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RESEARCH

PID4LaTe: a physics-informed deep learning model for lake multi-depth temperature prediction

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Abstract

Lake temperature plays a pivotal role in the physical and chemical processes in the water. It has a significant impact on the distribution of lake organisms. In lake temperature modelling, the physics-based models have the shortcomings of parameter calibration and generalization difficulties. The data-driven models are highly data dependent. This makes hybrid models an effective solution at present. In this paper, we explore the spatial and temporal co-evolution process for multi-depth lake temperature and propose a Physics-Informed Deep learning model for Lake multi-depth Temperature prediction, PID4LaTe. It consists of three sub-models, two of which are long short-term memory (LSTM) models for spatial and temporal prediction respectively, and the other is a physical model, the General Lake Model. The physical model offers simulation data based on its rich knowledge for data-driven model learning, while guaranteeing consistency between model results and physical mechanisms. We compared PID4LaTe with the Process-Based model (PB), the Deep Learning model (DL) and the Physics-Guided Recurrent Neural Networks model (PGRNN), and used Root Mean Square Error (RMSE), Mean Square Error (MSE), Mean Absolute Error (MAE) and Mean Absolute Percentage Error (MAPE) to assess the effectiveness of the models. Extensive experiments show the superiority of our hybrid model for lake multi-depth prediction over PB, DL and PGRNN with RMSE of 0.798, MSE of 0.644, MAE of 0.567 and MAPE of 4.367% in Mendota Lake and RMSE of 1.099, MSE of 1.261, MAE of 0.783 and MAPE of 7.936% in Sparkling Lake. The two-cases study indicates that the hybrid model combining the physics-based model with the data-driven model is a promising technique for multi-depth lake temperature predicting. This study provides a reference method for accurate prediction of temperature at multiple depths in lakes.

Keywords Hybrid model · Physics-informed · LSTM · Lake multi-depth temperature prediction

Introduction

The temperature status of lake is the basis for understanding various physicochemical processes and dynamical phenomena in lakes, and is one of the important environmental conditions affecting aquatic ecosystems (Staehr et al. 2010). Lake water temperature not only plays an important role in water balance calculations and evapotranspiration, but also in water quality analyses and material exchange at the soil-water interface (Ciampittiello et al. 2021). Lake water temperatures are distributed in layers with depth, which is called thermal stratification. Figure 1 shows the thermal stratification of a lake in summer. This thermal stratification usually consists of three layers: the epilimnion, the thermocline and the hypolimnion (Boehrer and Schultze 2008). Lake thermal stratification indirectly affects the plankton population structure and also limits the upward and downward mixing motion of turbulent flows (Spigel and Imberge 1987).

Meteorological conditions such as solar radiation, wind speed and precipitation affect the heating and mixing of lake water and have a significant effect on lake temperatures (Arhonditsis et al. 2004). Lake temperatures also exhibit significant seasonal stratification as a result of climatic conditions. In summer, the surface temperature of lakes tends to rise, while deeper layers maintain relatively cooler

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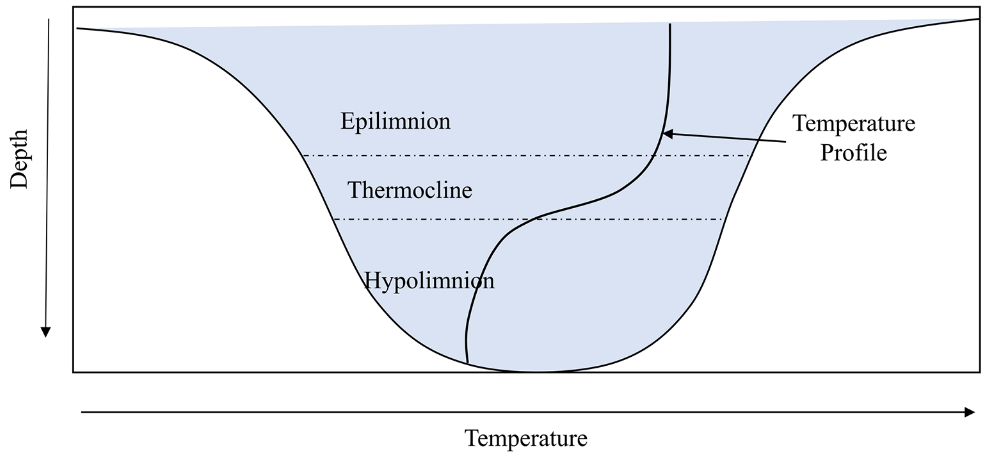

Fig. 1 Thermal stratification and temperature profile of lake in summer. During the summer months, thermal stratification of lakes usually results in the formation of three layers: the epilimnion, the thermocline and the hypolimnion. The epilimnion is warmer, the hypolimnion is cooler, and the water temperature drops sharply between the epilimnion and the hypolimnion, creating a transition zone known as the thermocline

temperatures, resulting in a discernible positive temperature stratification profile. In winter, the surface temperature of lakes is lower than that of the deep layers, showing inverse temperature stratification. The difference between the upper and lower water body temperatures in spring and autumn was small (Lampert and Somme 2007). Temperature prediction at multiple depths in lakes is a challenging task that requires comprehensive consideration of changes in meteorological conditions, modelling of thermal stratification phenomena, and the dynamics of water temperatures in different seasons and depths.

Some works related to lake temperature prediction have been proposed. Based on the technical approach, they can be divided into three categories: the physics-based methods, the data-driven methods, and the hybrid methods.

Researchers have focused on the physics-based methods that build complex functions to represent the physical and thermal processes between the lake and the atmosphere. Several models have been proposed to predict lake surface temperature, including regression methods (Kettle et al. 2004; Livingstone and Lotter 1998; Sharma 2008) and process-based numerical models (Martynov et al. 2010; Thiery et al. 2014). Due to their limitations of not being able to address some fundamental processes, Piccolroaz et al. (2013, 2016) proposed the air2water model that can reliably estimate lake surface temperature based on air temperature alone. The physical models for predicting lake temperature at multi-depths are more complex because they involve the vertical temperature distribution and variations within the lake. There have developed numerous models, such as the one-dimensional model Dynamic Reservoir Simulation Model (DYRESM) (Weinberger and Vetter 2012), the General Ocean Turbulence model (GOTM) (Burchard 2002) and the General Lake Model (GLM) (Read et al. 2017; Hipsey et al. 2019). We chose GLM as the primary physics-based model for predicting lake temperature because of its outstanding performance and extensive usage in lake modelling. It considers the effect of inflows/outflows, mixing and surface heating and cooling (Menció et al. 2017). The estimation and calibration of parameters in GLM models requires considerable observational data and computational resources. Accurate estimation and calibration of these parameters is a major challenge, especially for large lakes and complex environmental conditions.

With the advancement of big data era, the data-driven methods have emerged as a promising alternative for lake temperature prediction. It provides a flexibility and effective solution compared to the physics-based models (DeWeber and Wagner 2014). Some works have been reported that are adaptive network based on fuzzy inference system (Karabog and Kaya 2019), the standard multiple linear regression (Uyanık and Güler 2013), wavelet neural network (Alexandridis and Zapranis 2013) and deep learning neural network (Heddam et al. 2020). Recently, for lake surface temperature prediction, Yu et al. (2020) presented a hybrid prediction model that combines support vector regression (SVR), analytical hierarchy process (AHP), and backpropagation artificial neural network (BPANN) algorithms. This model was applied to simulate and estimate the surface temperatures of 11 lakes in the Yunnan-Guizhou Plateau, and the results showed low error rates and strong generalization capabilities. Willard et al. (2022) introduced entity information and proposed an entity-aware long and short-term memory network (EA-LSTM) to predict daily surface temperatures for lakes in the United States. Hao et al. (2023) proposed an Attention-GRU model, which combines the Self-Attention mechanism and GRU model for predicting lake surface temperature in Qinghai Lake. Di et al. (2023) used a machine learning algorithm by stacking multilayer perceptron and random forest (MLP-RF) for the prediction of lake surface temperatures. The result showed that the entity information is valuable for lake temperature prediction. While surface temperature prediction provides valuable insights, it fails to capture the complex thermal dynamics that occur below the lake surface. In this study, we emphasize the problem of temperature prediction at multiple depths. When multi-depth temperature data is available, researchers typically employ data-driven models to simulate temperatures at different depths separately (Saeed et al. 2016). Saber et al. (2020) used ANN to predict the future water temperature of Lake Mead at 22 different depths. Quan et al. (2022) proposed GA-SVR, a genetic algorithm with support vector regression model, to simulate the temperature of Longyangxia Reservoir at elevations of 2585, 2550 and 2495, respectively. The optimal parameters of SVR were obtained using GA.

The data-driven models demonstrate their excellent capability to a certain extent, but they require large amounts of high-quality data. High-quality data is hard to come by in complex scenarios, hindering the use of data-driven methods.

Recently, some hybrid models combining the data-driven model and the physical model have emerged for lake temperature prediction. These studies used the physical model to generate synthetics data or incorporated it to constrain the optimization objective. For lake multi-depth temperature prediction, Daw et al. (2022) proposed the physics-guided neural networks (PGNN) model that introduced the result of the physical model as a feature for the neural network and designed a loss function based on the relationship between lake depth and density to ensure the prediction coherence of the basic physical process. Subsequently, based on this work, Daw et al. (2020) proposed the Physics-Guided Architecture (PGA) model, which uses auto-encoder structure to extract temporal features and LSTM to mine spatial information to predict an intermediate physical quantity: density. PGA combines knowledge of density-depth physics on LSTM to have a monotonic recurrence relationship between predicted densities. Daw et al. (2020) have recognized that lake temperatures have a series relationship in both time and space, but PGA models have limited methods for mining time series information. Jia et al. (2021) proposed the Physics-Guided Recurrent Neural Networks model (PGRNN) model, which uses simulated data to pre-train data-driven model to address the problem of scarcity of observed data. PGRNN uses LSTM to exploit time-series relationships for lake temperatures, but neglects spatial-series relationships. The above models do not learn enough spatial and temporal information about lake temperatures and the integration with physical models could be further enhanced. Lake temperatures exhibit variations over time and depth. Therefore, the lake temperature prediction problem can be viewed as a spatiotemporal forecasting task, necessitating the extraction of information from both the temporal and spatial dimensions. In this paper, we propose a Physics-Informed Deep learning model for Lake multi-depth Temperature prediction, PID4LaTe. It consists of spatial, temporal and physical models. Extensive experiments show the superiority of our model.

The main contributions of this paper are follows:

(1) A hybrid method with a physics-informed deep learning model is proposed, where the physical model offers information that conforms to special theories to enhance and regularize the deep learning model.
(2) Considering the spatiotemporal change of lake temperature, two LSTMs are introduced to make temporal and spatial predictions respectively. The two views can clearly extract its latent trends from two different angles of view, which is simple but effective.
(3) The proposed model is compared with current popular models for predicting lake temperature, and the experimental results show the valid of our model in the datasets of Mendota and Sparkling lakes.

Table 1 Statistics of the datasets

Dataset	Time range	Time span	Depth range	Depth span	The number of observations
Mendota Lake	April 15,2009 to December 19,2017	1 day	0 m to 25 m	0.5 m	35,179
Sparkling Lake	April 29,2009 to November 13,2017	1 day	0 m to 18 m	0.5 m	26,098

Methods

In this part, we present the lake datasets used for training and testing our model and the overall framework of our proposed Physics-Informed Deep learning model for Lake multi-depth Temperature prediction (PID4LaTe).

Datasets

The datasets used in our experiments are temperature data from Lake Mendota and Lake Sparkling in the United States, which are publicly available from Read et al. (2019) and can be downloaded from https://doi.org/10.5281/zenodo.3497495. Observations of lake temperatures were obtained from North Temperate Lakes Long-Term Ecological Research Program (Read et al. 2019), specifically discrete temperature profile values. The sampling location for the Mendota Lake data is 43.099°N, -89.405°E, and for the Sparkling Lake data, it is 46.008°N, -89.701°E. The detailed information on the datasets is presented in Table 1. On some days we have observations at multiple depths, while on others there are few or no observations.

For Lake Mendota, we selected temperature measurements at every 0.5 m interval from the surface to a depth of 25 m. The dataset for Lake Mendota includes temperature observations from 15 April 2009 to 19 December 2017, for a total of 35,179 observations.

For Lake Sparkling, we selected temperature measurements at every 0.5 m interval from the surface to a depth of 18 m. The dataset for Lake Sparkling includes temperature observations from 29 April 2009 to 13 November 2017, for a total of 26,098 observations.

The features used in the experiments comprise daily climate conditions recorded between 2009 and 2017. Specifically, we focus on 10 features, including the day of the year, depth, shortwave radiation, etc., listed in Table 2. All meteorological features, except the depth feature and the predicted value generated by the GLM model, are measured or derived from the meteorological dataset. The meteorological dataset was recorded from stations located about 2 km and 10 km from Lake Mendota and Lake Sparkling. These features have consistent values across different depths on a given day. It is worth noting that the input features do not include historical lake temperature. Considering that there are some days when the temperature data is lost, we set up a mask vector, the vector consists of 0 and 1, where 0 means that the temperature data for that day is lost and 1 means that the temperature data for that day exists. The loss is calculated by multiplying the mask vector by the matrix of the difference between the true and predicted values.

Problem formulation

The aim of this paper is to predict the temperature at varying depths of the lake using given meteorological variables. We use $X = < X^1, X^2, ..., X^T > \in \mathfrak{R}^{T\times m}$ as the input sequence. $X^i \in \mathfrak{R}^m$ represents the i th feature vector. T represents the window size, while m refers to the feature dimension. $Y^T = \{y_i^T\}_{i\in Depth}$ represents the lake temperature at different depths at the time T. Hence, the lake temperature prediction task can be defined as to find the function $f : X \rightarrow Y^T$. The inputs X^i consist of short-wave radiation, long-wave radiation, wind speed, air temperature, relative humidity, rain, snow, as well as the value of depth and day of year.

Table 2 Details of the features used in this study

Name	Units
Day of Year (1-366)	days
Depth	m
Short-wave Radiation	W/m2
Long-wave Radiation	W/m2
Air Temperature	℃
Relative Humidity	%
Wind Speed	m/s
Rain	cm
Snow	cm
Physical model theoretical value	℃

Long-short term memory networks

Sequence prediction is a challenging class of prediction problems that need to capture sequence dependencies between input variables. Recurrent neural network (RNN) is a kind of neural network that can be used specifically to deal with sequence dependency. Long short-term memory network (LSTM) is a special kind of RNN. Memory units in LSTM are able to store and update information. It can store historical data to better predict future trends. The network structure is shown in Fig. 2.

The LSTM cell consists of an input gate i_t, an output gate o_t, a forget gate f_t and a cell gate c_t. The individual gates within the LSTM cell are calculated as follows:

$$f_t = sigmoid\left(W_f x_t + U_f h_{t-1} + b_f\right) \tag{1}$$

$$i_t = sigmoid\left(W_i x_t + U_i h_{t-1} + b_i\right) \tag{2}$$

$$o_t = sigmoid\left(W_o x_t + U_o h_{t-1} + b_o\right) \tag{3}$$

$$\tilde{c}_t = tanh\left(W_c x_t + U_c h_{t-1} + b_c\right) \tag{4}$$

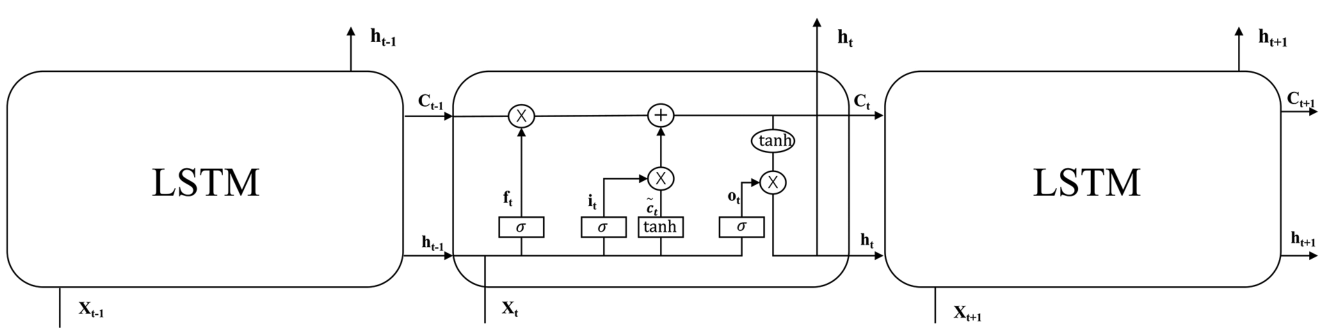

Fig. 2 The network structure of LSTM.

$$c_t = f_t c_{t-1} + i_t \tilde{c}_t \tag{5}$$

$$h_t = o_t \tanh(c_t) \tag{6}$$

where W_f, U_f, W_i, U_i, W_o, U_o, W_c and U_c stand for weights, b_f, b_i, b_o and b_c denote bias. $sigmoid$ is the sigmoid activation function. $tanh$ is the hyperbolic tangent activation function.

LSTM effectively solves the problems of gradient vanishing and gradient explosion in traditional RNNs through the gating mechanism. The gating mechanism enables the model to better capture long-term dependencies in sequence data, and is often able to achieve better results in sequence prediction tasks (Sherstinsky 2020). Therefore, we chose the LSTM as the prediction model for the sub-module.

PID4LaTe model

The overview of PID4LaTe is shown in Fig. 3, which consists of four major components: (1) Physical module that generates the predictions based on general physical knowledge. (2) Spatial prediction module that captures depth sequence information using LSTM. (3) Temporal prediction module that captures time series information using LSTM. (4) Modules-hybrid prediction that fuses the three modules to obtain the final predictions.

Physical module

In PID4LaTe, we use the GLM model as the physical model for predicting lake temperature. The GLM model considers surface heat exchange, vertical energy layer mixing and other factors. It gives a mapping function between the dynamic physical processes and water temperature. The GLM model takes meteorological time series data as input. In our work, the GLM model first needs to be calibrated. The calibration of the GLM model parameters can be expressed as the following optimization problem:

$$\min_{\theta} \sqrt{\frac{1}{s}\sum\nolimits_{(T,d)\in s}\left(y_d^T - y\_phy_d^T\right)^2} \tag{7}$$

$$s.t.\, y\_phy = f_\theta(X\_m\,|\theta)$$

where y_d^T represents the recorded temperature of the lake at time T and depth d, s is the sample size, y_phy denotes the theoretical value based on the physical model, which incorporates temperature at each depth from 1 to T time points, θ is the parameter sets, and X_m

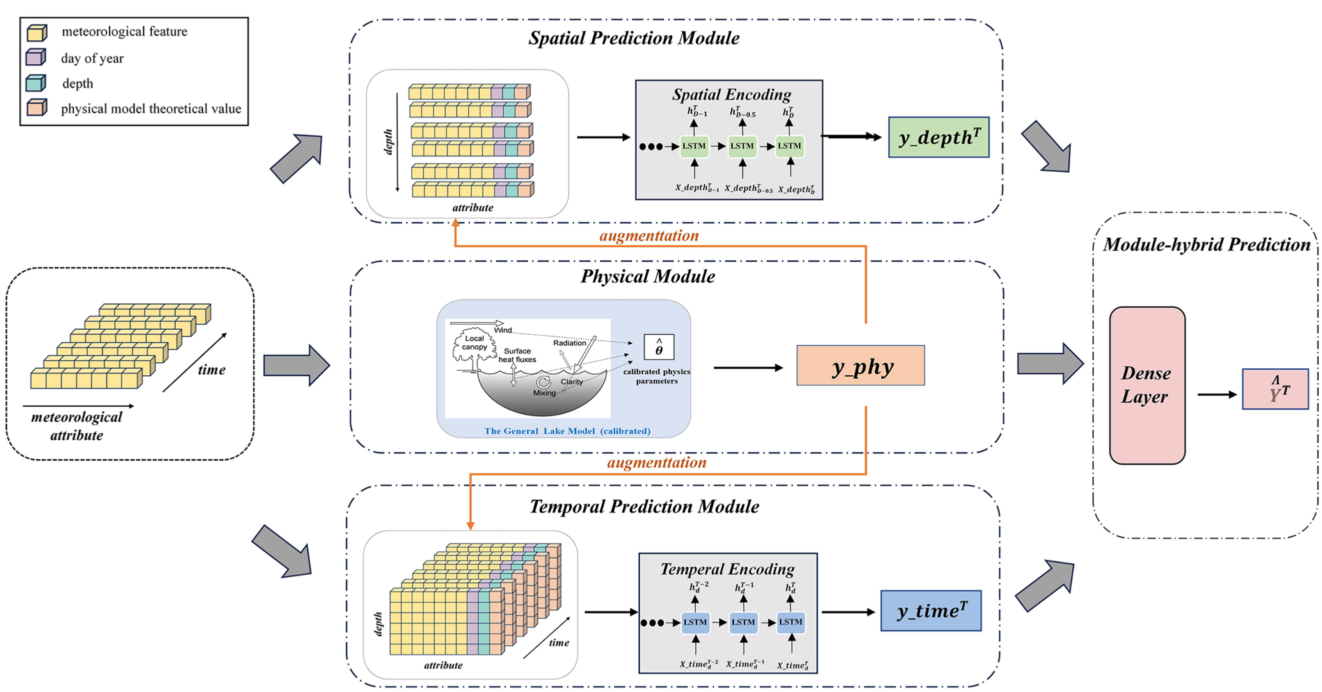

Fig. 3 The overview of PID4LaTe. In this model, the time interval is one day and the depth interval is 0.5 m. The PID4LaTe model can be divided into four modules: (1) Physical module generates the physical model theoretical values based on the meteorological time series data. (2) Spatial prediction module outputs the predicted values with spatial information based on the input features consisting of meteorological features, day of the year, depth, and the physical model theoretical values. (3) Temporal prediction module outputs the predicted values with temporal information based on the input features consisting of meteorological features, day of the year, depth, and the physical model theoretical values. (4) Modules-hybrid prediction: the outputs of Physical module, Spatial prediction module, and Temporal prediction module are passed through the Dense layer to get the final temperature predictions

is the meteorological data. The shape of X_m is $time\_window$*meteorological$_feature_number$.

The parameters of GLM model are linked to the location, depth, hypsographic curve, and other morphological characteristics of the lake. The objective is to select a set of parameter values, denoted as $\hat{\theta}$, that best matches the model output with the observed data. This optimisation is achieved through an adaptive evolution strategy of covariance matrix adaptive evolution strategy, resulting in the theoretical temperature values y_phy. The shape of y_phy is $time\_window$*d$epth_window$.

The GLM model is a general model for different lakes. It shows the significant relationship between temperature and factors such as morphology, hydrology, climatic conditions, and others.

The physical model generates simulated values at different depths, which are combined with known data to form series data at different depths. It plays the role of data augmentation, solving the problem of data shortage in practical application scenarios. At the same time, the simulation value of the physical model as a feature is in accordance with the physical law.

Spatial prediction module

Sequence data with different depth information are formed after the GLM model augmentation. Considering the spatial extent, the lake temperature shows a smooth evolving process over different depths. LSTM has gained popularity due to its ability to model long-term dependencies and ease of implementation. To capture this dependence relationship, we use LSTM to extract the concealed pattern of change in depth. The physical model theoretical values y_phy^T at time T are incorporated into the input, combined with the inputs X^T at time T to construct the input matrix X_depth^T. The size of the depth window is dw, with a depth interval of 0.5 m. The calculation formula for dw is:

$$dw = (D + 0.5)/0.5 \tag{8}$$

where D is the maximum depth of the lake. The shape of X_depth^T is $1*dw*feature\_number$. The spatial prediction module generates temperatures y_depth^T at different depth during a given time T based on depth series relationships. The shape of y_depth^T is $1*dw$.

Temporal prediction module

In PID4LaTe, the LSTM model is introduced to capture the temporal latent correlation. The input X_time to this module includes meteorological features X_m, day of the year, depth, and the physical model theoretical value. The shape of X_time is $dw*time\_window*feature\_number$. The meteorological features X_m comprise seven variables, namely short-wave radiation, long-wave radiation, wind speed, air temperature, relative humidity, rain, and snow. We include the theoretical value of physical model as a data augmentation feature, concatenated with X_m, day of the year and depth. The aim of this model is to extract the evolving temporal trend at a fixed depth. The output of this module is y_time^T which represents the temperatures at different depths at time T, calculated through the temporal sequence relationship. The shape of y_time^T is $dw * 1$.

Modules-hybrid prediction

Based on the physical module, the temporal prediction module and the spatial prediction module, the model derives three prediction values. These three values are initially transformed into one-dimensional data and subsequently passed through a dense layer with a single neuron to obtain the final temperature prediction $\hat{y}_d^T$, corresponding to time T and depth d:

$$\begin{aligned}\hat{y}_d^T =& f(w\_time * y\_time_d^T + w\_depth * y\_depth_d^T \\ &+ w\_phy * y\_phy_d^T + b)\end{aligned} \tag{9}$$

The function f is a linear activation function, while w_time ,w_depth and w_phy stand for weights, b denotes bias. The model generates more accurate prediction by considering the temporal and spatial dynamic correlations and physical principles.

The loss function is defined as the root mean square error between the predicted value and the true value:

$$loss_{rmse} = \sqrt{\frac{1}{s}\sum\nolimits_{(T,d)\in s}(y_d^T - \hat{y}_d^T)^2} \tag{10}$$

where s is the number of samples. We employ the loss function $loss_{Ec}$ developed by PGRNN (Jia et al. 2021) according to the energy conservation law to ensure reliable prediction of lake temperature. It guarantees the interpretability of the predicted results. PGRNN has already conducted thorough discussions on this topic, thus we will not repeat these analyses. The final loss function is obtained by adding the two:

$$loss_{all} = loss_{rmse} + \lambda_{Ec} loss_{Ec} \tag{11}$$

where λ_{Ec} is the coefficient of the energy conservation law loss function. The loss function is calculated and then backpropagated to update the model parameters.

Table 3 The inputs of PB, DL, PGRNN and PID4LaTe

Model	Inputs
PB	Short-wave Radiation, Long-wave Radiation, Air Temperature, Relative Humidity, Wind Speed, Rain, Snow
DL	Short-wave Radiation, Long-wave Radiation, Air Temperature, Relative Humidity, Wind Speed, Rain, Snow, Day of Year, Depth
PGRNN	Short-wave Radiation, Long-wave Radiation, Air Temperature, Relative Humidity, Wind Speed, Rain, Snow, Day of Year, Depth
PID4LaTe	Short-wave Radiation, Long-wave Radiation, Air Temperature, Relative Humidity, Wind Speed, Rain, Snow, Day of Year, Depth, Physical model theoretical value

Evaluation metrics

We choose Root Mean Square Error (RMSE), Mean Square Error (MSE), Mean Absolute Error (MAE) and Mean Absolute Percentage Error (MAPE) as evaluation metrics. They are calculated as follows:

$$RMSE = \sqrt{\frac{1}{s}\sum_{(T,d)\in s}(y_d^T - \overset{\Lambda}{y}{}_d^T)^2} \tag{12}$$

$$MSE = \frac{1}{s}\sum_{(T,d)\in s}\left(y_d^T - \overset{\Lambda}{y}{}_d^T\right)^2 \tag{13}$$

$$MAE = \frac{1}{s}\sum_{(T,d)\in s}\left|y_d^T - \overset{\Lambda}{y}{}_d^T\right| \tag{14}$$

$$MAPE = \frac{100\%}{s}\sum_{(T,d)\in s}\left|\frac{\overset{\Lambda}{y}{}_d^T - y_d^T}{y_d^T}\right| \tag{15}$$

where s is the number of test samples, y_d^T and $\overset{\Lambda}{y}{}_d^T$ are the true and predicted values at time T and depth d.

Experiments and results

We did experiments to evaluate the performance of PID-4LaTe. These experiments are summarized in the following research questions:

RQ1 How does the prediction performance of our proposed model PID4LaTe compare to the baseline models?

RQ2 How each module in the PID4LaTe contributes to the overall model performance?

RQ3 Which sub-module fusion approach has better prediction performance?

RQ4 How do PID4LaTe and the baseline models perform in time and depth?

Experiment settings

The experimental environment is as follows: Intel Core i9-10900 K CPU, NVIDIA 3090 GPUs. All codes are implemented in Python (3.7.6).

We have standardized all input features to predict lake temperature at different times and depths. The LSTM consists of 20 hidden neurons. The number of layers is 2. Epoch is a complete run of the process of forward and backward propagation of the entire training dataset through the neural network. In each epoch, all the samples in the training dataset are used to update the parameters of the model. The learning rate is the step size that controls the updating of the model parameters in each iteration. The number of training epoch is 600 and the learning rate is 0.001 for the Mendota Lake dataset. For the Sparkling Lake dataset, the epoch number is 400 and the learning rate is 0.005.

To compare with the baseline models, we follow an experimental design similar to as Read et al. (2019). We randomly select some continuous time periods as the test set, while the remaining time periods are used as the training set. We conduct five experiments, choosing a different test set for each experiment. In our experiments, the Mendota Lake dataset uses data of 980 dates as the training set and 540 dates as the test set. The Sparkling Lake dataset uses data of 500 dates as the training set and 540 dates as the test set.

Comparison methods

We choose the state-of-the-art models used for multi-depth temperature prediction in lakes as the baseline models. Table 3 shows the inputs to each model. The baseline models include:

PB (Read et al. 2017): A Process-Based model, which is the physical model. We select the GLM model. It is calibrated using the training sets of the two lakes, and the predicted results are evaluated on the test set.

DL (Jia et al. 2021): A Deep Learning model in which the meteorological indicators are features and LSTM is used to extract the time series relationships and generate the prediction.

PGRNN (Jia et al. 2021): This is a hybrid model which unites physical and data-driven models. The model employs LSTM to capture the temporal dynamic patterns of lake temperature. It is pre-trained using the output of the uncalibrated GLM model and further fine-tuned using a limited set of observations. The model also incorporates additional states derived from physical equations into the loss function to ensure energy conservation. In addition, PGRNN is another name for the Process-Guided Deep Learning (PGDL) model proposed by Read et al. (2019).

Hyperparameters study

We investigate the influence of the number of hidden neurons, the learning rate and the epoch on the model performance. Using an iterative approach, we systematically vary these parameters to assess their impact on the overall performance of the model. Hidden neurons $\in$ {10,20,30,40}, learning rate $\in$ {0.05,0.01,0.005,0.001,0.0005}, epoch $\in$ {100,200,300,400,500,600,700,800}.

Supplementary Table S1 shows the performance of the number of hidden neurons on the two datasets. The effect of this factor on the model performance is subtle. When the number of hidden neurons is set to 20, the model performs best on two datasets.

Supplementary Table S2 shows that the learning rate setting has a great impact on model performance. For Mendota Lake, the learning rate is set to 0.001 for best performance. For Sparkling Lake, the learning rate is set to 0.005 for best effect.

Supplementary Fig. S17 shows the optimal value for Mendota Lake when the epoch number is 600. The best value for Sparkling Lake is taken for an epoch number of 400.

Performance evaluation (RQ1)

The experimental results are given in Table 4. We can draw the following conclusions:

Our model demonstrates the superior performance than others on the two datasets. Table 4 shows the values of the evaluation metrics of our proposed model and other baseline models on the train and test datasets in Lake Mendota and Lake Sparkling. After five experiments, PID4LaTe performs best in both lakes, with an RMSE of 0.798, MSE of 0.644, MAE of 0.567 and MAPE of 4.367% in Lake Mendota, compared to an RMSE of 1.099, MSE of 1.261, MAE of 0.783 and MAPE of 7.936% in Lake Sparkling.

The hybrid models of PGRNN and PID4LaTe are all superior to the physics-based model and the data-driven model. As can be seen in Table 4, PB performs the worst with RMSE of 1.564, MSE of 2.511, MAE of 1.097, and MAPE of 8.787% in Lake Mendota and RMSE of 1.600, MSE of 2.619, MAE of 1.278, and MAPE of 11.804% in

Table 4 RMSE, MSE, MAE and MAPE of PB, DL, PGRNN and PID4LaTe on the train and test datasets for the two lakes. (**Bold** and *Italic* highlight the best and second-best model performance respectively.)

	Dataset	MODEL	RMSE	MSE	MAE	MAPE
Train dataset	Mendota Lake	PB	1.500	2.254	1.057	8.786%
		DL	1.074	1.159	0.786	4.099%
		PGRNN	*0.914*	*0.838*	*0.673*	*4.316%*
		PID4LaTe	**0.495**	**0.246**	**0.349**	**2.676%**
	Sparkling Lake	PB	1.468	2.159	1.097	10.524%
		DL	1.465	2.162	1.057	6.163%
		PGRNN	*1.294*	*1.688*	*0.952*	*6.687%*
		PID4LaTe	**0.437**	**0.194**	**0.315**	**2.995%**
Test dataset	Mendota Lake	PB	1.564	2.511	1.097	8.787%
		DL	1.074	1.157	0.786	6.397%
		PGRNN	*0.914*	*0.838*	*0.673*	*5.488%*
		PID4LaTe	**0.798**	**0.644**	**0.567**	**4.367%**
	Sparkling Lake	PB	1.600	2.619	1.278	11.804%
		DL	1.450	2.162	1.057	10.466%
		PGRNN	*1.281*	*1.688*	*0.952*	*9.402%*
		PID4LaTe	**1.099**	**1.261**	**0.783**	**7.936%**

Lake Sparkling, followed by DL with RMSE of 1.074, MSE of 1.157, MAE of 0.786 and MAPE of 6.397% in Lake Mendota and RMSE of 1.450, MSE of 2.162, MAE of 1.057 and MAPE of 10.466% in Lake Sparkling.

PID4LaTe has a better performance than PGRNN. The RMSE values of PID4LaTe are reduced by 12.7% and 14.2%, respectively. The improvement of PID4LaTe is significant when compared to PGRNN.

Ablation study (RQ2)

To investigate the role of each module in PID4LaTe, we design the ablation experiments. We calculate the mean of the results from five experiments, while discarding the highest and lowest values, to account for cases where certain models perform exceptionally well or poorly on specific datasets. The experimental results are shown in Fig. 4, where:

(1) PID4LaTe: the complete model.
(2) PID4LaTe-Tem: remove only the temporal prediction module.
(3) PID4LaTe-Spa: remove only the spatial prediction module.
(4) PID4LaTe-Phy: remove only the physical module.

The temporal prediction module shows superior performance in lake temperature prediction. Removing the temporal module results in a significant increase in errors, with a reduction of 42.2% for the Mendota Lake dataset and 21.6% for the Sparkling Lake dataset.

The spatial prediction module can help to reduce the prediction errors. The errors of PID4LaTe-Spa on the Mendota Lake and Sparkling Lake datasets increase by 3.4% and 17.5% respectively when the spatial module is removed. The role of the spatial prediction module is not as great as that of the temporal prediction module. However, it improves the accuracy of the lake temperature prediction to some extent.

The physical module plays a crucial role in improving the quantity and quality of the data, thereby enhancing the accuracy of prediction. Removing this module leads to an increase in errors, with an increase of 2.4% for the Mendota Lake dataset and 17.1% for the Sparkling Lake dataset. Therefore, the physical prediction module is also indispensable.

As a result, all three modules are crucial. They have a favorable impact on the prediction of lake temperature.

Analysis of the fusion procession (RQ3)

In addition, we explore different fusion processes for submodules and evaluate their performance. Four fusion techniques have been tested and compared:

Res: Residual model (San and Maulik 2018a, b; Wan et al. 2018). The final output of the model is the sum of the outputs of the three modules. It adopts data-driven method to correct the residual of the physical model.

Ave: This method is to sum the outputs of three modules and averages them as the final prediction.

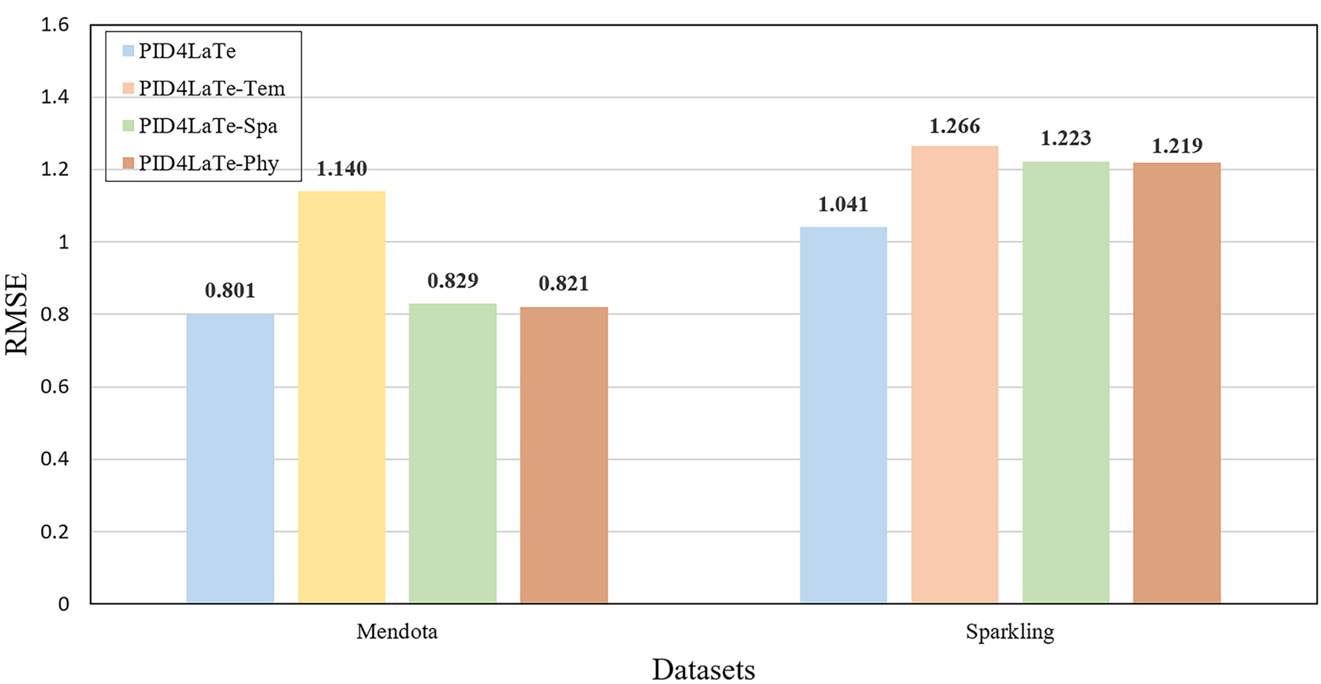

Fig. 4 RMSE values of prediction results for PID4LaTe, PID4LaTe-Tem, PID4LaTe-Spa and PID4LaTe-Phy

BLUE (Xue et al. 2022): It statistically integrates the model of the PID4LaTe removal physical prediction module with the theoretical value of the physical model based on the best linear unbiased estimator to get the final prediction. The best linear estimate (X_B) is:

$$X_B = \frac{{\sigma_P}^2}{{\sigma_P}^2 + {\sigma_D}^2} X_D + \frac{{\sigma_D}^2}{{\sigma_P}^2 + {\sigma_D}^2} X_P \tag{16}$$

where σ_P and σ_D are the root mean square errors of PID4LaTe-Phy and PB predictions, respectively. X_D and X_P are the temperature values from PID4LaTe-Phy and PB, respectively.

PID4LaTe: The final prediction is obtained by feeding the outputs of three modules into a dense layer. It learns the weights and gets the final prediction.

Table 5 shows the prediction results of different fusion techniques for the two lake datasets. Res gives the worst results at Lake Mendota with RMSE value of 0.943, MSE of 0.906, MAE of 0.673 and MAPE of 5.442%. In the residual model, the data-driven model acts as a corrective element, while the output of the physical model dominates the prediction. The data-driven model plays a lesser role. Ave gives better predictions than Res at Lake Mendota with RMSE value of 0.842, MSE of 0.717, MAE of 0.603 and MAPE of 4.658%. Ave assigns equal weight to the outputs of the temporal prediction module, the spatial prediction module, and the physical module. PID4LaTe and BLUE exhibit similar errors on Mendota Lake. BLUE has an RMSE of 0.797, MSE of 0.639, MAE of 0.585 and MAPE of 4.515%. PID4LaTe has an RMSE of 0.798, MSE of 0.644, MAE of 0.567 and MAPE of 4.367%. However, PID4LaTe significantly outperforms Blue on Sparkling Lake. As BLUE is a statistical fusion technique, it is clear from Eq. (16) that the results of the fusion are significantly limited by the RMSE of PID4LaTe-Phy and PB. The benefits of merging the two are only marginally improved. Figure 4 shows that the efficiency of PID4LaTe-Phy in Sparkling Lake is relatively low compared to that in Mendota Lake, which leads to the fusion result in Sparkling Lake not being as good as that in Mendota Lake.

Table 5 RMSE, MSE, MAE and MAPE of prediction results for Rse, Ave, BLUE and PID4LaTe. (**Bold** and *Italic* highlight the best and second-best model performance respectively.)

Dataset	MODEL	RMSE	MSE	MAE	MAPE
Mendota Lake	Rse	0.943	0.906	0.673	5.442%
	Ave	0.842	0.717	0.603	4.658%
	BLUE	**0.797**	**0.639**	*0.585*	*4.515%*
	PID4LaTe	*0.798*	*0.644*	**0.567**	**4.367%**
Sparkling Lake	Rse	1.135	1.314	*0.809*	8.092%
	Ave	*1.118*	*1.267*	0.820	**7.812%**
	BLUE	1.230	1.530	0.934	8.876%
	PID4LaTe	**1.099**	**1.261**	**0.783**	*7.936%*

These findings suggest that the fusion process in PID4LaTe enables better integration of the three modules, leading to improved forecast performance.

Performance of predicted temperature in time and depth (RQ4)

Due to the lack of lake observations during the winter months and the presence of fewer observations in some months, we chose data from the spring (May), summer (July and August), and autumn (October), when there were more observations, to assess the prediction effectiveness of the model across the seasons. Figures 5 and 6 show the results of the different evaluation metrics for PID4LaTe and the baseline models on the predicted values in these months for Lake Mendota and Lake Sparkling, respectively. For these four months, PID4LaTe performs best on almost all evaluation metrics, consistent with the overall performance evaluation results. For Lake Mendota, we selected data at 10 m from 30 April 2017 to 15 November 2017, and for Lake Sparkling, data at 8 m from 18 June 2010 to 15 November 2010 were selected. Figures 7 and 8 show the predicted compared to the true values for PID4LaTe and the baseline models for the selected time ranges at these two lakes. For Lake Mendota, we also compared model predictions with true values at depths of 0 m, 5 m, 15 m, and 20 m, with results shown in Supplementary Fig. S1 through S4. For Lake Sparkling, we also compared model predictions with true values at depths of 0 m, 4 m, 11 m, and 15 m, with results shown in Supplementary Fig. S5 through S8. Overall, the predictions of our model are closer to the true values.

In order to evaluate the prediction effectiveness of different models at different depths, we selected 25 depths from 0 m to 24 m with a depth interval of 1 m for Mendota Lake and 18 depths from 0 m to 17 m with a depth interval of 1 m for Sparkling Lake. Figures 9 and 10 show the performance of PID4LaTe and the baseline models for different evaluation metrics at different depths in Mendota Lake and Sparkling Lake. At shallow depths, PID4LaTe performs similarly to the best baseline model. At deeper depths, PID4LaTe shows a significant improvement in water temperature compared to the baseline models, which can better simulate temperature changes in the lakes. We selected lake temperatures at different depths on 28 May 2014 for Lake Mendota and 31 May 2011 for Lake Sparkling, and plotted the predicted versus true values of PID4LaTe versus the baseline models on both lakes, as shown in Figs. 11 and 12. For Mendota Lake, we also compared the model predictions with the true values on July 21, 2014, August 20, 2014, and October 30, 2014, as shown in Supplementary Fig. S9 to

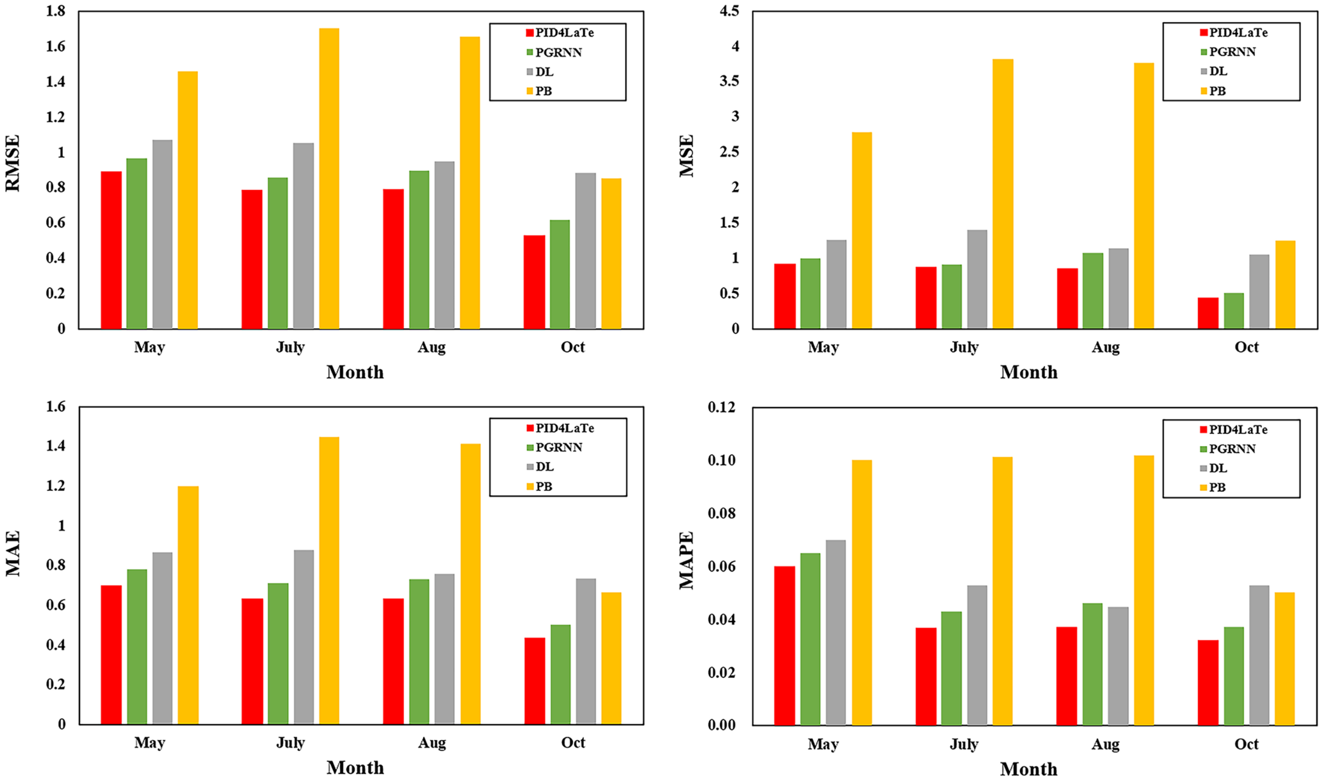

Fig. 5 RMSE, MSE, MAE and MAPE of prediction results for PB, DL, PGRNN and PID4LaTe on the Mendota Lake in May, July, August and October

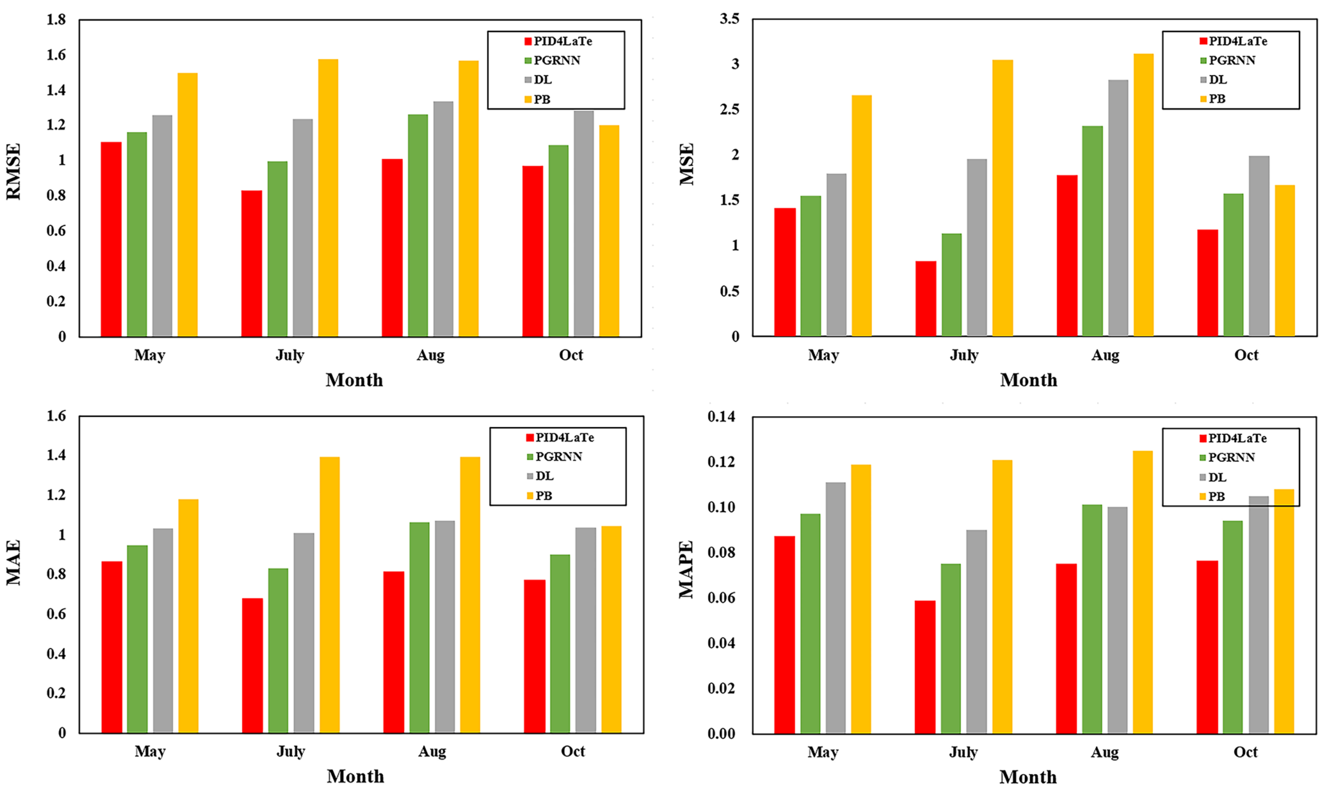

Fig. 6 RMSE, MSE, MAE and MAPE of prediction results for PB, DL, PGRNN and PID4LaTe on the Sparkling Lake in May, July, August and October

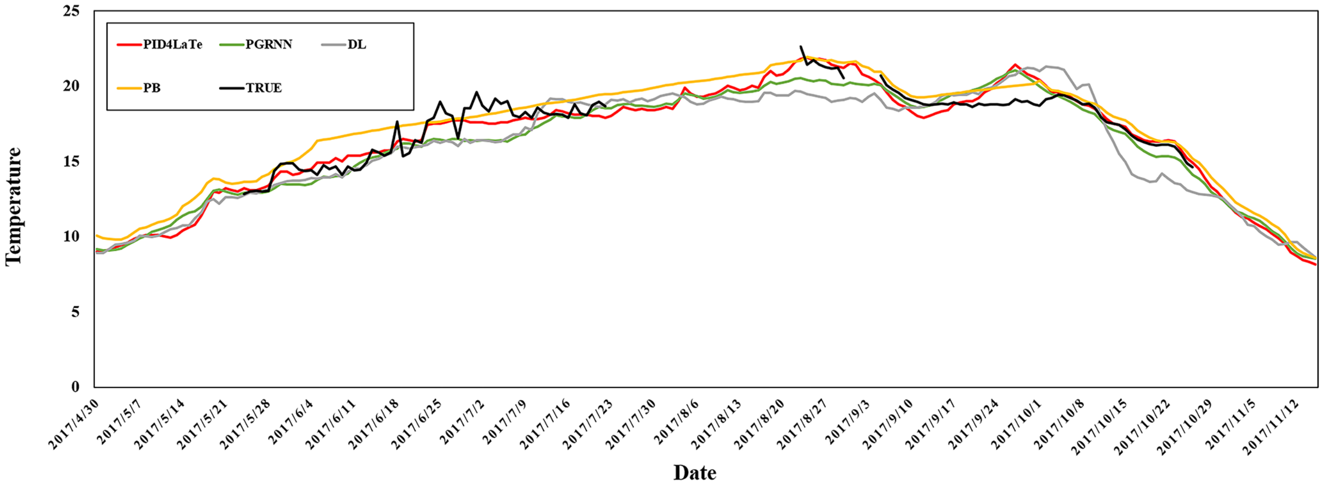

Fig. 7 Temperature predictions for PB, DL, PGRNN and PID4LaTe at 10 m in Lake Mendota from 30 April 2017 to 15 November 2017

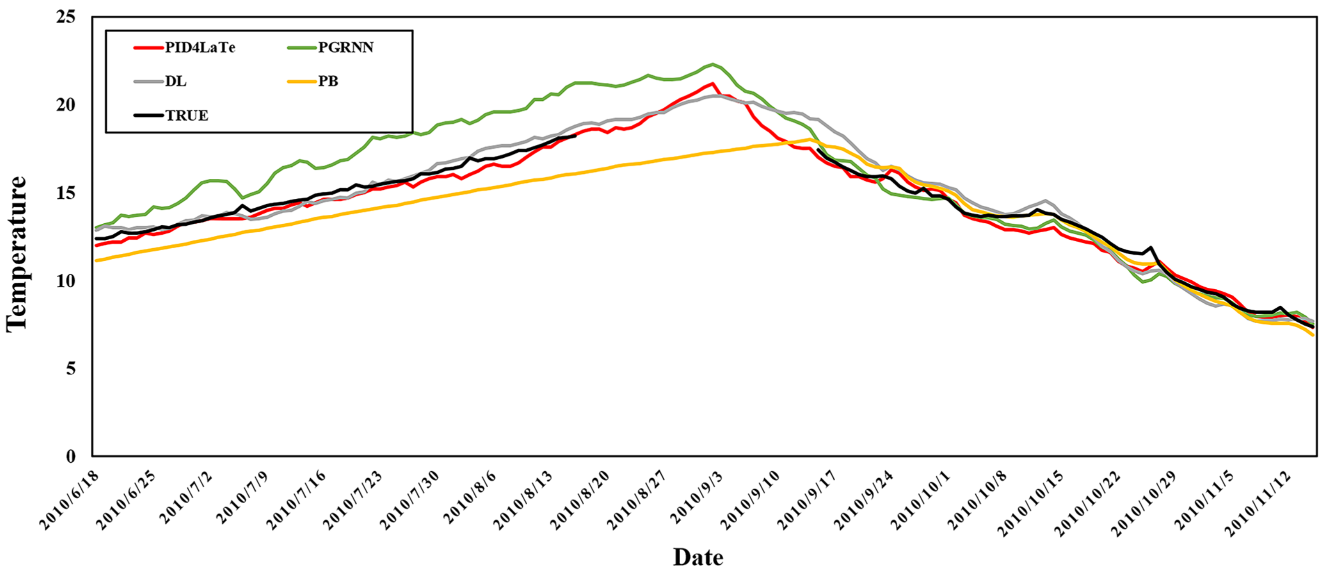

Fig. 8 Temperature predictions for PB, DL, PGRNN and PID4LaTe at 8 m in Lake Sparkling from 18 June 2010 to 15 November 2010

S11. For Sparkling Lake, we compared the model predictions with the true values on July 30, 2011, August 9, 2011, and October 6, 2011, as shown in Supplementary Fig. S12 to S14. The results show that the temperature distribution of PID4LaTe at deeper depths is closest to the true values.

Lake temperatures show a clear seasonal stratification phenomenon, with significant thermal stratification occurring in summer and winter, while in spring and autumn the lake undergoes an overturning phenomenon that reduces the temperature difference between the top and bottom of the lake. Due to the lack of winter observations and the presence of fewer observations in some months, we evaluated the prediction results for Lake Mendota and Lake Sparkling at different depths in summer (July, August), spring (May) and autumn (October). As shown in Supplementary Fig. S14 and S15, for Lake Mendota, the PGDL model performs better at shallower depths in May, July, and August. PID4LaTe is slightly worse than PGDL. PID4LaTe works better at deeper depths. In October, PID4LaTe outperforms the other models overall at various depths. For Sparkling Lake, PID4LaTe performs slightly better than the other baseline models at shallower depths in July and August, and significantly better at deeper depths. In May and October, PID4LaTe is similar to the optimal baseline model at shallower depths, and PID4LaTe performs better at deeper depths. This suggests that when the lake is thermally stratified, PID4LaTe can better simulate lake temperatures in the thermocline and deeper depths. Taken together, the prediction performance of PID4LaTe is similar to that of the optimal baseline model at shallow depths, and at deeper depths PID4LaTe can simulate the temperature change of the lake better than the baseline models. It can more accurately simulate

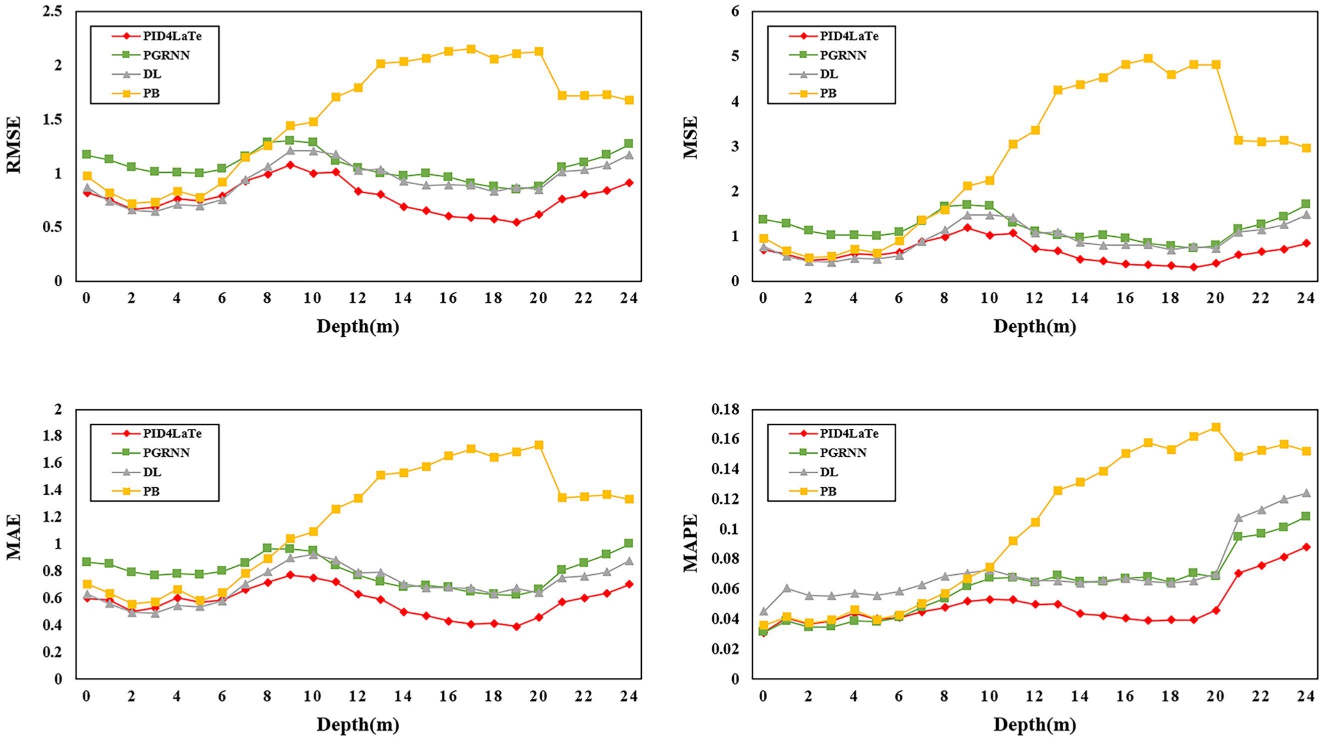

Fig. 9 RMSE, MSE, MAE and MAPE of prediction results for PB, DL, PGRNN and PID4LaTe on the Mendota Lake at different depths

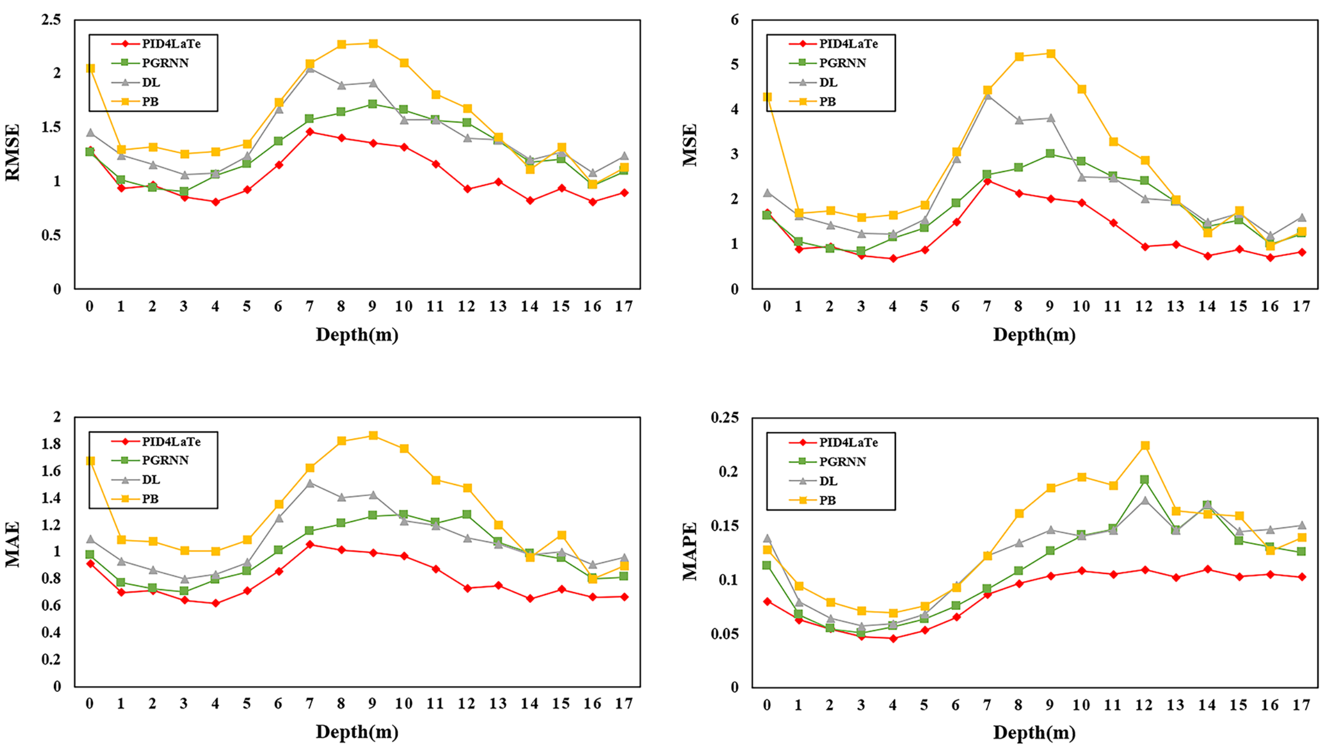

Fig. 10 RMSE, MSE, MAE and MAPE of prediction results for PB, DL, PGRNN and PID4LaTe on the Sparkling Lake at different depths

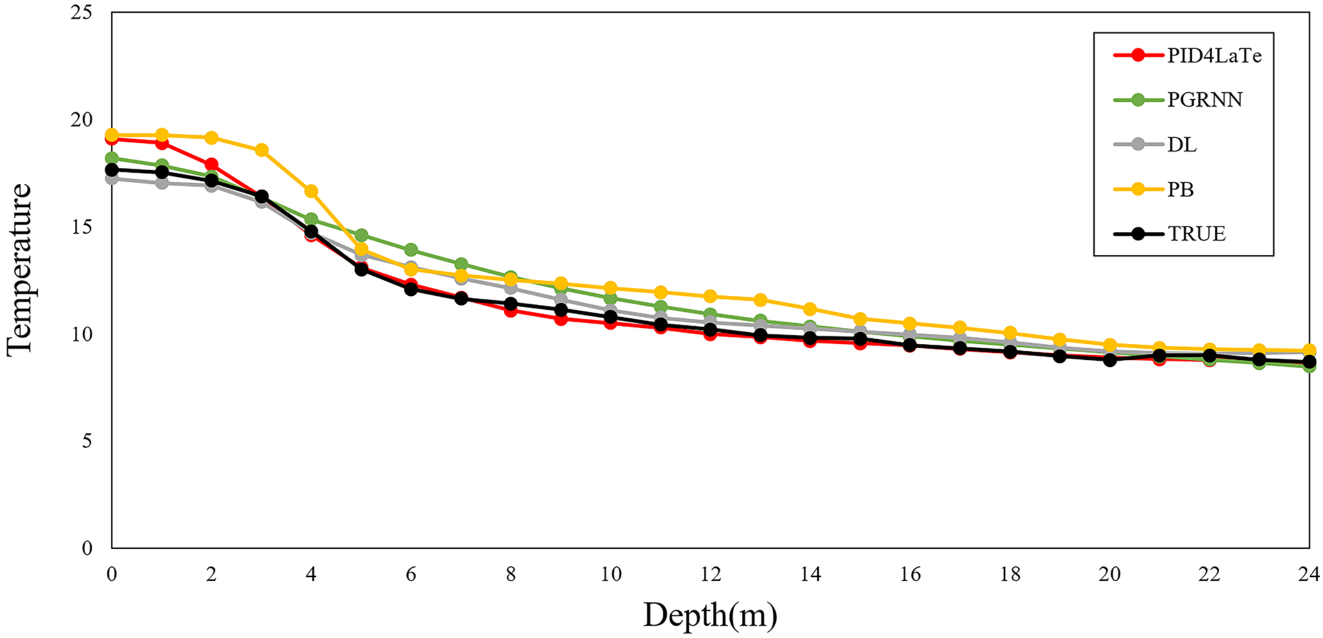

Fig. 11 Temperature predictions for PB, DL, PGRNN and PID4LaTe at different depths in Lake Mendota, 28 May 2014

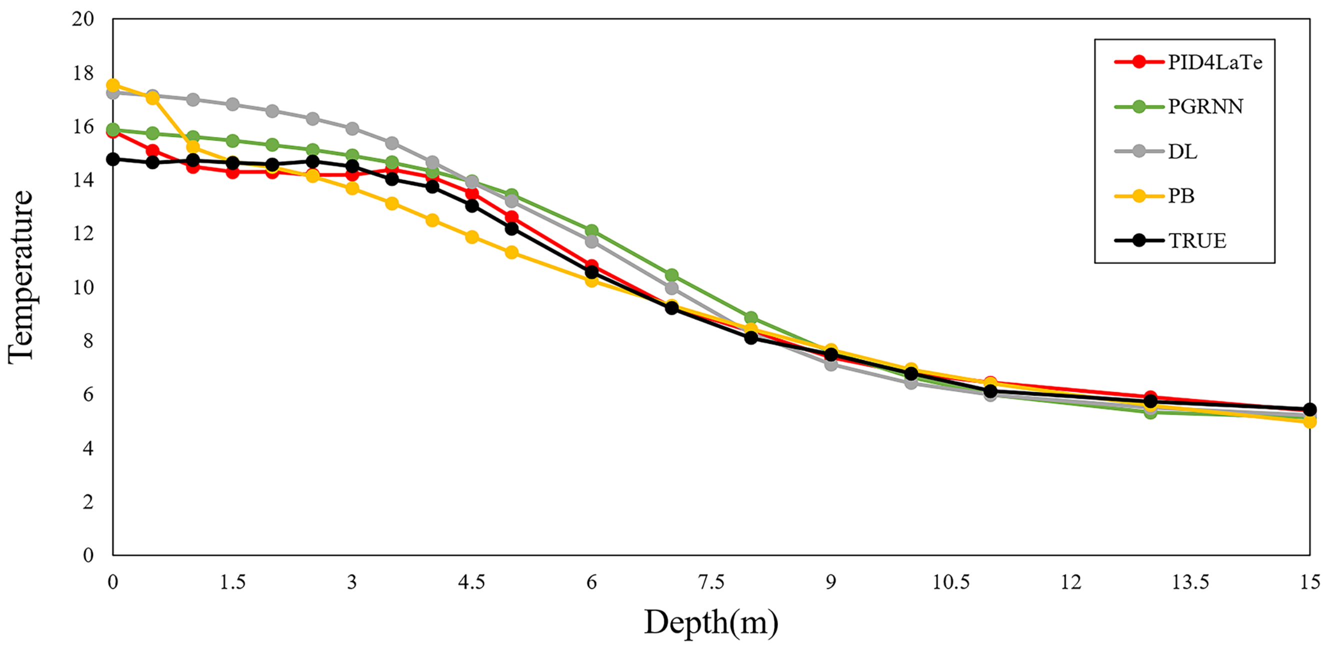

Fig. 12 Temperature predictions for PB, DL, PGRNN and PID4LaTe at different depths in Lake Sparkling, 31 May 2011

temperatures during periods of thermal stratification and mixing in lakes.

Discussion

Lake temperature plays a crucial role in maintaining a balanced underwater ecosystem (Prakash 2021). In this study, a hybrid model PID4LaTe that fuses the data-driven model with the physical model is proposed to predict lake temperatures at different depths. The results of the study show that combining the spatio-temporal mining module with the physical model could result in accurate multi-depth temperature modelling of lakes.

PGRNN and PID4LaTe have better prediction performance than DL and PB for both lakes. PB has the worst performance. PB simulates the dynamics of thermal stratification. However, predicting the stratification dynamics based on the underlying process is very challenging for the physical models including GLM. DL learns patterns from the data and is able to reduce prediction errors for complex processes in lakes. But a combination of physical and data-driven models is more effective. PID4LaTe is superior to PGRNN. One reason is that it takes into account depth sequences that the PGRNN does not. Its spatial prediction module helps to better mine the complex temperature variations at different depths. Another is that PID4LaTe benefits from the combination of the physical model and the data-driven model. All this highlights the advantages of PID-4LaTe over existing models by leveraging both depth and time series relationships and effectively utilizing the physical model to improve prediction.

PID4LaTe outperforms the PGRNN, DL and PB models in terms of prediction performance for selected lake temperatures in summer (July, August), spring (May) and autumn (October). In the shallow layer of the lake, the prediction performance of the PID4LaTe model is similar to that of the optimal baseline models. In the deeper layer, the PID4LaTe model is able to simulate the temperature variation of the lake better than the baseline models, showing an obvious enhancement effect. This improvement is due to the fusion effect of the physical model and the use of the physical model output as a feature for data augmentation in the depth prediction module, which learns more depth information. It can be concluded that the PID4LaTe model is able to simulate lake temperatures more accurately when thermal stratification and mixing occur.

The temporal prediction module, the spatial prediction module and the physical module of PID4LaTe are required. The temporal prediction module plays the main role, because most of the input features of the model change over time. The data contain more time series information. The mining of time series information by the temporal prediction module can greatly improve the prediction accuracy. Lake temperature prediction involves temperature at multiple depths. The same sequence relationship exists between the depths, which requires the spatial prediction module to mine the information. Although the model mines information in both temporal and spatial dimensions, the predictions made by the physical model based on complex physical knowledge cannot be ignored. The sub-modules fusion process of PID4LaTe allows the model to learn the weights of the sub-modules summation on its own to obtain more accurate predictions compared to Res, Ave and BLUE. The fusion method of PID4LaTe can combine the advantages of the sub-modules to a great extent, which can improve the prediction results.

There are some limitations in this study: due to the limited datasets of the studied lake, the applicability of the model proposed in this study to other lakes needs to be further analyzed. In addition, the spatio-temporal mining method of this model does not learn the spatio-temporal dynamic correlation, which needs to be studied by choosing a more advanced deep learning model.

Conclusions

The combination of data-driven model and physical model can improve the prediction of lake temperature at multiple depths more effectively. We consider the relationship between lake temperatures over time series and depth series, and fuse the spatio-temporal model with the physical model to propose a hybrid model: PID4LaTe. The model can effectively improve the accuracy of lake temperature prediction. Among the sub-modules of the model, the temporal prediction module plays the most important role, followed by the spatial prediction module, and finally the physical module.

By analyzing the prediction results in both temporal and spatial dimensions, we found that the PID4LaTe proposed in this paper has better prediction performance in summer (July, August), spring (May) and autumn (October) compared to PB, DL and PGRNN models. PID4LaTe outperforms the PB, DL and PGRNN models at all depths, especially at deeper depths, and is able to simulate temperatures during thermal stratification and mixing in lakes more accurately.

The results of this study will help future researchers in lake ecological studies, environmental protection and policy development. Further research could explore different neural network models and machine learning approaches, as well as more advanced fusion methods of data-driven and physical models to improve and increase the accuracy of lake temperature modelling.

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Author contributions Lingling Chen: Conceptualization, Methodology, Software. Li Wang: Writing-Reviewing and Editing, Supervision. Weixiang Ma: Writing-Original draft preparation. Xiaoya Xu: Visualization, Investigation. Hao Wang: Software, Validation. All authors reviewed the manuscript.

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Data availability No datasets were generated or analysed during the current study.

Declarations

Competing interests The authors declare no competing interests.

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