Supplemental material

Table S1. CE-QUAL-W2 parameter set for the Rappbode Reservoir

Parameter	Description	Value
DLTMIN	Minimum timestep (sec)	1
BETA	Fraction of incident solar radiation absorbed at the water surface	0.45
WSC	Wind sheltering coefficient (-)	1
AX	Longitudinal eddy viscosity (m^2 sec^{-1})	1
DX	Longitudinal eddy diffusivity (m^2 sec^{-1})	1
TSED	Sediment temperature (°C)	10
TSEDF	Heat lost to sediments that is added back to water column	1
Z0	Wind roughness height (m)	0.001
FI	Interfacial Friction (-)	0.015
EXH2O	Light extinction for pure water (m^{-1})	0.55
HWI	Coefficient of water-ice heat exchange (W m^{-2} $°C^{-1}$)	10
SHADE	Shade fraction coefficient (-)	1

S1. CE-QUAL-W2 setup and calibration for the Rappbode Reservoir

In CE-QUAL-W2 (hereafter W2), surface heat exchange was computed component-wise, i.e., shortwave and longwave radiation, sensible, and latent heat fluxes were each evaluated with the model's bulk-aerodynamic formulations. For scalar transport, we adopted the ULTIMATE advection scheme, which uses flux limiting to reduce numerical diffusion while preventing spurious overshoots/undershoots (i.e., maintaining monotonicity and boundedness). Vertical mixing was represented with the turbulent kinetic energy (TKE) closure; consistent with the W2 manual, the maximum vertical eddy viscosity was capped at 1 $m^2\ s^{-1}$.

Following the W2 documentation and prior reservoir applications (Carr et al. 2019; Sadeghian et al. 2018), three site-specific optical and meteorological exposure parameters were treated as calibration variables because they depend on local setting: the shading coefficient (SHADE), wind-sheltering coefficient (WSC), and the light-extinction coefficient (EXH_2O). Manual calibration against the observed thermal structure in the Rappbode Reservoir indicated optimum values of SHADE = 1, WSC = 1, and EXH_2O = 0.55 m^{-1}, which yielded the best overall skill in reproducing the seasonal stratification and temperature profiles. All remaining parameters were retained at W2's standard settings because they are physically based and not typically subject to site calibration (Cole and Wells 2006). The complete parameter set used for the Rappbode Reservoir is provided in Table S1.

S2. Background information on SHAP values

In our study, the final Shapley value for each predictor is obtained by taking a weighted average of these marginal contributions, thus yielding a unified and strictly additive measure of feature importance. For a model with *M* input variables, the Shapley contribution of feature *i* to a single prediction *f*(x) is defined as (Lundberg et al. 2020):

$$\varphi_i = \sum_{S \subseteq \mathcal{F}\{i\}} \frac{|S|!\,(M-|S|-1)!}{M!}\left[f_{S\cup\{i\}}\left(\mathbf{x}_{S\cup\{i\}}\right) - f_S(\mathbf{x}_S)\right]$$

where $\mathcal{F}$ ={1,…,*M*} is the full feature set, S is any subset that excludes i, and $f_S(\mathbf{x}_S)$=E$[f(x)|(\mathbf{x}_S)]$ denotes the conditional expectation of the model output when only the features in *S* are known. The combinatorial weight $\frac{|S|!(M-|S|-1)!}{M!}$ guarantees symmetry and fairness over all *M!* permutations of the input vector, thereby satisfying the axioms of efficiency and additivity.

S3. Thermal indices and model interpretation

Three thermal indices (e.g., Schmidt Stability, the bottom-to-surface temperature difference and mixed-layer depth, see 2.4.2) were applied to further evaluate stratification intensity based on the water temperature output W2, which were also used to illustrate the capability of XGBoost in reproducing the thermal feature of the reservoir. All three have been commonly adopted in previous studies to characterize the thermal structure of inland waters (Fang and Stefan 2009; Ladwig et al. 2021). Here, Schmidt Stability was defined as the energy per unit area required to fully mix a vertically stratified water to a uniform density state (Boehrer and Schultze 2008):

$$S = \frac{g}{A_s}\int_{0}^{z_{\max}} (z - z_*)(\rho_z - \rho_*)A_z dz$$

where S is the Schmidt stability (in J m^{-2}), g is the gravitational acceleration (m s^{-2}), A_s is the reservoir surface area (m^2) and z_{max} is the maximum reservoir depth (m), ρ_z and A_z denote the water density (kg m^{-3}) and horizontal cross-sectional area (m^2) at depth z, respectively. The mixed-layer depth was considered as the depth of minimum curvature of the temperature profile, where d^2T/dz^2 is at a minimum (see Kirillin et al. 2013).

All the statistical analysis and post-processing were performed in R version 4.2.2 (R core Team 2022). The packages "glmtools" (v0.16.0, Read et al. 2014) and "rLakeAnalyzer" (v1.11.4.1, Winslow et al. 2019) were applied for calculating the stratification indices mentioned above. The package "xgboost" (v1.7.8.1, Chen et al. 2015) was used to construct the XGBoost model and "SHAPforxgboost" (v 0.1.0, Liu and Just 2020) to calculate the SHAP value. The package "tidyr" (v1.3.0, Wickham H et al. 2023) was adopted to clean the original database, and "ggplot2" (v3.4.1, Wickham 2016) for visualization.

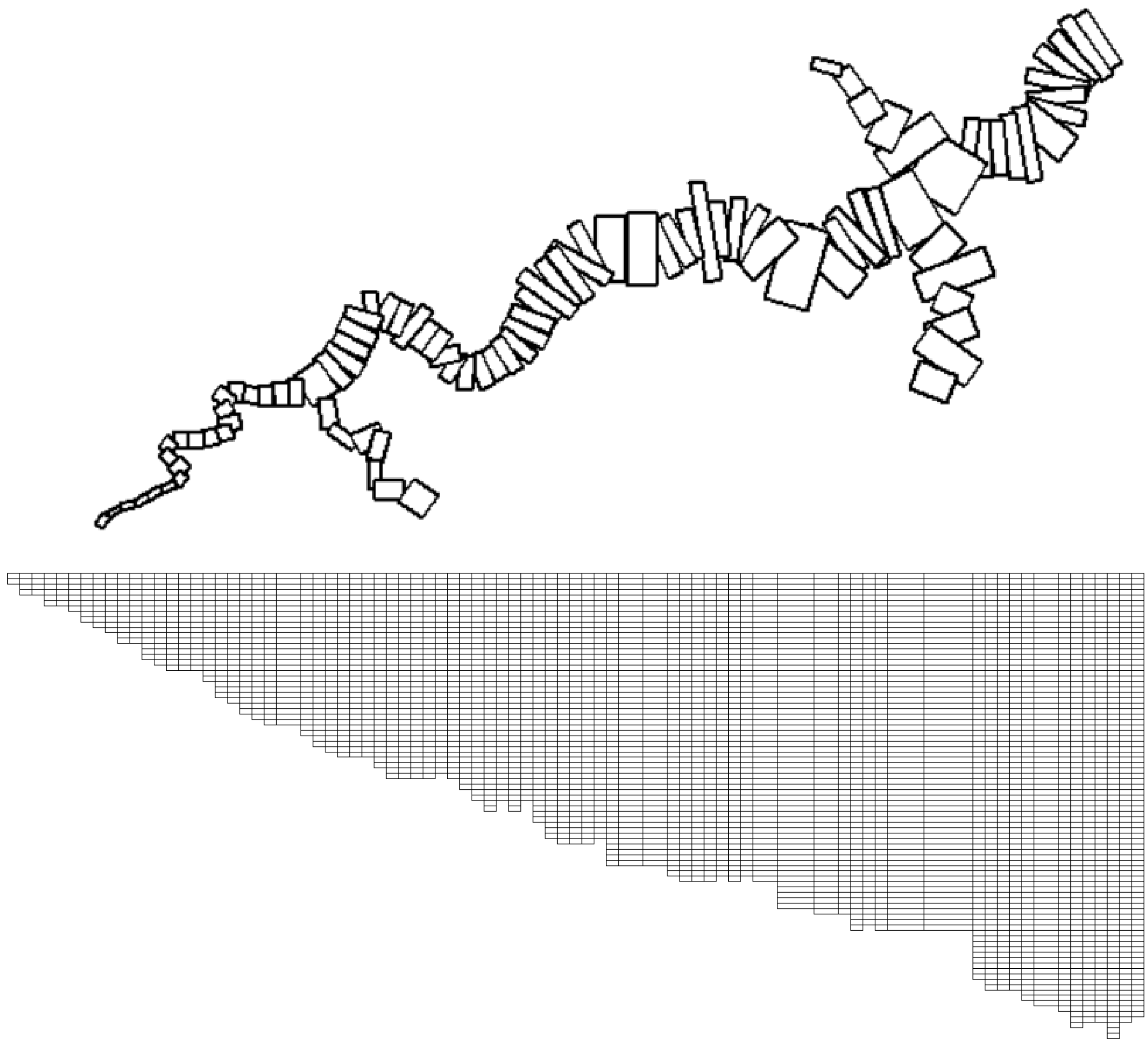

Figure S1. CE-QUAL-W2 grid definition for Rappbode Reservoir in plan (top) and profile view (bottom).

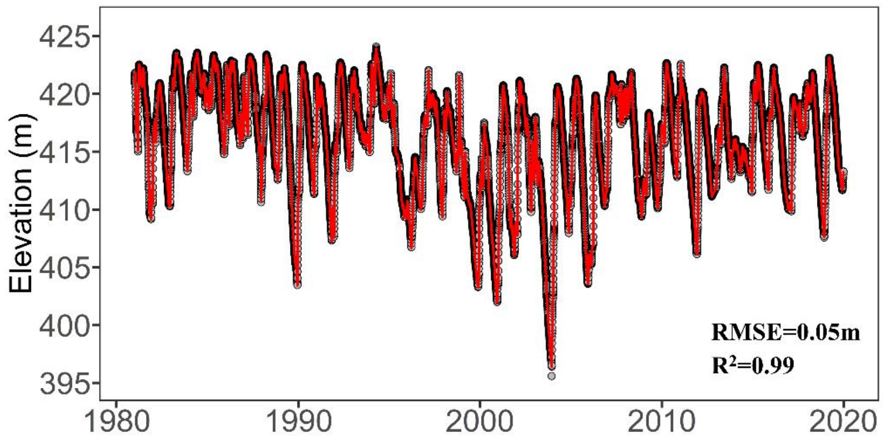

Fig.S2. Comparison of observed (the red line) and simulated (black points) water level, in Rappbode Reservoir, from 1981-2019

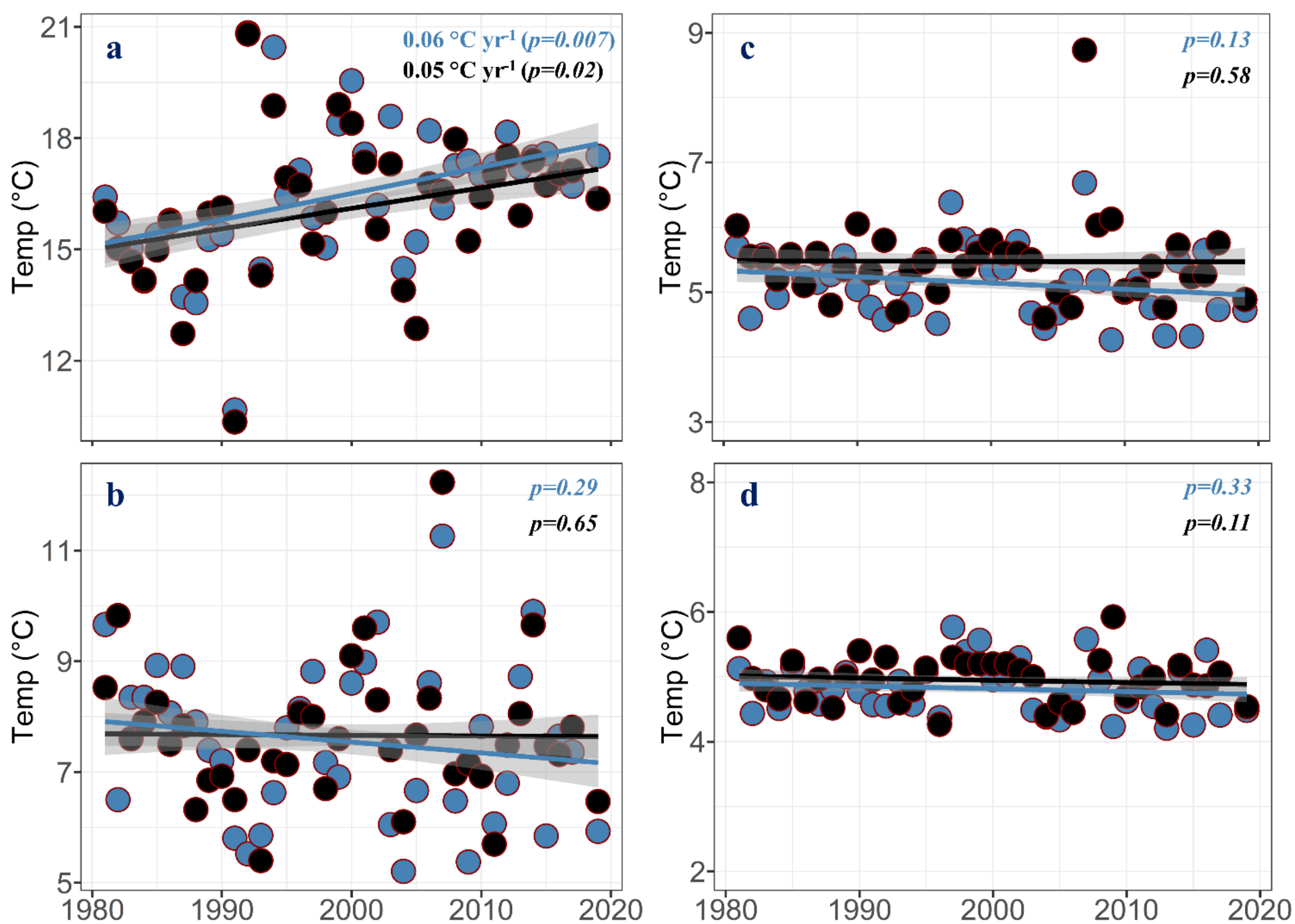

Fig.S3. Comparison of simulated (blue points) vs observed (black points) interannual variations in water temperature at different depths in the Rappbode Reservoir (a–d: 5 m, 15 m, 30 m, and 50 m, respectively)

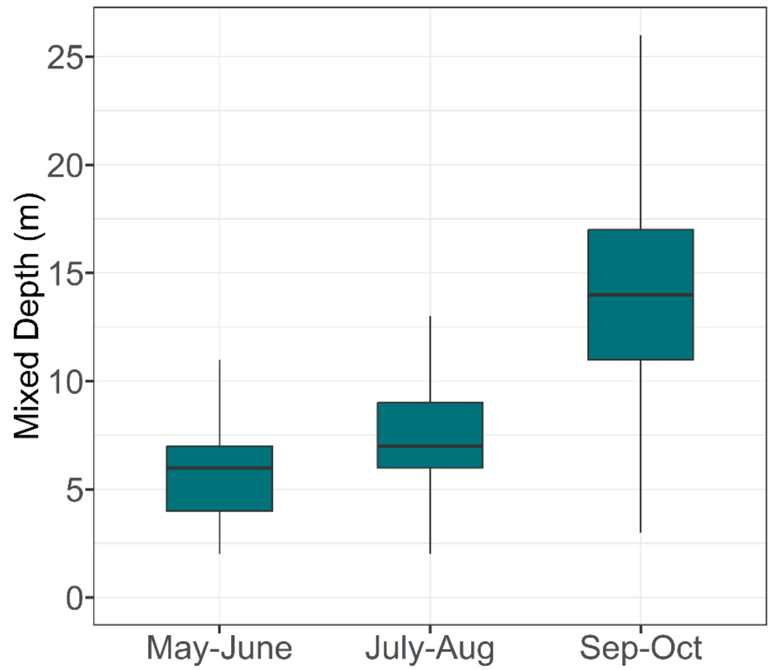

Fig.S4. Comparison of mixed-layer depth at different stages during the stratified period.

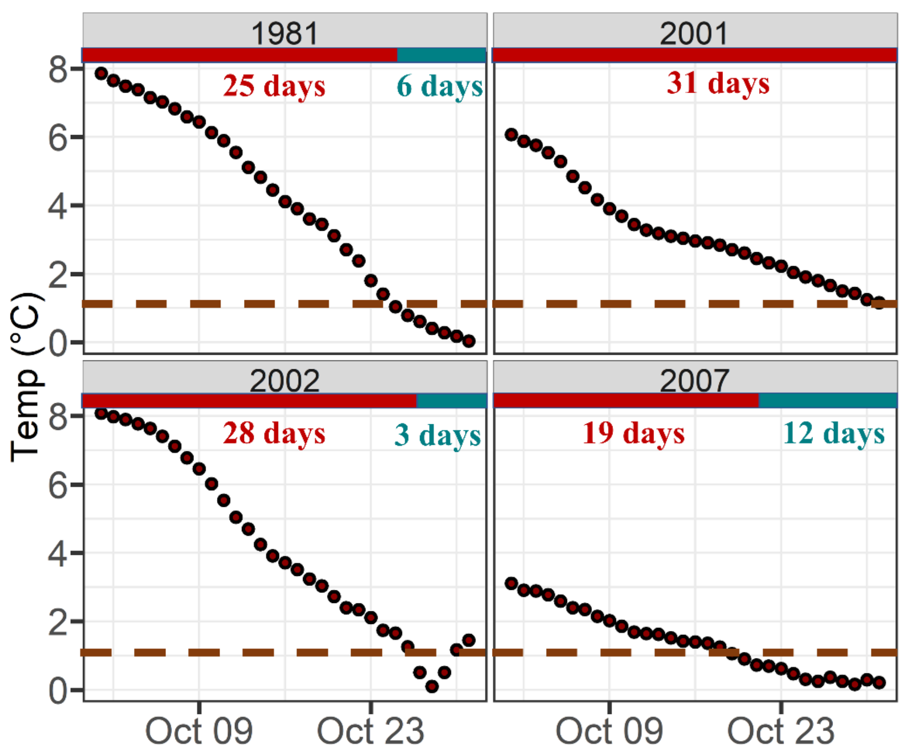

Fig.S5. Surface-to-bottom temperature difference at October during years of anomalously high bottom-layer temperatures (red text indicates stratification duration in that month; green text indicates mixing duration).

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