake Taihu, providing insights into the model's generalization, transferability and performance using different climatic forcing datasets.

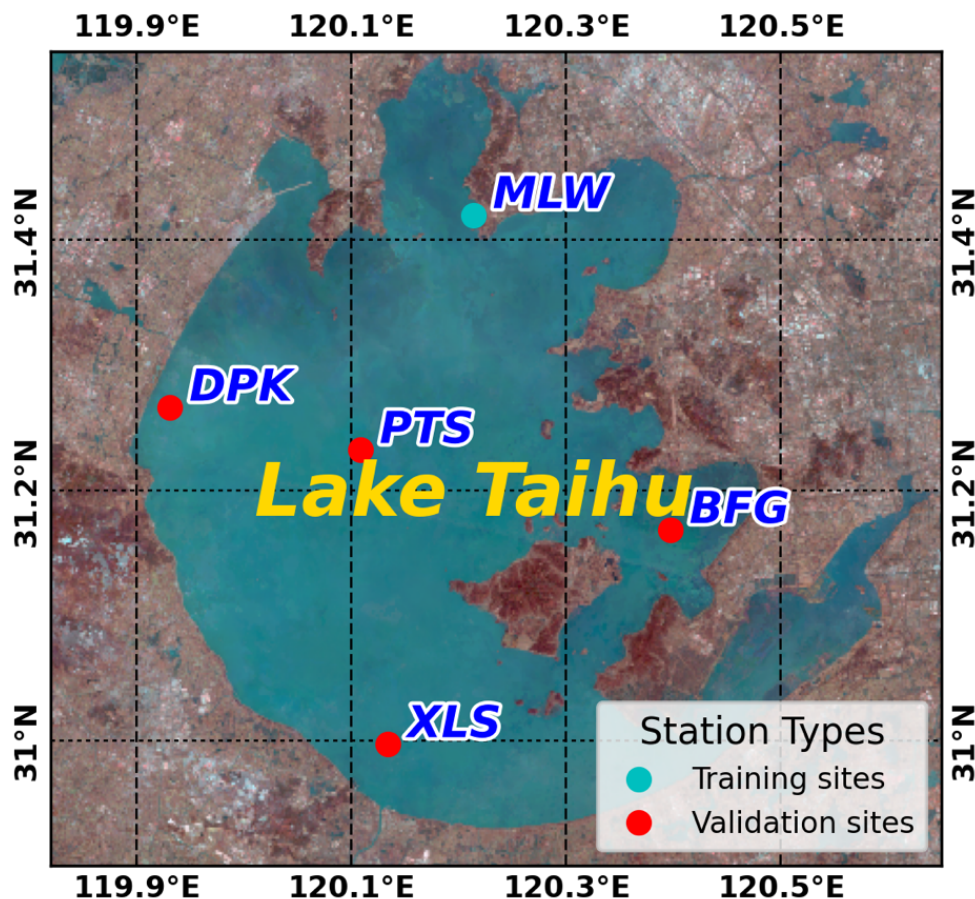


Figure 1: The locations of Lake Taihu and the five eddy covariance lake sites (MLW, DPK, BFG, XLS, and PTS) are shown in cyan and red bubbles, overlaid on a true-color image from Landsat 8. MLW as a training site was used to train BO-BLSTM-based surrogate, while the other validation sites were adapted as ungauged sites to validate the HyLake v1.0 performance.

Table 1. Information for selected lake sites in Lake Taihu.

Site	MLW	DPK	BFG	XLS	PTS
Lat. (°N)	31.4197	31.2661	31.1685	30.9972	31.2323
Lon. (°E)	120.2139	119.9312	120.3972	120.1344	120.1086
Start date	Jun 2010	Aug 2011	Dec 2011	Nov 2012	Jun 2013
Biology	Eutrophic	Super eutrophic	Submerged macrophyte	Transitional	Mesotrophic
Purpose	Train	Validation	Validation	Validation	Validation

145 **2.2 Model architecture of HyLake v1.0**

HyLake v1.0 is based on the backbone of physical principles from process-based lake models and then couple to a LSTM-based surrogate for LST approximation to further solve the untrained variables (e.g., LE, HE), as schematically shown in Figure 2. The following sections will introduce the architecture of HyLake v1.0 from the physical principles, LSTM-based surrogates and their training strategies, respectively.

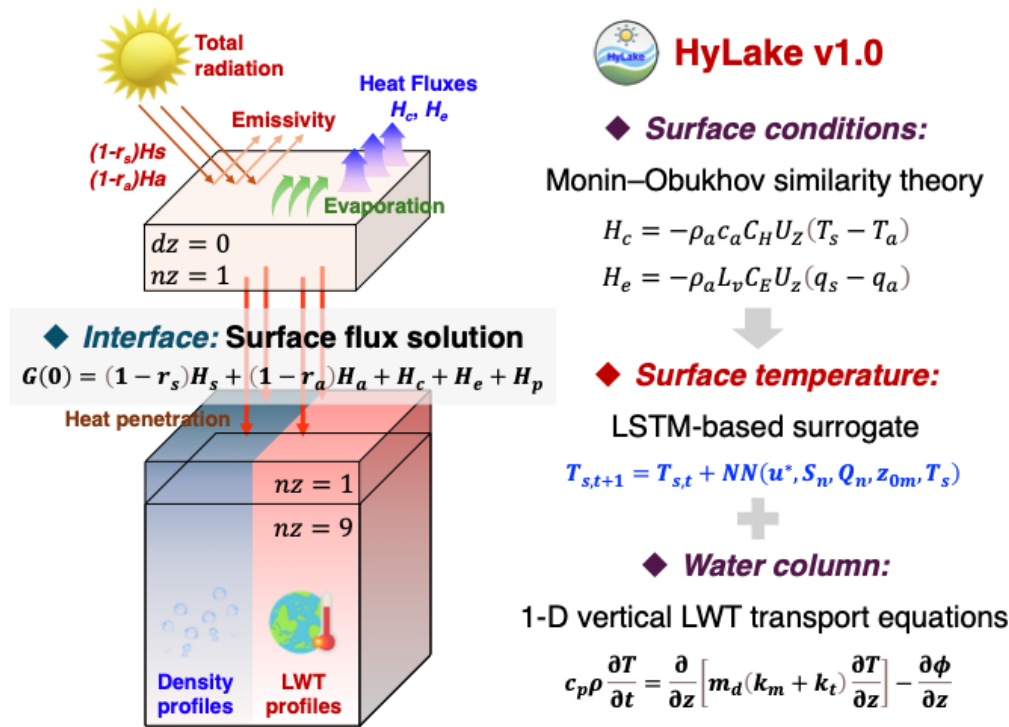


Figure 2: Conceptual model of HyLake v1.0. The LSTM-based surrogates were added to approximate the LST based on the surface conditions that calculated from Monin-Obukhov similarity theory, which further correct the LST in surface flux solution at the next timestep.

2.2.1 Physical principles for lake-atmosphere modeling systems

155 A process-based backbone lake model (PBBM) is separately constructed to serve as the backbone of HyLake v1.0, which
referred to the process-based lake models based on the governing equations and parameterization schemes of previously
validated lake physical processes (Sarovic et al., 2022). The conceptual model of PBBM is depicted in Figure 2 and Table 2.
Specifically, the lake-atmosphere modeling system in PBBM primarily involves energy balance equations for solving LE and
HE at the lake-atmosphere interface and the 1-D vertical lake water temperature transport equations within the water column
160 for solving LST (Piccolroaz et al., 2024).

The changes in LST are primarily driven by the net heat fluxes entering the lake surface. Therefore, the net heat flux is imposed
as a Neumann boundary condition at the upper boundary of the water column. Following Piccolroaz et al. (2024), the net heat
flux $G(0)$ (W/m^2) into the lake surface can be expressed by the energy balance equation:

$$G(0) = (1 - r_s)H_s + (1 - r_a)H_a + H_c + H_e + H_p \quad (1)$$

165 where H_s (W/m^2) and H_a (W/m^2) represent net downward shortwave and longwave radiation (also referred to the net solar and
thermal radiation in ERA5), respectively; r_s and r_a account for the shortwave and longwave albedos of water; the HE and LE
are denoted by H_c (W/m^2) and H_e (W/m^2); H_p represent the heat flux (W/m^2) brought from precipitation, often calculated via
an empirical equation to quantify (Sarovic et al., 2022). All heat fluxes are considered positive in downward direction. The net
shortwave and longwave radiation are derived from observation in Lake Taihu Eddy Flux Network and ERA5 reanalysis
170 datasets.

The sensible (HE, H_c) and latent (LE, H_e) heat fluxes follows the scheme by Verburg and Antenucci (2010) (Figures 2-3):

$$H_c = -\rho_a c_a C_H U_z (T_s - T_a) \quad (2)$$

$$H_e = -\rho_a L_v C_E U_z (q_s - q_a) \quad (3)$$

175 where ρ_a (kg/m^3) donated air density; $c_a = 1005 \text{ J/kg}\cdot\text{K}$ is the specific heat of air; $L_v \approx 2500 \text{ kJ/kg}$ is the LE of vaporization; C_E
and C_H are transfer coefficients for HE and LE derived iteratively with the Monin–Obukhov length based on bulk flux
algorithms; U_z (m/s) is the wind speed at observed height; T_s ($^\circ\text{C}$) accounts for LST solved by 1-D vertical lake water
temperature (LWT) transport equation; and T_a ($^\circ\text{C}$) present the air temperature. Further details on the heat flux calculations
can be found in Verburg and Antenucci (2010) and Woolway et al. (2015).

At the bottom boundary of the 1-D lake model, the zero-temperature-gradient boundary and the zero-flux boundary are
180 imposed as shown in Figure 2, which can be expressed as:

$$\partial T_z / \partial z = 0 \quad (4)$$

$$G(z_{max}) = 0 \quad (5)$$

where T_z ($^\circ\text{C}$) present the lake water temperature; z means the mean lake depth; $G(z_{max})$ (W/m^2) account for the heat exchange
between water column and sediment, which is set to 0 at the bottom boundary.

185 To simulate vertical temperature profiles in the water column (Figure 2), PBBM solves a 1-D vertical lake water temperature
transport equations within a cylindrical water column assumption of constant surface area as follows:

$$c_p \rho \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left[m_d (k_m + k_t) \frac{\partial T}{\partial z} \right] - \frac{\partial \phi}{\partial z} \quad (6)$$

where c_p is the specific heat capacity of water, which is set to 1006 J/kg·K; ρ (kg/m³) present water density, which can be calculated from lake water temperature (T , °C) at different depths; t (s) and z (m) is simulated time and depth of water column respectively; m_d is the enlarge coefficient of thermal conductivity, which is also set to 5 in PBBM; k_m and k_t (W/m·K) are the molecular and turbulent thermal conductivity, respectively; ϕ (W/m²) is defined by the heat flux that penetrate into the lake from net solar radiation. The specific parameterization of PBBM follows the lake module in CLM v5.0 (Subin et al., 2012). The PBBM provides a backbone for HyLake v1.0, which adapted a LSTM-based surrogate to solve the LST instead of solving 1-D vertical lake water temperature transport equations by the implicit Euler scheme (Figure 3a).

2.2.2 LST approximation using LSTM-based surrogates

In PBBM, LST along with the LWT in the 1-D vertical lake water temperature transport equations (Eq. (6)) are typically solved simultaneously using an implicit Euler scheme for numerical stability (Sarovic et al., 2022). This can be expressed in matrix form as:

$$MT^{n+1} = AT^n + B \quad (7)$$

where, M , A and B jointly form the tridiagonal system of equations based on implicit Euler scheme, which can be further decomposed into equations (8) to (10):

$$M = \begin{cases} \frac{-k_m - k_{t,j-1/2}}{z_j - z_{j-1}}, & z = j - 1 \\ \frac{\Delta z_j c_p \rho_j}{\Delta t} + \frac{k_m + k_{t,j+1/2}}{z_{j+1} - z_j} + \frac{k_m + k_{t,j-1/2}}{z_j - z_{j-1}}, & z = j \\ \frac{-k_m - k_{t,j+1/2}}{z_{j+1} + z_j}, & z = j + 1 \end{cases} \quad (8)$$

$$A = \frac{\Delta z_j c_p \rho_j}{\Delta t} \quad (9)$$

$$B = \phi_{j+1/2}^n - \phi_{j-1/2}^n \quad (10)$$

where j denotes the index of each water-column layer (from 1 to 10 in this study); n represents the time step. Δz_j and ρ_j are the thickness and density at j^{th} water column, respectively. The terms $k_{t,j-1/2}$ and $\phi_{j-1/2}^n$ refer to the molecular diffusivity and residual radiation at middle location between $j-1^{\text{th}}$ and j^{th} at n step. All other variables in these equations follow the same notations and definitions as given previously.

It has been demonstrated that LSTM could capture historical time-step dependencies and handle variable-length input sequences using gradient optimization combined with backpropagation in hydrological applications (J. Liu et al., 2024). Bayesian LSTM (as an improved LSTM) adapts probability distributed weight parameters, which reduces the model overfitting, thereby providing robust predictions in hydrology (D. Li et al., 2021; Lu et al., 2019). The development of LSTM-based surrogates offers the possibility of accurate predictions in addressing the critical processes in lake-atmosphere modeling systems. HyLake v1.0 and other hybrid lake models, including Baseline and TaihuScene, employed LSTM-based surrogates rather than the implicit Euler scheme in process-based models to solve LST for each time step (Figure 3a). Specifically, several

sequence-to-one LSTM-based surrogates are adapted to be trained to approximate ΔLST (the difference of LST between two time steps) based on dynamic inputs, including time series of historical 24-step variables of LST, friction velocity (u^* , m/s), surface roughness length (z_{0m} , m), and $G(0)$. These dynamic parameters were calculated from the outputs of surface flux solutions based on the observations. Thus, to address the numerical stability of autoregressive prediction in iterations, the LST increments can be expressed by:

$$T_{s,t+1} = T_{s,t} + \Delta T = T_{s,t} + NN(u^*, S_n, Q_n, z_{0m}, T_s) \quad (11)$$

where $NN(\cdot)$ donates different LSTM-based surrogates within HyLake v1.0, Baseline and TaihuScene, which will activate to approximate the increment of lake surface temperature for each time step. Such LSTM-based surrogates have shown stable autoregressive prediction capabilities in hydrological modeling (J. Liu et al., 2024) and can readily be coupled with PBBM to provide numerically robust predictions of lake surface temperature. The other untrained variables, such as LE, and HE, were derived from the module of surface flux solutions (Eq. (1-3)).

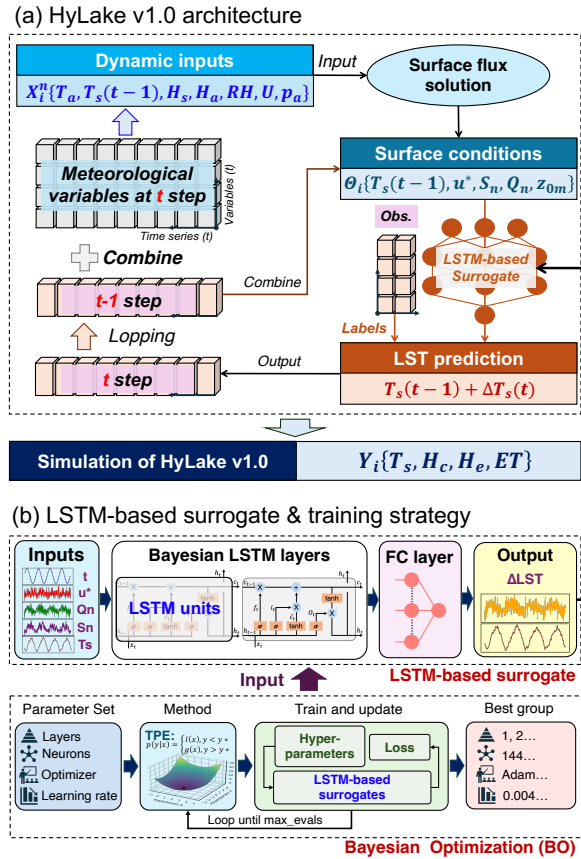


Figure 3: The general architecture of HyLake v1.0. (a) Coupling strategy of physical principles and LSTM-based surrogates and (b) training strategy of LSTM-based surrogates in HyLake v1.0. X_t^n , θ_t , and Y_t represent dynamic inputs for forcing surface flux solution in PBBM, surface conditions calculated from surface flux solution, and the outputs calculated from HyLake v1.0, respectively.

2.2.3 **Training** strategy of LSTM-based surrogates

The LSTM-based surrogates in HyLake v1.0 are composed by the stacked LSTM or Bayesian LSTM (BLSTM) units and fully-connected layers (Figure 3b), including two different units to separately construct LSTM-based surrogates in HyLake v1.0 that trained on observations. LSTM units are a type of Recurrent Neural Network (RNN) designed to avoid vanishing gradients problem, making them particularly suited for time series forecasting (Sherstinsky, 2020). Here, this study constructed a LSTM surrogate for Baseline and a BLSTM surrogate for HyLake v1.0 to couple in PBBM (Table 2). Specifically, the LSTM unit comprises three gates: the forget gate, the input gate and the output gate, which controls whether information should be retained or updated (Hochreiter, 1997). The forget gate was firstly introduced by Gers et al. (2000), which can be expressed as follow:

$$f_t = \sigma(W_f x_t + U_f h_{t-1} + b_f) \quad (12)$$

$$\tilde{c}_t = \tanh(W_{\tilde{c}} x_t + U_{\tilde{c}} h_{t-1} + b_{\tilde{c}}) \quad (13)$$

where f_t is a resulting vector of the forget gate; $\sigma(\cdot)$ and $\tanh(\cdot)$ are the logistic sigmoid and hyperbolic tangent functions; W_f , U_f and b_f represent the trainable parameters in two weight matrices and a bias vector of the forget gate; $W_{\tilde{c}}$, $U_{\tilde{c}}$ and $b_{\tilde{c}}$ are another set of trainable parameters to calculate the next hidden state in LSTM unit. x_t and h_{t-1} are the current input and last hidden state, respectively, to calculate a potential update vector $\tilde{c}_t$. The input gate determines which information of $\tilde{c}_t$ will be used to update the cell state in the current time step:

$$i_t = \sigma(W_i x_t + U_i h_{t-1} + b_i) \quad (14)$$

$$c_t = f_t \odot c_{t-1} + i_t \odot \tilde{c}_t \quad (15)$$

where i_t is a resulting vector in the input gate, determining which new information will store in $\tilde{c}_t$ (Kratzert et al., 2018); W_i , U_i and b_i are trainable parameters in input gate. The output vector of the input gate c_t is updated by [Eq. \(15\)](#). Specifically, $\odot$ represents element-wise multiplication. The last gate is the output gate controlling the information of c_t that flows into the new hidden state h_t , which can be calculated from:

$$O_t = \sigma(W_o x_t + U_o h_{t-1} + b_o) \quad (16)$$

$$h_t = \tanh(c_t) \odot O_t \quad (17)$$

where O_t is a resulting vector; W_o , U_o and b_o are the trainable parameters for the output gate. The new hidden state h_t is calculated by combining the results from [Eq. \(14-15\)](#), allowing for an effective learning from long-term dependencies in historical time series (Kratzert et al., 2018). By stacking multiple LSTM layers on the top of the neural networks, LSTM-based surrogates used a fully-connected layer or Bayesian fully connected layer to connect the results from the last hidden state in LSTM to a single output neuron to acquire the final prediction. The basic formula of these layers is given by the following equation:

$$y = W_d h_n + b_d \quad (18)$$

where y is the prediction variable, which is LST in this study; h_n is the output from the last LSTM layer. In the fully-connected layer, W_d and b_d are deterministic constants learned during training, while in the Bayesian fully-connected layer, W_d and b_d are instead modeled as random variables from Gaussian distribution to capture uncertainty of parameters.

The hyperparameters of these LSTM-based surrogates are both adjusted to be optimal. Specifically, the LSTM-based surrogate in Baseline that was trained with an Adam Optimizer consists of two layers with 256 LSTM units and 1 fully-connected layer, with a batch size of 32, and a learning rate of 0.01. This surrogate was adjusted manually to achieve the optimal performance. The BLSTM-based surrogate was composed by 4 layers with 467 LSTM units and 1 Bayesian fully-connected layer, with a batch size of 64, a learning rate of 0.00096, and an optimizer of RMSprop. The BLSTM surrogate in HyLake v1.0 was adjusted using Bayesian Optimization (BO-BLSTM), which is a powerful tool for the joint optimization of design choices using less computational power to compute better solution (Shahriari et al., 2016), with a hyperparameter space of the number of layers and units, learning rate and optimizer to search for the optimal group of hyperparameters (Figure 3b). The BO-BLSTM-based surrogate in TaihuScene comprised 7 layers with 836 BLSTM units and 1 Bayesian fully-connected layer, with a batch size of 145, a learning rate of 0.2538, and an optimizer of AdamW using Bayesian Optimization to search for the optimize group of hypermeters. The hyperparameter space included the number of hidden layers (ranging from 1 to 8), neurons per layer (ranged from 16 to 1,024), optimizer (Adam, or RMSprop), batch size (ranging from 8 to 256), and learning rate (ranging from 1E-6 to 1E-2). The hyperparameters in BO-BLSTM-based surrogates were optimized using BO with a maximum of 100 iterations, 1000 epochs for each iteration, and 50 patience in an EarlyStopping strategy. A Tree-structured Parzen Estimator (TPE) is adopted in BO, performing 20 to 100 iterations of surrogate training and updates. Training, validation, and test datasets for each lake site were divided by 80%, 10% and 10% of the length of time series (2013-2015), respectively. They are divided into 2013-01-01 00:00:00 to 2015-05-26 04:00:00, 2015-05-26 04:00:00 to 2015-09-12 14:00:00, and 2015-09-12 14:00:00 to 2015-12-30 23:00:00.

2.3 Numerical experiments design and evaluation metric

2.3.1 Numerical experiments for model intercomparison

To address the generalization and transferability of HyLake v1.0 in studied (MLW) and ungauged lake sites (DPK_BFG_XLS and PTS) (Table 1), this study further conducted three numerical experiments, including MLW experiment, Taihu-obs experiment, Taihu-ERA5 experiment, and Chaohu experiment, using distinct models and forcing datasets (Table 2 and 3), including FLake, Baseline, and TaihuScene to intercompare. Baseline and TaihuScene serve as extended models of HyLake v1.0 that are composed of the same physical principles and distinct LSTM-based surrogates using different training strategies were used to intercompare with HyLake v1.0. The descriptions of these models are described as follows:

- PBBM as a backbone of HyLake v1.0 is a simplified process-based lake model was constructed based on the energy balance equations and the 1-D vertical lake water temperature transport equations.

- FLake is a bulk model based on a two-layer parametric representation of the evolving temperature profile and on the integral budgets of heat and of kinetic energy for the layers, which is widely used as a lake module for simulating lake-atmosphere interactions in Earth System Models (ESMs) (Huang et al., 2021; Mironov et al., 2010). FLake served as a well-known traditional process-based lake model is suitable for model intercomparison.
- Baseline is a hybrid lake model that is coupled to an LSTM-based surrogate trained on outputs of PBBM, which is used to intercompare the performance with HyLake v1.0.
- TaihuScene is another hybrid lake model that is coupled to a BO-BLSTM-based surrogate trained on observations from all sites (MLW, BFG, DPK, PTS, and XLS) in Lake Taihu, which is different from the HyLake v1.0. The purpose of TaihuScene is to compare the performance of using a larger training dataset to train a surrogate model with that of using a small dataset from HyLake v1.0.

The PBBM performed like FLake in MLW site, indicating a high reliability and accuracy (Figure S2). Except for PBBM, the LST, LE and HE calculated from models in all experiments were initially intercompared in each lake site from Lake Taihu. FLake and TaihuScene was additionally intercompared using the forcing datasets from ERA5 datasets in Taihu-ERA5 experiment. The specification of the datasets used, surrogate, and the descriptions for each model can be found in Table 2. Furthermore, this study implemented the HyLake v1.0 into Lake Chaohu, the 5th-largest shallow freshwater lake in China, which has experienced heavy eutrophication and harmful algal blooms (Yang et al., 2020), to assess its transferability to other lakes. A LST dataset in Lake Chaohu was obtained from MODIS/Terra Land Surface Temperature/Emissivity Daily L3 Global 1km SIN Grid V061 imageries (MYD11A1, <https://www.earthdata.nasa.gov/data/catalog/lpcloud-mod11a1-061>), which were used to validate the performance of LST derived from HyLake v1.0. The computational efficiency for each 1-time prediction was recorded using a 16G 10-Core Apple M4 processor based on the established HyLake v1.0 model in this study. The training of the above-mentioned surrogates was run using a 24G NVIDIA GeForce RTX 4090 GPU.

Table 2. Specification of each model for intercomparison.

Model	Forcing datasets	Surrogate	Training datasets	Description
PBBM	\	\	\	Backbone for HyLake v1.0
FLake	ERA5; observations	\	\	A process-based freshwater lake model for intercomparison
Baseline	MLW	LSTM	PBBM outputs	A baseline experiment using PBBM outputs for model intercomparison
TaihuScene	ERA5; observations	BO-BLSTM	All observations	A numerical experiment using large train dataset to train surrogate
HyLake v1.0	ERA5; observations	BO-BLSTM	MLW observations	Proposed hybrid lake model in this study

2.3.2 Metrics for model evaluation and intercomparison

To evaluate the performance of these numerical experiments, the Pearson correlation coefficient (R), Root Mean Square Error (RMSE), and Mean Absolute Error (MAE) was used in this study to compare the accuracy of LST and heat fluxes between simulations and observations. Specifically, the R is proposed to measure the linear correlation of the observed and modeled values, RMSE and MAE assess if the models over or underestimate the observations with the same data units (Piccolroaz et al., 2024). The calculation of R, RMSE, and MAE can be expressed by:

$$R = \frac{\sum(x_i - \bar{x}_i)(y_i - \bar{y}_i)}{\sqrt{\sum(x_i - \bar{x}_i)^2 \sum(y_i - \bar{y}_i)^2}} \quad (17)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \bar{y}_i)^2} \quad (18)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \bar{y}_i| \quad (19)$$

where x_i and $\bar{x}_i$ are the observations and its average; while y_i and $\bar{y}_i$ are the results of model and its average; n represents the length of time series.

3 Results

3.1 Validation of HyLake v1.0 in MLW experiment

The PBBM, a backbone of HyLake v1.0, has already been validated in Figure S2 by comparing with FLake model and observations from MLW site, indicating a robust prediction with a R of 0.98 and RMSE of 1.78 °C in LST, a R of 0.85 and RMSE of 38.34 W/m² in LE and a R of 0.89 and RMSE of 9.37 W/m² in HE. FLake demonstrated a slightly better performance to PBBM in LST and HE while performed poorer in LE (LST: R = 0.98, RMSE = 1.76 °C; LE: R = 0.82, RMSE = 42.73 W/m²; HE: R = 0.84, RMSE = 7.24 W/m²). These results fully indicated that the backbone provided from PBBM for HyLake v1.0 is reasonable for all variables.

This study separately validated Baseline, TaihuScene, HyLake v1.0 and their adapted LSTM-based surrogates using MLW observations to address the performance of integrated models (Figure 4, 5 and Figure S3). Firstly, the results from HyLake v1.0 and its BO-BLSTM-based surrogate was individually validated based on MLW observations. Specifically, this study separately assessed the accuracy of the BO-BLSTM-based surrogate of HyLake v1.0 in the training, validation, and test sets, aiming to evaluate their ability to describe the physical principles between climate change and LST (Figure 4). The Δ LST obtained from observations was used to train surrogate in HyLake v1.0. For the BO-BLSTM-based surrogate in HyLake v1.0, a higher consistency between predictions and observations was observed (Figure 4). Specifically, the Δ LST results for the BO-BLSTM-based surrogate showed RMSE values of 0.1945 °C and MAE of 0.1306 °C in the training dataset, RMSE of 0.3359 °C and MAE of 0.1925 °C in the validation dataset, and RMSE of 0.2271 °C and MAE of 0.1461 °C in the test dataset, respectively.

345 Considering the model intercomparison, the LSTM-based surrogate-derived Δ LST in Baseline model, which is trained from process-based simulations of PBBM, also performed superior performance, indicating a great capacity for learning physical principles (Figure S3a-c). The results indicated a RMSE of 0.0580 °C and a MAE of 0.0112 °C in the training dataset, RMSE of 0.0079 °C and MAE of 0.0058 °C in the validation dataset, and RMSE of 0.0161 °C and MAE of 0.0094 °C in the dataset. These results suggest that the LSTM-based surrogate can capture approximately about 90% of the physical principles even

350 during validation and testing. When applied to Lake Taihu, another BO-BLSTM-based surrogate in TaihuScene was used to train with observations from all lake sites. It demonstrated a close match to observations, with RMSE values of 0.2363 °C and MAE of 0.1537 °C in the training dataset, RMSE of 0.3342 °C and MAE of 0.1880 °C in the validation dataset, and RMSE of 0.2281 °C and MAE of 0.1480 °C in the test dataset. These results were somewhat lower than HyLake v1.0 due to the larger dataset size in training for Δ LST. Therefore, these surrogates, improved on the basis of purely LSTM-based surrogates, ensure

355 robust capacity for autoregressive prediction of Δ LST while maintaining numerical stability, laying a solid foundation for algorithms coupled to HyLake v1.0 backbone.

After validating the accuracy of all LSTM-based surrogates in Baseline, TaihuScene and HyLake v1.0, this study conducted MLW experiments to predict the LST, LE and HE by using Baseline and HyLake v1.0 that integrated these surrogates, then compared with the outputs of traditional process-based FLake model using MLW observations (Figure 5 and Table 3).

360 Compared to FLake, Baseline which utilized the LSTM-based surrogate trained on outputs from PBBM performed slightly poorer, with an R of 0.96 and RMSE of 2.71 °C for LST, an R of 0.74 and RMSE of 51.77 W/m² for LE, and an R of 0.75 and RMSE of 14.63 W/m² for HE. The physical principles learned from these simulations is limited but enabled the surrogate to provide predictions similar to those of PBBM. For LST, HyLake v1.0 outperformed both FLake and Baseline, with an R of 0.99 and RMSE of 1.08 °C (Figure 5a). For heat fluxes calculated from the energy balance equations of surface flux solution,

365 HyLake v1.0 also outperformed FLake and Baseline, with an R of 0.94 and RMSE of 24.65 W/m² for LE and an R of 0.93 and RMSE of 7.15 W/m² for HE (Figure 5b-c). These results demonstrate the HyLake v1.0 that using BO-BLSTM-based surrogate as a module of the HyLake backbone to solve LST and thereby compute LE and HE in the subsequent time step offers numerical stability and predictability. Furthermore, HyLake v1.0 proves capable of estimating lake-atmosphere interactions, surpassing FLake in the integration of deep-learning-based and process-based models, which offered a robust way for applying

370 in ungagged locations. TaihuScene was used to intercompare with HyLake v1.0 in model generalization and transferability across all lake sites and different forcing datasets, which will be discussed in the section 3.3.

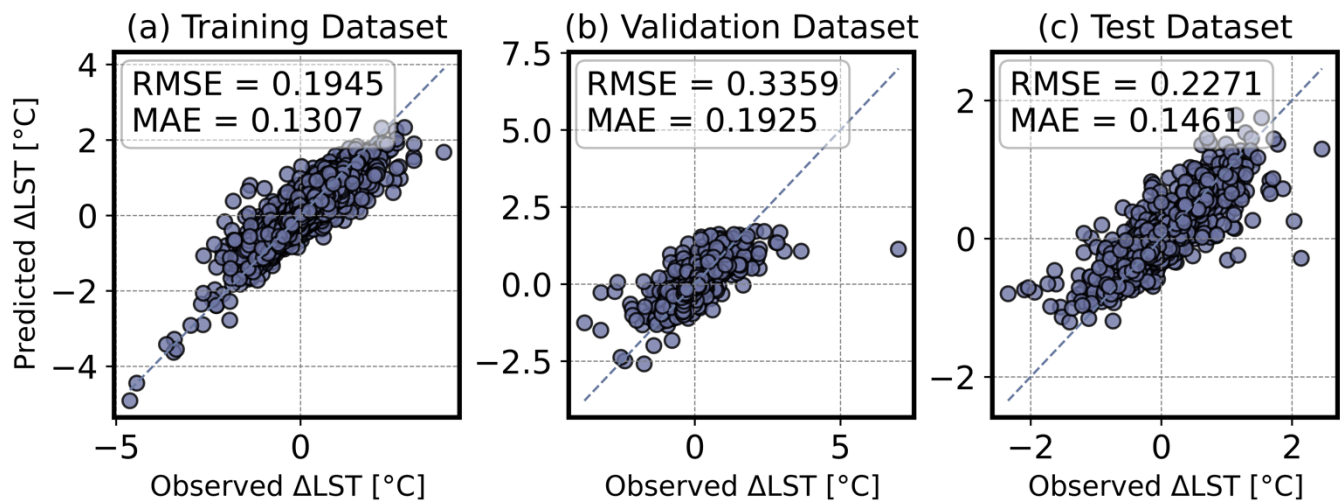


Figure 4: The validation of BO-BLSTM-based surrogate in HyLake v1.0 for (a) training, (b) validation and (c) test datasets.

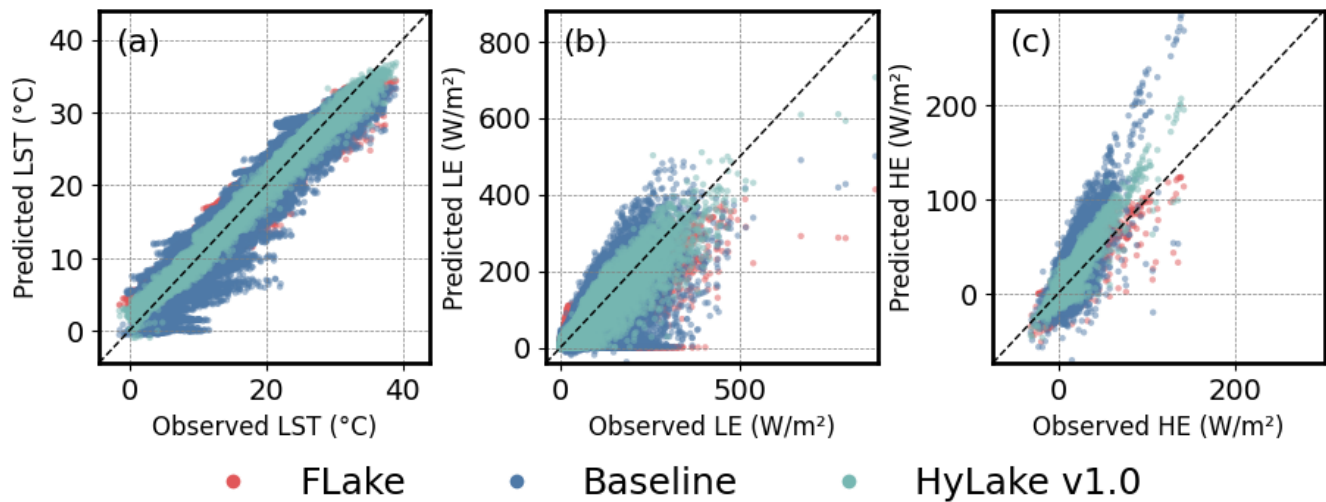


Figure 5: Comparison of predicted (a) LST, (b) LE and (c) HE by using FLake (red points), Baseline (blue points), HyLake v1.0 (green points) and observations in MLW experiments.

Table 3: Intercomparison of model performance across different experiments conducted in diverse regions with different forcing datasets. Observations from all lake sites (MLW, DPK, BFG, XLS, and PTS) on Lake Taihu, were used to drive models in the Taihu-obs experiment. Bold values in the table present the best-performing model with each group of experiments. Computational efficiency is reported as the runtime for a single simulation.

<u>Exp</u>	<u>Model</u>	<u>Forcing</u>	<u>R</u>			<u>RMSE</u>			<u>MAE</u>			<u>Efficiency</u> (s)
			<u>LST</u>	<u>LE</u>	<u>HE</u>	<u>LST</u>	<u>LE</u>	<u>HE</u>	<u>LST</u>	<u>LE</u>	<u>HE</u>	
<u>MLW</u>	<u>PBBM</u>	<u>MLW</u>	0.98	0.85	0.89	1.78	38.34	9.37	1.38	23.54	6.22	189.49
	<u>FLake</u>	<u>MLW</u>	0.98	0.82	0.84	1.76	42.73	7.24	1.35	24.76	5.01	16.40

	<u>Baseline</u>	<u>MLW</u>	<u>0.96</u>	<u>0.74</u>	<u>0.75</u>	<u>2.71</u>	<u>51.77</u>	<u>14.63</u>	<u>2.11</u>	<u>33.52</u>	<u>9.30</u>	<u>151.46</u>
	<u>HyLake v1.0</u>	<u>MLW</u>	<u>0.99</u>	<u>0.94</u>	<u>0.93</u>	<u>1.08</u>	<u>24.65</u>	<u>7.15</u>	<u>0.85</u>	<u>15.18</u>	<u>4.73</u>	<u>270.21</u>
	<u>FLake</u>	<u>All sites</u>	<u>0.97</u>	<u>0.61</u>	<u>0.74</u>	<u>2.24</u>	<u>15.46</u>	<u>69.11</u>	<u>1.69</u>	<u>41.95</u>	<u>10.44</u>	<u>89.00</u>
<u>Taihu-obs</u>	<u>TaihuScene</u>	<u>All sites</u>	<u>0.99</u>	<u>0.82</u>	<u>0.89</u>	<u>1.52</u>	<u>14.93</u>	<u>43.49</u>	<u>1.23</u>	<u>29.53</u>	<u>10.63</u>	<u>6928.44</u>
	<u>HyLake v1.0</u>	<u>All sites</u>	<u>0.99</u>	<u>0.81</u>	<u>0.90</u>	<u>1.36</u>	<u>11.19</u>	<u>39.20</u>	<u>1.03</u>	<u>24.79</u>	<u>7.88</u>	<u>2693.23</u>
	<u>FLake</u>	<u>ERA5</u>	<u>0.98</u>	<u>0.63</u>	<u>0.69</u>	<u>1.82</u>	<u>12.31</u>	<u>67.24</u>	<u>1.46</u>	<u>50.94</u>	<u>9.68</u>	<u>19.60</u>
<u>Taihu-ERA5</u>	<u>TaihuScene</u>	<u>ERA5</u>	<u>0.99</u>	<u>0.68</u>	<u>0.73</u>	<u>1.60</u>	<u>13.00</u>	<u>64.83</u>	<u>1.29</u>	<u>47.78</u>	<u>10.11</u>	<u>652.25</u>
	<u>HyLake v1.0</u>	<u>ERA5</u>	<u>0.99</u>	<u>0.71</u>	<u>0.78</u>	<u>1.12</u>	<u>11.05</u>	<u>49.48</u>	<u>0.90</u>	<u>35.02</u>	<u>7.97</u>	<u>236.78</u>
	<u>FLake</u>	<u>ERA5</u>	<u>0.97</u>	<u>\</u>	<u>\</u>	<u>2.28</u>	<u>\</u>	<u>\</u>	<u>1.76</u>	<u>\</u>	<u>\</u>	<u>70.40</u>
<u>Chaohu</u>	<u>HyLake v1.0</u>	<u>ERA5</u>	<u>0.97</u>	<u>\</u>	<u>\</u>	<u>2.07</u>	<u>\</u>	<u>\</u>	<u>1.57</u>	<u>\</u>	<u>\</u>	<u>972.83</u>

3.2 Intercomparisons of LST, LE and HE from 2013 to 2015

This study conducted a comprehensive intercomparison of daily and hourly trends in LST, LE and HE from [MLW experiment](#) in the MLW site during the period from 2013 to 2015, including FLake, Baseline, and HyLake v1.0 (Figures 6-8).

As shown in Figure 6, the temporal changes in LST for the period of surrogates training ([2013-01-01 00:00:00 to 2015-05-26 04:00:00](#)), validation ([2015-05-26 04:00:00 to 2015-09-12 14:00:00](#)), and test datasets ([2015-09-12 14:00:00 to 2015-12-30 23:00:00](#)) were compared. For daily changes in LST, HyLake v1.0 and FLake showed a closer match to observations, whereas Baseline, trained with process-based simulations, exhibited a larger error in comparison to the observed values ($R = 0.96$, $RMSE = 2.71$ °C, Figure 5a). HyLake v1.0 demonstrated a greater capability in capturing the daily changes in LST, particularly in mid-winter for each dataset, thus indicating long-term stability in LST modeling ($R = 0.99$, $RMSE = 1.08$ °C, Figure 5a). Specifically, FLake provided a good match to observations at a daily-average scale, which, however, showed poorer performance in capturing diurnal variations of LST ($R = 0.98$, $RMSE = 1.76$ °C, Figure 5a). This study randomly selected two subperiods from the training, validation, and test periods (Figure 5b and c), where the diurnal variations of LST observations exhibited a significant bias compared to FLake, indicating that FLake is not able to accurately describe variations at the diurnal scale. Meanwhile, Baseline primarily captured the long-term trends of LST from PBBM but did not effectively represent diurnal variations due to the limitations of the datasets and physical principles provided by PBBM. In contrast, HyLake v1.0 was able to capture more information about the diurnal variations of LST from the observations, thereby outperforming both FLake and Baseline. Overall, HyLake v1.0, coupled with the BO-BLSTM-based surrogates trained on observations, offers a robust way for predicting LST trends at a finer temporal resolution.

The LE and HE were calculated using the energy balance equations, where the LST, updated by LSTM-based surrogates in HyLake, served as an essential input. Consequently, it is necessary to validate the variations in these heat fluxes outputted by HyLake v1.0 to assess its capacity for modeling lake-atmosphere interactions. This study validated the observed LE and HE at the MLW site on both daily and hourly scales (Figures 7-8).

Regarding the changes in LE (Figure 7), HyLake v1.0, which used LST calculated from the BO-BLSTM-based surrogate, demonstrated a minor bias in estimating LE ($R = 0.94$, $RMSE = 24.65 \text{ W/m}^2$, Figure 5b), outperforming both FLake ($R = 0.82$, $RMSE = 42.73 \text{ W/m}^2$, Figure 5b) and Baseline ($R = 0.74$, $RMSE = 51.77 \text{ W/m}^2$, Figure 5b). Notably, using an improved LSTM-based surrogate resulted in a slightly and significant improvement of LE compared to the FLake and Baseline. Specifically, Baseline showed more similar performance to FLake, capturing the major trends of these heat fluxes. The LE predicted by HyLake v1.0 reproduces both the peak and trough magnitudes more closely to the MLW observations than FLake and Baseline models (Figure 7b-c), indicating its overall superior capacity for describing the diurnal variations. Still, some biases persisted in the validation and test periods. For example, HyLake v1.0 overestimated to the observations during 2015-08-20 and 2015-08-23 (Figure 7c).

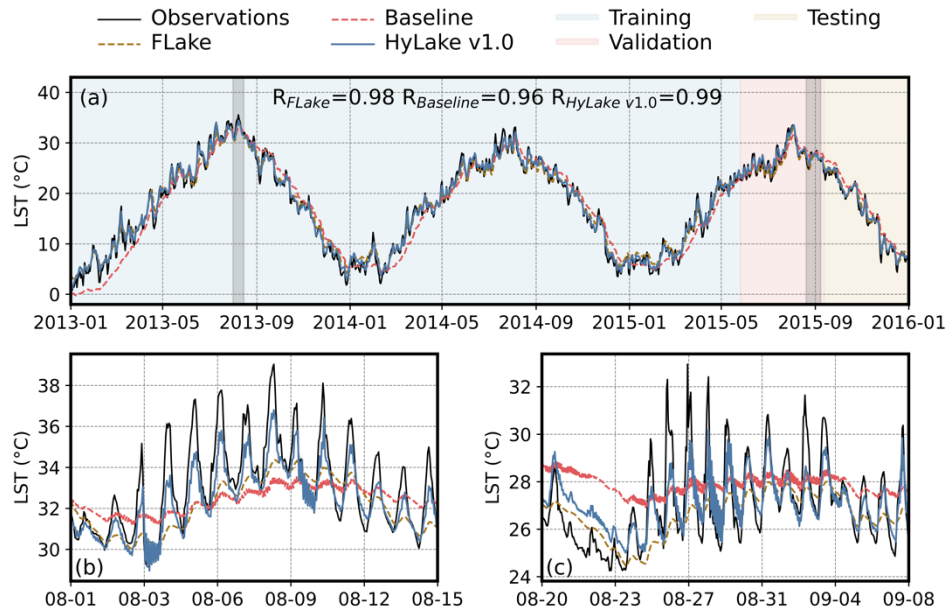
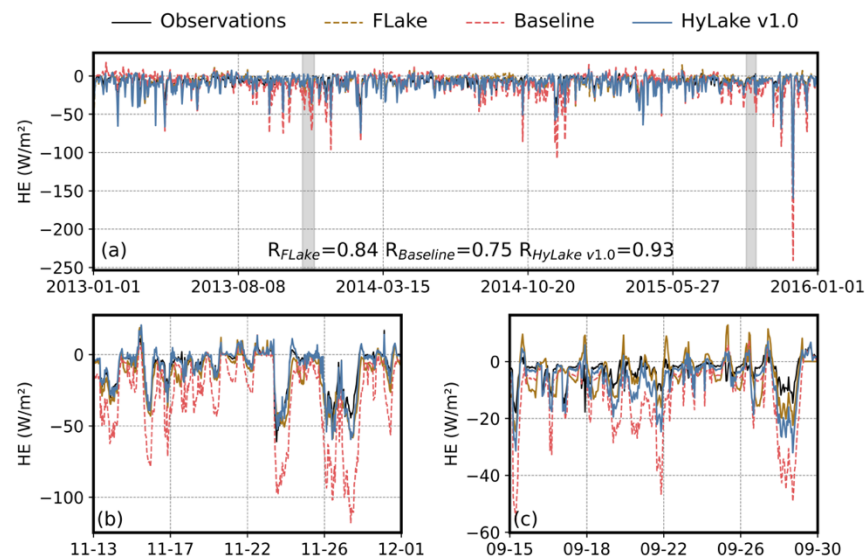


Figure 6: Comparison of observations and predictions by FLake, Baseline, and HyLake v1.0 in temporal trends of LST. Comparison of (a) the full time series and (b-c) partial time series of models derived LST and observations from 2013 to 2015. All results in (a) were presented at a daily-average scale by resampling. Blue, red, and yellow regions represent the period for the train, validation, and test datasets, respectively. Black solid, brown dashed, red dashed, and blue solid lines represent LST from observations, FLake, Baseline, and HyLake v1.0, respectively.

For HE, which exhibited relatively insignificant diurnal and seasonal variations during the studied period, HyLake v1.0 ($R = 0.93$, $RMSE = 7.15 \text{ W/m}^2$, Figure 5f) outperformed both FLake ($R = 0.84$, $RMSE = 7.24 \text{ W/m}^2$, Figure 5f) and Baseline ($R = 0.75$, $RMSE = 14.63 \text{ W/m}^2$, Figure 5f) in simulating variations of both hourly and daily trends. The results were found that Hylake v1.0 is capable of correcting some of the partial biases in HE estimation by integrating the BO-BLSTM-based surrogate (Figure 8b-c), leading to more accurate simulations of these heat fluxes. Besides that, the HE calculated from both FLake and Baseline was difficult to accurately estimate the minor variations in hourly scale during simulations, which could accumulate bias in subsequent time steps. This issue was especially evident in the validation and test datasets (Figure 8c), whereas HyLake

425 v1.0 showed minimal bias due to its improved representation of LST. In summary, HyLake v1.0 that coupled PBBM to a BO-
 BLSTM-based surrogate provided a more robust and reasonable prediction of LST, leading to better corrections for untrained
 variables (LE and HE) produced by the other modules. This improvement ensures HyLake v1.0's capability in accurately
 describing lake-atmosphere interactions with improved performance.



430 **Figure 7: Comparisons of observations and predictions by FLake, Baseline, and HyLake v1.0 in temporal trends for LE.** Comparison
 of (a) full and (b-c) partial time series of model derived LE and observations from 2013 to 2015.

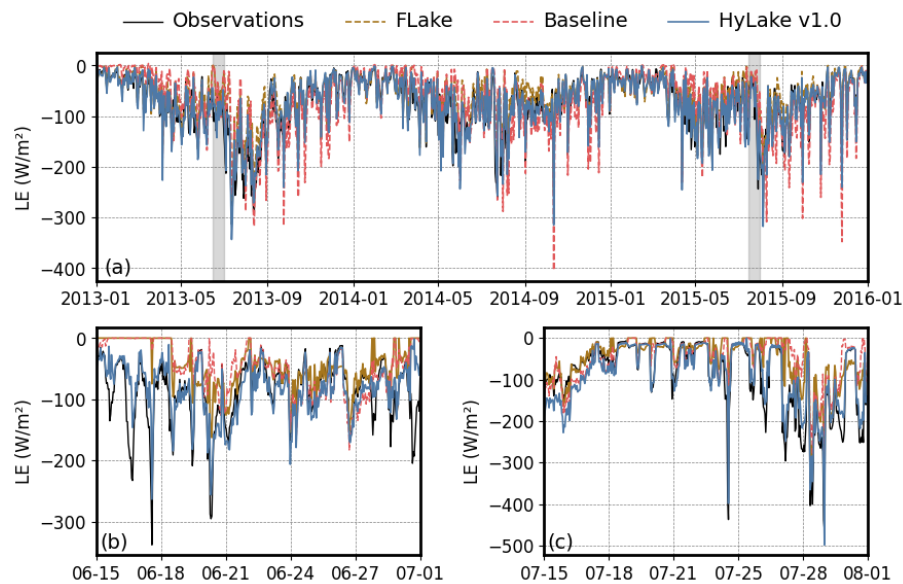


Figure 8: Comparisons of observations and predictions by FLake, Baseline, and HyLake v1.0 in temporal trends for HE. Comparison
 of (a) full and (b-c) partial time series of model derived HE and observations from 2013 to 2015.

435 3.3 Validation across observational sites in Lake Taihu

A successful hybrid model that unified physical principles and deep learning techniques requires strong generalization, evidenced by a remarkably small gap between its performance on training and test datasets (Zhang et al., 2021), and strong transferability, defined as the ability to generalize well to a novel task for domain adaptation (Long et al., 2015). The transferability and generalization of traditional deep-learning-based models remain challenging (T. F. Xu & Liang, 2021).
440 However, integrating process-based models with deep learning-based models can mitigate these issues to some degree. To address these challenges with HyLake v1.0, this study specially developed a TaihuScene (Table 2), another hybrid lake model which enlarges the size of training datasets by incorporating data from 5 lake sites in Lake Taihu to train its BO-BLSTM-based surrogates and evaluate the potential difference from HyLake v1.0. The primary objectives of TaihuScene are to (1) offer a theoretically optimal coupled model (previous studies allocated that larger train datasets improve deep-learning-based models' performance (Halevy et al., 2009)) for simulating lake-atmosphere interactions in Lake Taihu, and (2) compare with HyLake
445 v1.0 in generalization and transferability for ungauged regions.

Given to the experiment TaihuScene trained with large datasets, HyLake v1.0 still performed the best in predicting LST (MAE = 1.03 °C), HE (MAE = 24.79 W/m²), and LE (MAE = 7.88 W/m²) among FLake and TaihuScene (Figure 9). While FLake performed the worst in each variable, with a MAE of 1.69 °C in LST, a MAE of 41.95 W/m² in LE and a MAE of 10.44 W/m²
450 in HE, respectively. TaihuScene performed moderately, with a MAE of 1.23 °C in LST, a MAE of 29.53 W/m² in HE and a MAE of 10.63 W/m² in LE, respectively.

Involving the relative bias (the difference between simulation and observation), the median biases (the dashed lines) and distribution of outputs by TaihuScene indicated an overestimation of LST (Figure 9a), which may contribute to the underestimation of heat fluxes derived from the common physical principles learned from large datasets during step-by-step
455 iterative calculations (Figure 9b-c). While HyLake v1.0 exhibited an opposite estimation, with a slightly underestimation in LST and overestimation in HE and LE. This suggests that BO-BLSTM-based surrogates trained with observations from MLW site provide more reliable results than those trained with data from all sites due to the more clearly physical principles for training. But it is worthy to note that TaihuScene still far outperformed FLake, as evidenced by a denser distribution of biases. These results challenge the assumption that larger datasets always improve the performance of deep-learning-based models
460 (T. F. Xu & Liang, 2021; W. Zhong et al., 2020), with the results suggested that HyLake v1.0, trained on relatively smaller datasets, performs better than TaihuScene in Lake Taihu.

The results of intercomparison in each lake site for FLake and TaihuScene experiments further explain the reasons for this phenomenon (Figure S4). HyLake v1.0 performed best at the MLW, PTS, and XLS sites but showed poorer results at the BFG and DPK sites. Specifically, HyLake v1.0 outperformed FLake and TaihuScene at the MLW site, with a MAE of 0.85 °C,
465 15.18 W/m², and 4.73 W/m² for LST, LE, and HE, respectively. In contrast, TaihuScene performed relatively worse, with a MAE of 1.38°C, 15.54 W/m², and 8.33 W/m². FLake showed moderate performance, with MAE values of 1.35 °C, 24.76 W/m², and 5.01 W/m² for LST, LE, and HE, respectively (Figure S4a-c). A similar pattern was apparent at the PTS and XLS

sites. At PTS, HyLake v1.0 also showed the best performance (LST: MAE = 0.79 °C; LE: MAE = 20.12 W/m²; HE: MAE = 6.90 W/m²), while FLake performed moderately (LST: MAE = 1.22 °C; LE: MAE = 24.77 W/m²; HE: MAE = 6.93 W/m²), and TaihuScene performed the worst (LST: MAE = 1.47 °C; LE: MAE = 39.66 W/m²; HE: MAE = 15.11 W/m²) (Figure S4j-i). Similarly, at the XLS site, HyLake v1.0 performed the best (LST: MAE = 1.86 °C; LE: MAE = 20.40 W/m²; HE: MAE = 6.61 W/m²), while FLake performed moderately (LST: MAE = 1.33 °C; LE: MAE = 30.00 W/m²; HE: MAE = 7.69 W/m²), and TaihuScene performed the worst (LST: MAE = 1.29 °C; LE: MAE = 32.20 W/m²; HE: MAE = 12.19 W/m²) (Figure S4m-o). However, at the BFG and DPK sites, TaihuScene outperformed the other models in estimating LST, LE, and HE, with MAE values of 1.06 °C, 27.92 W/m², and 9.73 W/m² at BFG and 1.00 °C, 26.05 W/m², and 8.43 W/m² at DPK (Figure S4d-i). Specifically, TaihuScene performed slightly better than HyLake v1.0 (BFG: LST: MAE = 1.32 °C, LE: MAE = 32.88 W/m², HE: MAE = 10.47 W/m²; DPK: LST: MAE = 1.29 °C, LE: MAE = 34.71 W/m², HE: MAE = 10.54 W/m²) but was far superior to FLake (BFG: LST: MAE = 2.32 °C, LE: MAE = 65.05 W/m², HE: MAE = 16.53 W/m²; DPK: LST: MAE = 2.16 °C, LE: MAE = 62.71 W/m², HE: MAE = 15.56 W/m²).

It is clear that HyLake v1.0 demonstrated outstanding capacity to apply for ungauged regions, surpassing traditional lake-atmosphere interaction models such as FLake in prediction accuracy for each variable, which demonstrated a strong transferability for future applications. TaihuScene, though capable of predicting changes across all sites in Lake Taihu, also exhibited a superior overall performance at specific sites when compared to HyLake v1.0. This highlights HyLake v1.0 offers promising potential for extending its application to these ungauged lakes or sites with similar characteristics by effectively learning physical principles.

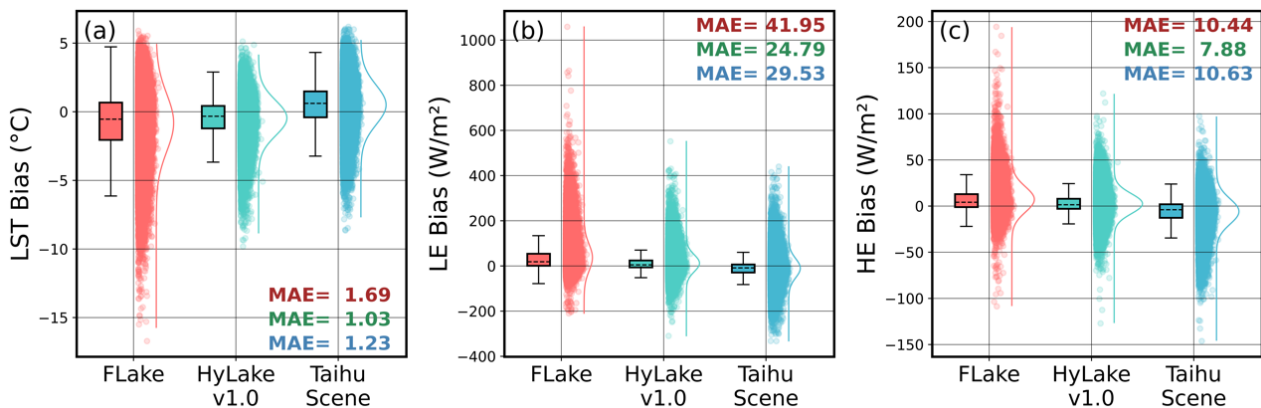


Figure 9: Comparisons of (a) LST, (b) LE, and (c) HE between observations, FLake, HyLake v1.0 and TaihuScene in five sites (MLW, BFG, DPK, PTS, and XLS) of Lake Taihu based on the Taihu-obs experiment. Dashed lines in boxplot represent median biases between observations and predictions simulated by FLake, HyLake v1.0, and TaihuScene, respectively. The scatterplots and probability distribution curves illustrate the data distribution of LST, LE and HE. The Numbers at the top or bottom right of subfigures with same color to boxes indicate the MAE of outputs for FLake, HyLake v1.0, and TaihuScene, respectively.

3.4 Performance comparison of models in Lake Taihu based on ERA5 datasets

This study additionally conducted Taihu-ERA5 experiment to demonstrate transferability of HyLake v1.0, which proves its superior capability to apply for the ungauged locations based on different forcing datasets. The meteorological variables from ERA5 dataset, which are widely used as forcing datasets for process-based models (Albergel et al., 2018; Hersbach et al., 2020), were selected to force FLake, TaihuScene and HyLake v1.0 and then compared their performance on LST, LE and HE observations from the Lake Taihu Eddy Flux Network. The spatial resolution of ERA5 dataset covers 5 grid cells that encompass the studied lake sites, among the 11 grids for the entire Lake Taihu. These grids include portions of the land surface surrounding the lake, inevitably introducing uncertainty due to the scale mismatch between climatic forcing datasets and the lake model (Hersbach et al., 2020).

Despite these limitations, it was surprising to find that the evaluation showed that HyLake v1.0 exhibited performance similar to or even superior to that of FLake for each lake site, with consistent spatial patterns for LST, LE, and HE (Figure 10, 11 and Figure S5). From the statistical properties, HyLake v1.0 still exhibited an incomparable performance in overall datasets, with MAE values of 0.90 °C, 35.02 W/m², and 7.94 W/m² for LST, LE and HE, respectively, which following with TaihuScene performed with MAE values of 1.29 °C, 47.78 W/m², and 10.11 W/m² for LST, LE and HE, far outperforming FLake with MAE values of 1.46 °C, 50.94 W/m², and 9.68 W/m² for LST, LE and HE, respectively (Figure 10). From spatial patterns observed, LST in the middle of the lake was relatively higher for all experiments (Figure 11c and d), while LE was higher in the southern and western shore (Figure 11b and e), and HE showed higher values in the northwestern shores of Lake Taihu (Figure 11c and f). Both HyLake v1.0 and TaihuScene revealed similar patterns of average across all variables, except for a slight overestimation of LE and underestimation of HE in the southeastern and northeastern shores of Lake Taihu in HyLake v1.0, respectively (Figure 11a-c). However, TaihuScene predicted relatively higher values in LE and HE, and lower in LST than the other models although it still followed similar spatial patterns for LST, LE, and HE (Figure 11d-f). This indicates that HyLake v1.0, coupled with a small dataset-trained BO-BLSTM-based surrogate, can still provide robust and reasonable predictions for estimating spatial patterns of Lake Taihu.

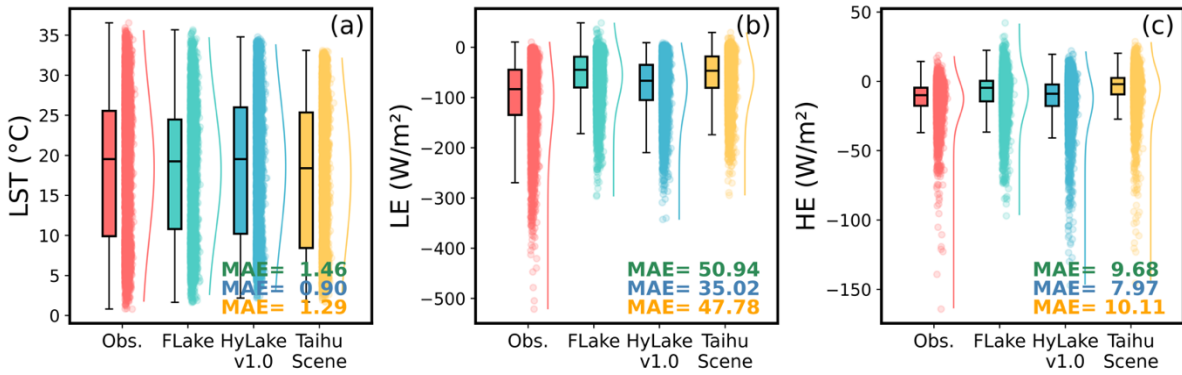


Figure 10: The statistical characteristics and spatial average of LST, LE and HE for observations, FLake, HyLake v1.0 and TaihuScene in all sites using ERA5 forcing datasets. Green, blue and yellow texts in figures represent the MAEs of LST, LE and HE for FLake, HyLake v1.0 and TaihuScene, respectively.

HyLake v1.0 in Taihu-ERA5 experiments exhibited superior performance for each lake site, showing a strong transferability using ERA5 datasets (Figure S5). At the MLW site (Figure S5a-c), which located on the northern shore of Lake Taihu, HyLake v1.0 outperformed both FLake (LST: MAE = 1.68 °C; LE: MAE = 33.84 W/m²; HE: MAE = 9.68 W/m²) and TaihuScene (LST: MAE = 1.17 °C; LE: MAE = 22.53 W/m²; HE: MAE = 8.98 W/m²), with MAE values of 1.05 °C, 31.46 W/m², and 9.12 W/m² for LST, LE, and HE, respectively. The train datasets used for the BO-BLSTM-based surrogate in HyLake v1.0 contributed to its powerful performance at this site, while predictions from TaihuScene performed farther from the observations. HyLake v1.0 still performed considerable well in ungauged sites by learning physical principles from MLW observations (Figure S4d-o). TaihuScene showed robust predictions but outperformed HyLake v1.0 only at the XLS and MLW sites. For the BFG site (Figure S5d-f), HyLake v1.0 outperformed both FLake and TaihuScene, with MAE values of 0.94 °C, 42.30 W/m², and 9.94 W/m², respectively. TaihuScene performed the worst among these models, with MAE values of 1.85 °C, 60.32 W/m², and 15.73 W/m². FLake exhibited a moderately performance with MAE values of 1.15 °C, 49.52 W/m², and 10.77 W/m² for LST, LE and HE, respectively. At the DPK site (Figure S4g-i), HyLake v1.0 performed better than FLake for LST but performed slightly worse for LE and HE, with MAE values of 0.68°C, 52.82 W/m², and 8.43 W/m². TaihuScene performed the worst in this site (LST: MAE = 1.49 °C; LE: MAE = 69.67 W/m²; HE: MAE = 12.40 W/m²). FLake performed the moderate in this site (LST: MAE = 1.14 °C; LE: MAE = 56.12 W/m²; HE: MAE = 9.11 W/m²). At the PTS site (Figure S4j-l), HyLake v1.0 (LST: MAE = 0.75°C; LE: MAE = 22.28 W/m²; HE: MAE = 6.43 W/m²) outperformed FLake for LST, LE, and HE (LST: MAE = 1.89 °C; LE: MAE = 57.12 W/m²; HE: MAE = 9.84 W/m²) and TaihuScene (LST: MAE = 0.94°C; LE: MAE = 31.75 W/m²; HE: MAE = 6.74 W/m²). HyLake v1.0 showed a slightly better performance at the XLS site (Figure S4m-o), with MAE values of 1.05 °C, 24.29W/m², and 5.69 W/m², while TaihuScene performed slightly worse for LE (MAE = 37.94W/m²) and HE (MAE = 6.79W/m²), FLake performed the worst with MAE values of 1.49 °C, 58.78 W/m², and 9.01 W/m².

Overall, both HyLake v1.0 and TaihuScene showed reliable performance across lake sites in Lake Taihu. Specifically, HyLake v1.0 performed the best in 14 of 15 variables (included LST, LE and HE for 5 lake sites) in Lake Taihu among these 3 models;

TaihuScene outperformed HyLake v1.0 in 1 of 15 variables and outperformed FLake in 8 of 15 variables in Lake Taihu. HyLake v1.0 providing superior results in most cases, proving its potential for extensive application in ungauged lakes under different forcing datasets. However, the prediction accuracy of these models based on ERA5 datasets were almost reduced due to the potential uncertainty in lake-atmosphere modeling systems. The current coupling strategies of HyLake v1.0 ensured the numerical stability and superior performance in validation due to the robust capability of auto-regressive predictions by proposed LSTM-based surrogates and to avoid the numerical divergence or error accumulation in step-by-step iteration loops. The results evidenced that HyLake v1.0 coupled with BO-BLSTM-based surrogate is suitable for discovering the potential physical principles for lake-atmosphere interactions systems, indicating that the integration of deep learning-based surrogates as a module with process-based models is effective for improving predictions in ungauged lakes.

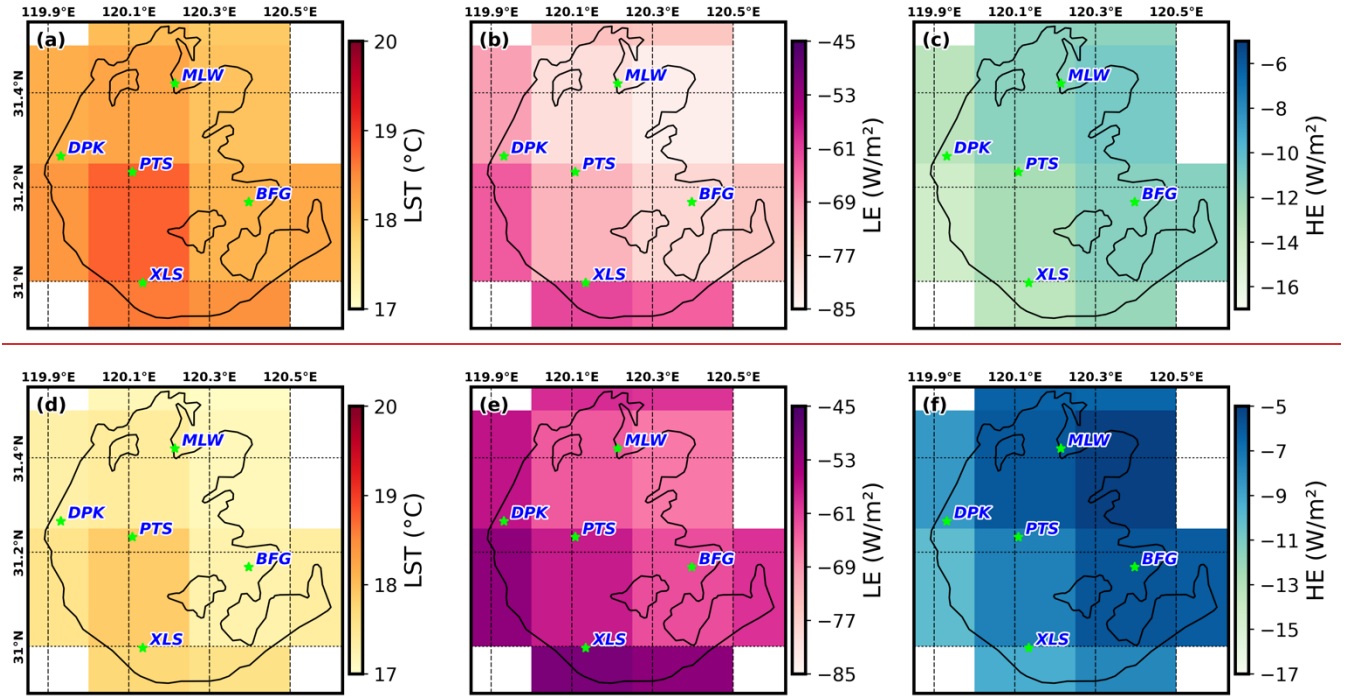


Figure 11: The statistical characteristics and spatial average of predicted LST, LE and HE for HyLake v1.0 and TaihuScene drove by ERA5 forcing datasets. (a-c) represent LST, LE and HE for HyLake v1.0, respectively; (d-f) represent LST, LE and HE for TaihuScene, respectively. The green stars noted in all figures are lake sites in Lake Taihu.

4. Discussion

4.1 Limitations of HyLake v1.0

In this study, we firstly utilized the in-house programed python-based 1-D process-based lake model PBBM, and then replaced traditional LST approximation methods with a LSTM-based surrogate trained on observations from the Lake Taihu Eddy Flux Network to construct a novel lake model named HyLake v1.0, which is a hard-coupled and auto-regressive hybrid model. To

address issues related to model performance, generalization, and transferability in ungauged locations, three additional numerical experiments, including FLake, Baseline, and TaihuScene, were proposed for intercomparison and a framework for applying HyLake v1.0 to another lake, such as Lake Chaohu, with a deeper lake depth of 3.06 m and lake area of 760 km² (Figure S6, Jiao et al., 2018), to validate the potential capacity of model application. These experiments were compared using observed meteorological datasets and ERA5 datasets, then validated for both spatiotemporal patterns of LST at Lake Taihu and Lake Chaohu (Tables 2-3). Similarly, ERA5 dataset-derived HyLake v1.0 outperformed FLake in estimating LST ($R = 0.97$, $RMSE = 2.07\text{ }^{\circ}\text{C}$, $MAE = 1.57\text{ }^{\circ}\text{C}$) in Lake Chaohu, compared to MYD11A1 datasets (Table 3 and Figures S7-9). The results demonstrated that HyLake v1.0 indicated outstanding performance in validation and robust predictions in ungauged lake sites under ERA5 reanalysis datasets, highlighting its superior capacity for lake-atmosphere interaction modeling systems.

However, several limitations exist, primarily involving data scarcity, computation efficiency, model architecture, explainability, and coupling strategies.

One challenge is the scarcity of observed radiation and energy fluxes, as it is expensive to collect long-term, multi-site microclimate and water temperature datasets from a large number of lakes for model forcing (Erkkilä et al., 2018; Nordbo et al., 2011). Although several reanalysis datasets (e.g., ERA5, NLDAS-2, GLSEA) have been used to drive lake models (Kayastha et al., 2023; Monteiro et al., 2022; Notaro et al., 2022; J. L. Wang et al., 2022), the lack of extensive observational data impedes the understanding of the relationships within lake-atmosphere interactions on a ground-truth scale. Due to the sparse observations, attempting to accurately predict the changes in lake-atmosphere modeling systems or parameterize the process-based models based on deep learning models and reanalysis datasets has to be popular (Almeida et al., 2022; Guo et al., 2021; Read et al., 2019). As a result, the relationships between reanalysis datasets and observation that learned by deep-learning-based surrogates may introduce additional biases, potentially influencing the learned relationships between climate change and lake surface conditions in models. Despite this, the results of this study still demonstrate that the relationships revealed by observations using deep-learning-based surrogates can be robust and generalizable to ungauged regions with reasonable training strategies. Incorporating deep-learning-based surrogates with process-based models based on adequate and high-quality observations holds promise for developing a general HyLake model on a global scale, improving the understanding of lake-atmosphere interactions.

Moreover, simplified parameterizations in traditional process-based lake models are commonly adopted (Golub et al., 2022; Mooij et al., 2010), which influence the coupling strategies in HyLake v1.0. The two critical components, including energy balance equations and 1-D vertical lake water temperature transport equations, compose the physical principles of lake-atmosphere interaction modeling systems, which also possess simplification to some degrees. For example, the calculation of friction velocity (u^*) and surface roughness length (z_{0m}) in surface flux solutions has improved over time from constant empirical models to iterative routines (Hostetler et al., 1993; Woolway et al., 2015), but substantial discrepancies still exist between simulation results and observations (Figure S6), which in turn influence the physical principles between land surface conditions and LST. The current approaches for solving energy balance equations uses bulk aerodynamic method based on the Monin–Obukhov similarity theory (Monin and Obukhov, 1954) and is the vital module in process-based lake models (e.g.,

FLake (Mironov et al., 2010), GLM (Hipsev et al., 2019), WRF-Lake (Gu et al., 2015)). However, it remains challenges to construct explainable approaches to quantify the relationships between surface conditions and fluxes and LST due to inadequate observations. These potential differences in physical processes lead to uncertainties in training deep-learning-based surrogates, contributing to the insufficient/limited knowledge during model training and thereby introducing large uncertainties in hybrid models. Furthermore, the long-term trends and diurnal variations in lake water temperature profiles remain challenging to accurate approximate using the finite difference method (e.g., Crank-Nicholson solution, implicit Euler scheme) (Piccolroaz et al., 2024; Sarovic et al., 2022; Subin et al., 2012). On top of the extensive observations of water temperature, several hybrid models that integrate deep-learning-based and process-based models have been constructed in previous studies, achieving improved performance in model comparisons (He et al., 2025; Ladwig et al., 2024; Read et al., 2019). These models and their training strategies generally perform better on training and test datasets due to their complex coupling strategies and higher computational requirements, while their generalization and transferability need further validation. Lake Taihu, as one of typical shallow, eutrophic, and large Chinese lakes with almost complete mixing throughout the year and subject to complex chemical and biological influences in its aquatic ecosystem, requires a suitable model as part of the temperature-solving module in the water column to predict lake water temperature and estimate other potential ecological implications under thermodynamic changes. HyLake v1.0, developed based on in situ observations from Lake Taihu, has been proven to be reliable and rigorously validated in Lake Chaohu (Table 3), demonstrating a faster and more accurate framework for enhancing the understanding of hybrid hydrological modeling.

LSTM networks have been regarded as community benchmarks for daily hydrograph metrics (J. Liu et al., 2024). HyLake v1.0 integrates a BLSTM network with Bayesian Optimization, which enhances robustness and stability during long-term auto-regressive predictions compared to traditional LSTM networks. However, we found that HyLake v1.0 required slightly higher computational costs compared to process-based models, which depend on the hyperparameters of LSTM-based surrogates, despite achieving greater performance (Table 3). In an individual case of MLW prediction, HyLake v1.0 took about 9 times longer to run compared to FLake, with a cost of 151.46 seconds. To compare different experiments of hybrid lake models, Baseline, coupled to an LSTM-based surrogate with 1 layer and 256 neurons per layer, indicated the lowest cost. While TaihuScene, constructed by an LSTM-based surrogate with 7 layers and 836 neurons per layer, showed the most expensive in predictions. Given the sophisticated architecture of LSTM-based surrogates, which inevitably leads to higher costs in training and prediction, developing novel algorithms for approximating LSTMs is urgently needed. Furthermore, the recent research progress demonstrated that LSTM-based surrogates are more suited for short-term predictions compared to the prevalent Transformer-based family, which is suited for long-term predictions and commonly used in global weather forecasting systems (K. F. Bi et al., 2023; L. Chen et al., 2023). This limitation restricts the performance and robustness of LSTM-based surrogates for long-term predictions. Future improvements should incorporate more powerful deep-learning-based surrogates with enhanced long-term prediction, generalization, and transferability capabilities. Recent advances in state-of-the-art deep-learning models, such as Transformers, Graph Neural Networks, Temporal Convolutional Networks, TimesNet, and Kolmogorov-Arnold Networks, have shown exceptional performance in time series forecasting (Bai et al., 2018; Z. Liu et

al., 2024; Wen et al., 2022; Wu et al., 2022), and are increasingly being applied in hydrological modeling (Sun et al., 2021; Z. C. Wang et al., 2024). To address the expensive computational demands, robustness of auto-regressive predictions, these novel deep-learning models need to be further validated and improved with additional modifications (Koya & Roy, 2024; J. Liu et al., 2024). However, developing powerful surrogates such as the Fuxi and Pangu models, which involve large parameters, requires not only large size of observations but also substantial computational power and efficiency (K. Bi et al., 2023; Lei Chen et al., 2023).

While the interpretability of HyLake v1.0 is better than that of purely data-driven models due to its hard-coupling structure, which retains the energy balance equations and utilizes a BO-BLSTM-based surrogate to solve LST, it still lags behind process-based models. LSTM-based surrogates, while offering powerful performance, introduce a "black-box" aspect that reduces their explainability (Chakraborty et al., 2021; de la Fuente et al., 2024). Developing deep-learning-based surrogates that incorporate knowledge from physical principles is an ongoing effort and has gained more attention recently (Piccolroaz et al., 2024; Read et al., 2019; Willard et al., 2023). For example, Read et al. (2019) proposed a process-guided deep-learning model with a loss function based on the simplified energy budget model from GLM and tested it on 68 lakes. Ladwig et al. (2024) developed a modular compositional learning framework for a 1-D Hydrodynamic Lake model, integrating four deep-learning models for each term and an eddy diffusion approach to improve performance in lake water temperature predictions at Lake Mendota. However, the simplified parameterizations, unclear relationships within the modules, and high computational demands hinder further development and limit the generalization and transferability of these models.

4.2 Future improvements

HyLake v1.0 has been applied to Lake Chaohu and achieved superior performance in comparison to the MYD11A1 LST observations, showing a promising way for more applications. Future improvements to HyLake v1.0 should focus on investigating the scaling laws of datasets, development of surrogate architectures, and extension of coupled modules. Currently, HyLake v1.0 has been validated primarily in Lake Taihu, utilizing high-quality training data provided by the Lake Taihu Eddy Flux Network (Zhang et al., 2020). However, in some exceptional cases, the lake may be influenced by regional inflows/outflows, or it may be covered by snow/ice for a long period, and the processes at the lake-air interface may differ from those in our experiments (Woolway et al., 2020). As a result, our model may not be quantifiable for these situations. Its surrogate will be required for more high-quality local datasets to retrain or finetune. Future development of HyLake v1.0 needs

to collect more observations, including heat fluxes and water temperature, and searching for more variables in datasets to train LSTM-based surrogates and acquire more general models at a larger scale. However, it is important to note that the performance of HyLake may not always improve with an increase in the training data size. The training datasets with higher representation of physical principles help improve the model performance. Similar phenomenon has already been observed in many deep-learning-based large models, demonstrating that directly training models using all datasets would neglect heterogeneous functional samples and thereby hinder performance gains (Wang et al., 2025). Therefore, this study assumed that an individual-site-trained LSTM-based surrogate would have better capacity in representing lake-atmosphere interactions,

which was collectively matched to the above-mentioned hypotheses. Due to insufficient observations at other lake sites (DPK, PTS, and XLS), to some degree, the surrogates trained on their datasets performed closely in estimating Δ LST except for XLW (Table S1). For the relatively complete observed datasets in BFG (although its biological characteristics cannot represent the whole Lake Taihu), the surrogate performed poorer than the proposed BO-BLSTM-based surrogate in terms of diurnal patterns of LST of HyLake v1.0 (Figure S10). As HyLake is extended to larger scales or more lakes, the computational architecture will need to accommodate large training datasets, which may limit performance for specific lakes. Specifically, the scaling laws for deep-learning models indicate that model performance does not continue to increase indefinitely with the stacking of neurons and layers (Hestness et al., 2017). Adapting more powerful deep-learning-based surrogates will further improve HyLake v1.0 performance, leading to a better representation of lake-atmosphere interactions in ungauged lakes. BO-BLSTM-based surrogate exhibits superior performance in estimating LST for HyLake v1.0. This study adapted BO and EarlyStopping strategies to ensure BLSTM provides accurate and reliable estimates in prediction but increases the computational demands for training due to its ability to converge from its more complex Bayesian architecture (Peng et al., 2025; Ferianc et al., 2021). In addition, the mere 1 Bayesian fully connected layer that was adapted in this surrogate only captures limited data uncertainty, which may lose several important aspects of probabilistic prediction (Klotz et al., 2022). Given the importance of uncertainty quantification for BLSTM, it is worth noting that HyLake v1.0 has the potential to assess the variance of predictions and probabilities of lake extreme events occurrence by developing its surrogate in future (Kar et al., 2024; Gawlikowski et al., 2023). Major limitations, including high computational demands and insufficient model performance, should be addressed by developing a novel deep-learning-based surrogate based on a more efficient architecture and larger datasets.

Moreover, the proposed hard-coupling strategies in HyLake v1.0 provide possibilities for coupling additional modules, such as lake water temperature, methane and carbon dioxide dynamics, oxygen dynamics, and lake-watershed interactions. Previous 1-D process-based lake models have often been developed as a backbone for coupling with these various modules (Saloranta & Andersen, 2007; Stepanenko et al., 2016). For example, Lake 2.0 was proposed by Stepanenko et al. (2016) first coupled methane and carbon dioxide modules to investigate oxygen, methane, and carbon dioxide dynamics in Kuivajärvi Lake, and MyLake proposed by Saloranta & Andersen (2007) gradually coupled modules such as DOC degradation, DO dynamics, microbial respiration, several gas exchange models, sediment-water interactions, dynamic light attenuation, nitrogen uptake and floating solar panels (Couture et al., 2015; Exley et al., 2022; Holmberg et al., 2014; Kiuru et al., 2019; Markelov et al., 2019; Pilla & Couture, 2021; Salk et al., 2022). These hydro-biogeochemical processes have typically been described by PDEs or empirical models, which remain simplified and introduce uncertainty to some degrees (L. Li et al., 2021). The flexible structure of HyLake v1.0 allows for better capability to couple with different deep-learning-based surrogates for approximating lake water temperature changes, gas exchange, and DO dynamics, likely achieving better performance than purely process-based or data-driven models.

Overall, HyLake v1.0 holds significant potential for improvement, as current process-based lake models are overly simplistic and fail to capture the full range of hydro-biogeochemical processes accurately. Future efforts should mainly focus on improving the representation of heat and gas transport in the water column to better simulate aquatic ecosystems.

5. Conclusion

This study introduced a novel hybrid lake model, HyLake v1.0, by hard-coupling a BO-BLSTM-based surrogate trained with observations from the MLW lake site in Lake Taihu. It replaced the implicit Euler scheme typically used in traditional process-based lake models with this BO-BLSTM-based surrogate, enabling the prediction of LST, LE, and HE at the lake-atmosphere interface by collectively using energy balance equations. The HyLake v1.0 was proposed to offer more accurate prediction and flexibility in development of hybrid hydrological models. Specifically, in three numerical experiments (MLW, Taihu-obs, and Taihu-ERA5), including three models (FLake, Baseline, and TaihuScene), this study intercompare the performance of HyLake v1.0 by adapting different surrogates, training strategies, and forcing datasets. Additionally, this study used different forcing datasets, including observations from 5 lake sites in Lake Taihu and the ERA5 datasets, to evaluate the and transferability of HyLake v1.0 in ungauged regions and unlearned datasets. The experiments demonstrated that HyLake v1.0 effectively learns the physical principles governing lake-atmosphere interactions, highlighting its potential for application in ungauged lakes. Major conclusions are summarized as follows:

(1) The BO-BLSTM-based surrogate in HyLake v1.0 performed well in representing changes in Δ LST of test dataset (RMSE = 0.2587 °C, MAE = 0.1594 °C), outperforming TaihuScene while underperforming Baseline;

(2) HyLake v1.0 showed superior generalization capacity in LST ($R = 0.99$, RMSE = 1.08), LE ($R = 0.94$, RMSE = 24.65), and HE ($R = 0.93$, RMSE = 7.15) at both daily and hourly scales compared to observations, FLake and Baseline model, indicating that integrating physical principles with LSTM-based surrogates improves model accuracy and better captures changes in lake-atmosphere interactions;

(3) HyLake v1.0 demonstrated its capability of transferability in ungauged regions of Lake Taihu and with low-resolution ERA5 forcing datasets. The results of intercomparison across lake site showed HyLake v1.0 presented the best capability in representation of LST (MAE = 1.03 °C), LE (MAE = 24.79 W/m²) and HE (MAE = 7.88 W/m²) than FLake and TaihuScene. Specifically, it performed the best in MLW, PTS, and XLS, but slightly poorer in BFG and DPK sites than TaihuScene. Regarding the capability of spatial transferability using ERA5 forcing datasets, results indicated HyLake v1.0 performed the most closely matched the observations in Lake Taihu compared to FLake and TaihuScene in 14 of 15 variables (LST, LE and HE in 5 lake sites).

These intercomparison experiments highlighted that HyLake v1.0, when coupled with a BO-BLSTM-based surrogate, offers excellent flexibility and is capable of capturing the underlying physical principles, providing more accurate predictions than traditional process-based models in ungauged regions. This also demonstrates the model's promising potential for application

725 in ungauged lakes. Future work should focus on expanding HyLake v1.0 by exploring different architectures, utilizing larger training datasets, and incorporating additional coupled modules.

Code and data availability. The datasets, codes and scripts of HyLake v1.0 and other models (e.g., Baseline, TaihuScene) used in this study are available at <https://doi.org/10.5281/zenodo.15289113> (He et al., 2025). FLake model was run via LakeEmsemblR tool (<https://aemon-j.github.io/LakeEmsemblR/>). The ERA5 reanalysis datasets can be downloaded from the Climate Data Store (<https://cds.climate.copernicus.eu/>). Observations of lake surface water temperature, latent and sensible heat fluxes at Lake Taihu are available at Harvard Dataverse (<https://doi.org/10.7910/DVN/HEWCWM>; Zhang et al., 2020).
730 **Author contributions.** YH designed the HyLake model, wrote the code, organized the experiments, ran the simulations, performed the results, and wrote the original manuscript. XY contributed to the design and writing of the paper.

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

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