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Resolving spatially complex interactions between hydrodynamics and biogeochemical processing in a large reservoir with metalimnetic oxygen deficits

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Abstract:

Metalimnetic oxygen minima (MOM) typically occurs during the mid to late stages of limnetic stratification. To investigate the mechanism of MOM during stably stratified periods in the Panjiakou Reservoir, northern China, 4 years of in-situ monitoring was conducted in parallel with longitudinal-vertical 2D modeling. The model simulated the hydrodynamic, water quality, algal, and DO processes in 2017 and 2020, and was calibrated and verified by the measurements. Three scenarios were designed to test the impact of hydrological processes and the high oxygen-consuming sedimentation zones (HOCSZ). We concluded that the stratification and the corresponding advection generated in the metalimnion are the driving forces of MOM in the reservoir, and the limnetic eutrophication-related benthic HOCSZ are the seedbeds of the metalimnetic low oxygen. This unique spatial setting driving the biogeochemical processing and MOM dynamics required a new generation of modelling that includes spatial inhomogeneities of sediment characteristics and a sophisticated resolution of hydrodynamics. Hypolimnetic currents, sedimentation hot spots and the formation of high oxygen consumption zones became the major initiation processes leading to MOM. The numerical modeling not only represented the occurrence, development, and extinction of MOM but also comprehensively explained the spatial differences in the vertical morphology of MOM and its inter-annual variations. Our studies help to identify management strategies to mitigate the impacts of MOM on aquatic ecology and water quality, thus supporting the optimization of reservoir regulation and management.

Keywords: (Metalimnetic oxygen minima, Oxygen advection in metalimnion, Stratified reservoir, Benthic high-oxygen consumption, CE-QUAL-W2, upwelling in hypolimnion)

1. Introduction

Deep lakes located between 35 and 50 degrees latitude tend to be strongly and stably stratified in summer (Lewis, 1987). Density gradients in the metalimnion strongly limit vertical mixing between the hypolimnion and epilimnion in stratified lakes, resulting in biogeochemical concentration stratification(Boehrer and Schultze, 2008a). Dissolved oxygen (DO) is involved in most biochemical reactions and is highly sensitive to environmental stressors, including seasonal weather patterns, trophic status, organic pollution and hydrological regime, making it an important indicator in water quality management of lakes and reservoirs.

Hypoxia usually emerges in the metalimnion or hypolimnion during the mid to late stages of the limnetic stratification period, threatening the habitat of benthic invertebrates and fish. Hypolimnetic hypoxia is mainly caused by oxygen depletion from sediments and decomposition of sediment organic matter and is initiated at the sediment-water interface(Chen et al., 2020). Hypolimnetic hypoxia is therefore exacerbated as the productivity and trophic status of the water body increases. In contrast, the interpretation of potential process chains leading to metalimnetic oxygen minima (MOM) remains controversial.

The earliest records of metalimnetic oxygen minima in stratified lakes or reservoirs date back to 1906 in Lake Mendota (Wiebe, 1939a). Vertical oxygen profiles collected from 235 reservoirs in Missouri during 1989-2007 showed MOM, probably related to mesotrophic or eutrophic conditions and intense and stable thermal stratification(Jones et al., 2011). Metalimnetic metabolic processes rates exhibited high day-to-day variability in all trophic states(Giling et al., 2017). The study of dissolved oxygen dynamics in Lake Constance, covering a period of more than 30 years from eutrophication to oligotrophication, has shown that severe oxygen depletion in the metalimnion occurred during periods of moderate (1988-1999, TP between 10 and 40 μg L^{-1}) and oligotrophic (2000-2010, TP<10 μg L^{-1}) rather than during periods of high eutrophication (1977-1987, TP>40μg L^{-1}), indicating that MOM was not simply coordinated with nutrients (Rhodes et al., 2017). McDonald et al. (2022) concluded from high-frequency observations of oxygen depletion at multiple depths that DO consumptions in the metalimnion were synchronised with DO deficits in the hypolimnion over time. Shapiro (1960) proposed three possible causes of metalimnetic oxygen minima: 1) in situ oxygen depletion; 2) invasion of low oxygen inflows; and 3) basin morphological features associated with horizontal water movement.

Many studies have identified the cumulative effect of in situ oxygen depletion due to the following aspects：(a) phytoplankton respiration beyond its photosynthetic activity(Effler et al., 1998; Wentzky et al., 2019); (b) zooplankton respiration(Schram and Marzolf, 1994; Shapiro, 1960), and (c) bacterial respiration from organic matter decomposition(Boehrer and Schultze, 2008b; McDonald et al., 2022; Saeed, 2020), all of which are considered to be Shapiro's first explanation. Based on the hydrodynamic properties due to stratification. Kreling et al. (2017) suggested that the high density gradient retards sedimentation of surface organic matter, making the metalimnion a hotspot for organic matter degradation, implying that the corresponding vertical positions for oxygen consumption are in the metalimnion. As a contribution to primary productivity, most live blue-green algae accumulate in the euphotic zone, and dying or dead algae float briefly to the surface where they are decomposed by bacteria and then sedimented. Mitchell and Burns (1979) pointed out that zooplankton respiration accounted for less than 10% of the maximum oxygen depletion in the metalimnion in one year, but more in the other two years in Lake Johnson. Schram and Marzolf (1994) calculated zooplankton respiration accounted for 26-31% of the observed oxygen loss, except in midsummer when it accounted for 15%, Estimated bacterial respiration accounted for >44% of the observed oxygen loss. In a study of the northern Baltic Sea, microbial decomposition accounted for 80% and mesozooplankton respiration for 20% of the metalimnetic oxygen consumption(Raateoja et al., 2010). Algae deposition partly contributed to the oxygen depletion in the hypolimnion, and the proportions of dead algae decomposed in the metalimnion and in the hypolimnion are unclear. Terry et al. (2017) inverted the inter-annual variation in sediment oxygen demand (SOD) by modelling in an ice-covered lake in winter and concluded that maximum summer Chl_a concentrations determined winter sediment oxygen demand, suggesting that mortal algae were mostly deposited on the bed rather than fully decomposing in the metalimnion. The in-situ theory deduces that the local metalimnetic DO depletion can be predicted from the local biomass in a vertical water column, and the horizontal spatial variability in lakes or reservoirs should be related to the algal heterogeneity in the current year. In addition, Mi et al. (2020) indicated that approximately 60% of the oxygen consumption is from benthic processes, with the remainder from pelagic processes.

Furthermore, in some studies the formation of MOM was mainly due to exogenous inflow. The incoming density currents carried oxygen-depleted water towards the dam, forming biogeochemical gradients limited to their characteristic density and temperature, respectively (Wiebe, 1939b). During the flood season, the oxygen demand of the inflowing water can be very high due to large amounts of organic matter, and such inflow-borne loading can induce corresponding dissolved oxygen changes in the reservoir (Lyman, 1944; Nix, 1981). During low flow periods, upstream water containing some algae was incorporated into a density current and transported through the metalimnetic region, and this process was proposed to support the formation of metalimnetic dissolved oxygen minima in DeGray Reservoir (Nix, 1981).

The third hypothesis of MOM has received little research attention, while the morphological features that generate environmental properties are being reviewed. In stratified estuarine regions, the combination of upwelling along the coastal shelf in the underlying high-density layer and river plumes in the surface layer regulates sedimentation and pelagic processes, resulting in the spatial distribution of hypoxia on the shelf bed，the so-called 'shelf effect' (Jacox and Edwards, 2011; Wei et al., 2021). Unlike estuaries inland reservoirs tend to be seasonally stratified, with similar benthic hypoxia typically occurring first at the tail bottom during the stratification. It is rarely mentioned whether there is the similar upwelling along the hypolimnetic slope that acts on the tail-bed hypoxia in the stratified reservoirs. The spatial variation in sediment properties posed by flow velocity-sieved sedimentation from the tail to the head of a reservoir (Chen et al., 2021). The exchange of solutes between sediment and water is influenced by temperature and dissolved oxygen concentration (Dadi et al., 2023). In a stratified reservoir, the flux of reducing agents at the sediment-water interface appeared to be unevenly distributed (Wang et al., 2021).

Numerical models can be useful to study the formation of MOMs and even to quantify the contribution of different processes. One-dimensional (1D) coupled physical-ecological models provided information on the dissolved oxygen dynamics along the vertical changes and emphasized the vertical turbulent diffusivity (K_z) (Antonopoulos and Gianniou, 2003). In 1D models, the pelagic respiration term is considered to be the most important factor controlling the formation and intensity of MOM, and the effect of SOD on MOM may be negligible (Joehnk and Umlauf, 2001; Saeed, 2020). However, 1D models grounded on the in-situ theory and ignore horizontal evolutions, which may miss some information(Weber et al., 2017). The two-dimensional (2D) CE-QUAL-W2 is widely used in water allocation and quality management(Lindenschmidt et al., 2019). The 2D modelling results also showed that the oxygen depletion would be intense if the withdrawal at the dam was at the same level as the metalimnion(Williams, 2007). The 2D model of Rappbode reservoir was well calibrated by the amount of observation data in different time periods, whereas there was only one monitoring site at the head of the reservoir and it was difficult to interpret the MOM formation comprehensively (Mi et al., 2020).

A 4-year monitoring campaign was conducted in a dimictic stably stratified reservoir in northern China, and by combining the monitoring results from the literature, we found that MOM showed spatial differences and year-to-year variation in the reservoirs. The established references could explain certain driving factors of MOM, but not enough to predict the whole MOM process and guide the reservoir operation. For the reservoir monitor, water temperature, dissolved oxygen, chemical indices, algae and sediments are relatively easy to measure, but the systematic and high-resolution assessment of hydrodynamics in stratified reservoirs is challenging. A solution to this problem can be provided by numerical models. In this study, in addition to the field survey, we use CE-QUAL-W2 to simulate the hydrodynamics and associated water quality and phytoplankton dynamics in Panjiakou Reservoir (PJKR). The model is driven by observed meteorological, hydrological and water quality data at the boundaries to represent the dynamics of currents, nutrients, algae and especially oxygen processes in the regulated limnetic ecosystem. A major novelty of our study is the detailed spatial structure of biogeochemical processing in a large reservoir with very complex morphometry. We provide evidence that spatial heterogeneities, particularly with respect to sediment properties, can play a major role in structuring and driving water quality dynamics in large reservoirs. A comprehensive understanding of MOM formation of the reservoir will help to secure ecological safety and implement scientific management.

2. Date and Methods

2.1 Study area and Observed data

The Panjiankou Reservoir, located in northern China (40°26'N, 118°16'E) on Luan River (Fig. 1), has a multi-year capacity of 1.6 billion m^3 and a maximum depth of 68.9 m at the target water level of 225 m. Since its construction in the 1970s, the water intakes have been located at the bottom of the dam. The inflow to the PJKR has been significantly reduced by about 70% since the late 1990s, and the hydraulic retention time (HRT) has increased to 2-3 years in recent years. The PJKR suffered from severe eutrophication due to net-pen fish farming in the reservoir, non-point source imports and upstream pollution. Since 2016, following the implementation of nutrient reduction measures, the concentration of total phosphorus (TP) and total nitrogen (TN) in the PJKR has decreased significantly, mainly due to the ban on aquaculture and the pollution control from the catchment.

[Insert Figure 1 about here]

The study collected several categories of data: daily hydrological data, water quality data, satellite remote sensing data, meteorological data and literature data. The inflow contributions of the two tributaries are about 74% and 22% respectively, and the net distributed inflow from the reservoir basin minus evaporation and infiltration is about 4%. The meteorological data come from a small meteorological monitoring station on the dam. There are 24 water quality indicators measured based on the Chinese Environmental Quality Standards for Surface Water (GB 3838-2002), including water temperature, dissolved oxygen (DO), permanganate index (COD_{Mn}), chemical oxygen demand (COD), ammonia nitrogen (NH_4-N), TN and TP. Water was typically sampled monthly from April to October only at a depth of about 1.5 m. However, in-situ vertical profiling campaigns in PJKR from the tail to the dam using a YSI-EXO multiparameter probe were conducted in 2017, 2019 and 2020 at different times of the year following the routine monitoring sites (Fig. 1). Among these years there was a higher sampling frequency in 2020. In addition to these probe-based measurements, we also obtained monthly averaged surface spatial distributions of Chl_a and total dissolved solids (TDS) through remote sensing interpretation.

2.2 Model description and set up

The longitudinal-vertical 2D model CE-QUAL-W2 was chosen to simulate water quality dynamics and hydrodynamics. In the hydrodynamic model, water temperature and density are mandatory items in the hydrodynamic module， in which the density is taken into account. The eddy viscosities, Chezy coefficient, and wind shelter coefficient are the parameters for the hydrodynamics and solute transport. In the vertical direction, CE-QUAL-W2 uses z-coordinates with fixed meshes at a vertical resolution of 1 m. The water quality module is coupled with the hydrodynamic model and can reflect feedbacks between water quality and hydrodynamic variables, while it can be updated less frequently than hydrodynamics in order to save computational time. The model is well suited to PJKR, which is relatively long and narrow has longitudinal and vertical temperature and water quality gradients. The horizontal grid spacing ranges from 221.97m to 2278.32m and the vertical grid spacing is 1m, as shown in Fig. 1(b)

According to the laboratory analysis of algae, the phytoplankton in PJKR is mainly composed of Bacillariophyta, Cyanophyta and Chlorophyta, among which Bacillariophyta is the most dominant one. The state variables modelled for water quality include nutrients, dissolved oxygen and three algal groups, namely diatoms, cyanophytes and green algae. Twenty-four active constituents, including orthophosphate (PO4), ammonia-N (NH4), nitrate-N (NO3), DO, dissolved and particulate matters, labile and refractory matters, and eight derived constituents, including TN, TP, Chl_a, are modelled.

The transport and reaction equation used to model the dynamics of water quality or temperature variables is:

$$\frac{\partial B\Phi}{\partial t}+\frac{\partial UB\Phi}{\partial x}+\frac{\partial \mathrm{WB}\Phi}{\partial z}=\frac{\partial}{\partial x}\left(BD_x\frac{\partial \Phi}{\partial x}\right)+\frac{\partial}{\partial z}\left(BD_z\frac{\partial \Phi}{\partial z}\right)+q_\Phi B+S_\Phi B \tag{1}$$

In which, Φ is lateral averaged concentration of active constituents mentioned before and water temperature, mg L^{-1} and °C B is control volume width, m; U is x-direction velocity, m s^{-1}; W is z-direction velocity, m s^{-1}; D_x is longitudinal dispersion coefficient, m^2s^{-1}. D_z is vertical temperature and constituent dispersion coefficient, m^2s^{-1}; q_Φ = lateral inflow or outflow mass flow rate of constituent per unit volume, $gm^{-3}s^{-1}$; S_Φ = laterally averaged source/sink term, $gm^{-3}s^{-1}$.

The D_x specification is a user-defined input, it can also be set to be a function of the mean velocity. D_z is internally computed within the model using the Reynold's analogy, where D_z is computed from the vertical eddy viscosity A_z, as $D_z = 0.14A_z$, There are several methods available in CE-QUAL-W2 to calculate A_z, we chose the turbulent kinetic energy (TKE) approach.

According to equation (1), the changes in temperature or actived constituents in a unit grid are composed of four elements: (a) the convection term driven by the currents; (b) the dispersion generated by mixing intensity and gradients; (c) the inflow or outflow; and (d) the source and sink terms. The source and sink terms here describe the rates of change due to biogeochemical reactions between active constituents. Here, the source and sink terms for DO are described by equation (2).

$$
\begin{aligned}
S_{DO} = {} & \underbrace{\sum (K_{ag} - K_{ar})\delta_{OMa}\Phi_a}_{algal\ net\ production} + \underbrace{\frac{A_{sur}}{V_{sur}} K_L(\Phi_{SDo} - \Phi_{DO})}_{aeration} - \underbrace{K_{RPOM}\delta_{OM}\gamma_{OM}\Phi_{RPOM}}_{refractory\ POM\ decay} - \\
& \underbrace{K_{LPOM}\delta_{OM}\gamma_{OM}\Phi_{LPOM}}_{labile\ POM\ decay} - \underbrace{K_{RDOM}\delta_{OM}\gamma_{OM}\Phi_{RDOM}}_{refractory\ DOM\ decay} - \underbrace{K_{LDOM}\delta_{OM}\gamma_{OM}\Phi_{LDOM}}_{labile\ DOM\ decay} - \\
& \underbrace{K_{sed}\delta_{OM}\gamma_{OM}\Phi_{sed}}_{1st-oroder\ sediment\ decay} - \underbrace{SOD\gamma_{OM}\frac{A_{sed}}{V}}_{0-order\ SOD} - \underbrace{\sum K_{CBOD}R_{CBOD}\theta^{T-20}\Phi_{CBOD}}_{CBOD\ decay} - \\
& \underbrace{K_{NH4}\delta_{NH4}\gamma_{NH4}\Phi_{NH4}}_{nitrification} - \underbrace{\delta_{Fe2-O2}K_{Fe2}\Phi_{Fe2}}_{oxidation} \qquad (2)
\end{aligned}
$$

In which, Φ_i describes the oxygen concentrations, mg·L^{-1}; δ_i is the oxygen stoichiometric coefficient of *i*; γ_i is the temperature rate multiplier for *i*; K_i is the growth, respiration or decay rate of *i*, s^{-1}; V_{sur} is volume of the surface cell, m^3; T is temperature, °C; A_{sur} is water surface area, m^2; A_{sed} is sediment surface area, m^2.

The net production of oxygen by algae is given by photosynthetic production minus respiration. Aeration processes are restricted to the surface cells in calculation, while the sediment oxygen demand is met by the benthic layers. A fraction of the organic matter released by algal mortality enters the detritus compartment as particulate organic matter(POM), while the remainder becomes labile dissolved organic matter(LDOM). The transformation of POM into DOM is a first order process with a transformation rate, as is the mineralisation of DOM.

The inflow boundary conditions were set at the upper reaches of Luan River and Pu River, and the outflow boundary was at Dam. According to the frequency of in-situ vertical monitoring and the representativeness of the measurements, we chose the years 2017 and 2020 for modelling and analysis. A small amount of missing input data is calculated using the linear interpolation method.

The trophic status of PJKR is reviewed to give an insight to the nutrient cycle. In addition to high N and P loads, the high algal biomass leads to high sedimentation and high oxygen consumption. The yearly average Chl_a concentrations at sites 1, 3, 5 and 8 and the yearly average TP concentrations and the yearly maximum Chl_a concentrations at sites 1, 3, 5 and 8 from 2010 to 2020 are shown in Fig. 2. Chl_a concentrations decreased significantly from 2010 to 2020, and TP concentrations reached high values in 2015~2017 and then decreased dramatically, and the correlation between annual mean Chl_a and TP concentrations is not obvious. In general, Chl_a concentrations were higher at site 8 than at sites 1, 3 and 5. The oxygen consumption of reservoirs in different years can refer to the algal biomass of that year or the previous years.

[Insert Figure 2 about here]

The distributed sediment condition was mainly based on a reservoir sediment survey (Wang et al., 2021). Ammonia nitrogen, nitrite and nitrate in sediments were sampled in May 2020 and the internal loading of the reservoir was analyzed. According to the nutrient flux at the sediment-water interface during the static release experiment in Fig. 2(c, d, e), the release of ammonia nitrogen was about more than 10 times higher than that of nitrite, while nitrate was a sink. Spatially, the largest ammonia releases were at site 3, followed by the second largest releases at 1, 2 and 8, and small ammonia releases at 4, 5, 6 and 7, which were about 1/3 or 1/2 of those at 1, 2 and 8. Among these 8 sites, the smallest ammonia release flux was at 7. In the investigation of the oxygen consumption in 11 European lakes (Steinsberger et al., 2020), the flux of reduced compounds from the sediment was in good agreement with the sediment oxygen uptake. The estimated fluxes were converted to oxygen equivalents (F_{red}, mmol O_2 m^{-2} d^{-1}) (Matzinger et al., 2010; Müller et al., 2012) as follows:

$$F_{\mathrm{red}} = 2 \cdot J_{CH_4} + 2 \cdot J_{NH_4} + 0.5 \cdot J_{Mn(II)} + 0.25 \cdot J_{Fe(II)} \quad (3)$$

In which, J is fluxes of reduced substances J (mol m^{-2} s^{-1}). Although the components of CH_4, Mn(II) and Fe(II) fluxes were not tested in the reservoir, the NH_4 flux at different sites can be used as a reference for the SOD distributions.

A schematic diagram of the corresponding SOD value in the range of 1~9 g·m^{-2}·day^{-1} in PJKR can be seen in Fig. 3. The SOD values in 2017 were higher than those in 2020 considering the annual Chl_a and TP concentrations, which was also reflected in the model calibration in different years.

[Insert Figure 3 about here]

The main parameters used in the model and their values are given in Table 1. Some parameters refer to the CE-QUAL-W2 manual or to the model documents, others come from the calibration.

Table 1. Parameters calibrated or referenced in PJKR model

Parameter	Description	Value	Source
AX	Hor. Eddy Viscosity , $m^2 \cdot s^{-1}$	1.0	Manual
DX	Hor. Eddy Diffusivity, $m^2 \cdot s^{-1}$	1.0	Manual
AZC	Vertical Eddy Viscosity	TKE	Manual
AZSLC	Vertical Transport Hor. Momentum	IMP	Manual
CBHE	Sediment Heat Exchange Coeff. ($W \cdot m^{-2} \cdot s^{-1}$)	1.0	Calibration
SEDK	Sediment decay rate, day^{-1}	0.05	Calibration
SOD	SOD, $g \cdot m^{-2} \cdot day^{-1}$	0.2~9 (2017)	Calibration
		0.2~6 (2020)	Calibration
SODT1	Lower temperature for sediment decay (°C)	4	Manual
SODT2	Upper temperature for sediment decay (°C)	30	Manual
AT1	Lower temperature for 3 ALG growth (°C)	2, 6, 16	Calibration
AT2	Lower temperature for maximum 3 ALG growth (°C)	3, 14, 27	Calibration
AT3	Upper temperature for maximum 3 ALG growth (°C)	8, 16, 29	Calibration
AT4	Upper temperature for 3 ALG growth (°C)	10, 31, 36	Calibration

PO4R	Sediment Release rate of phosphorus, $g \cdot m^{-2} \cdot day^{-1}$	0.050(2017), 0.025(2020)	Calibration
NH4R	Sediment release rate of ammonium, $g \cdot m^{-2} \cdot day^{-1}$	0.40(2017), 0.25(2020)	Calibration

2.3 Scenarios designed

Three hypothetical scenarios were designed to identify the hydrodynamic and sedimentary factors on MOM. Scenarios aimed at the role of algae on MOM were also calculated by switching algae on and off, and similar results with Mi (2020) were found that MOM without SOD disappears, whether with or without the algae process. In this study, 3 scenarios (S-A, S-B and S-C for short), mainly based on the conditions of 2017, are designed to analyze the mechanism of MOM formation in the reservoir.

In scenario A (S-A), a quiescent reservoir with temperature and biochemical processes is set up by removing inflow, outflow and wind to test the exogenous hydrodynamic effects. Vertical water movements due to the changing stratified water temperature are still present, while the advection and circulation driven by inflow, outflow and wind disappear. The initial conditions of temperature and water quality, meteorological conditions and SOD settings are the same as in 2017. In scenario B (S-B) and scenario C (S-C), except for the spatial SOD patterns, the boundary condition, initial condition and parameters are the same as in the 2017 simulation. The downstream and upstream SOD, bounded by location 7 in Figure 3, are set to 0 in S-B and S-C, respectively. The Algal processes are calculated in three scenarios. The detailed setting options for the three scenarios are given in Table 2.

Table 2. Model setting options for each scenario.

	Flow and wind	Upstream SOD	Downstream SOD	Chemical reaction and Algae
Scenario A	-	+	+	+
Scenario B	+	+	-	+
Scenario C	+	-	+	+

"+"means switch on, "-" means switch off.

3. Results

3.1 Model calibration

The hydrodynamic changes are the fundamental processes for the water environment, while there are fewer observations of velocities or eddies, except for water levels. The hydrodynamic calibration uses the daily observed water levels to check the modelling results to validate the inflow and outflow balance as they influence the heat budget. The calculated water levels in 2017 and 2020 are in good agreement with the measurements, which are not shown in this paper.

The model temperature and oxygen profiles are calibrated using in-situ vertical monitoring data from 2017 and 2020. Sites 1 to 8 are therefore shown in Fig. 1. The comparisons between computed and measured water temperature and DO profiles in 2017 are shown in Fig. 4, and the comparisons of 2020 are shown in Fig. 5.

[Insert Figure 4 about here]

[Insert Figure 5 about here]

We mainly compared Chl_a and TP with the measured data, as shown in Fig. 6. The contour plots of computed (a) diatom, (b)blue-green algae and (c)cyanobacteria concentrations in 2020 at monitoring site 1 in PJKR are shown in Fig. 7.

[Insert Figure 6 about here]

[Insert Figure 7 about here]

The algae were calibrated against the measured Chl_a concentration. According to the measurements in 2020, the Chl_a concentration from site 8 to site 1 were in the range of 0.2~7.4 ug/L, and the concentration at site 8 was higher than that at site 3 and site 1, TP concentrations were 0.017~0.057mg/L. PJKR was in mesotrophic condition. The low Chl_a level, indicating low algal biomass, causes the intense oxygen minima locally, which is doubtful.

The calculation of water level and vertical water temperature has a high accuracy, while the vertical oxygen has a lower accuracy but a good fit in the metalimnion. The simulation accuracy of the water quality indicators is slightly less good. The local mass inputs and the uneven distribution of meteorological factors could be the sources of uncertainty due to the large catchment area of the reservoir. The error analysis data are presented in Table 2.

Table 2. Summary of the performance indicators for the W2 modeling of hydrodynamic and water quality variables, RMSE= root mean squared error, R^2 = coefficient of determination, NSE=Nash-Sutcliffe efficient

Simulated Variables	RMSE	R^2	NSE
Water level (WL) (m)	0.06	0.99	0.98
Water temperature (T) (°C)	0.46	0.95	0.95
DO (mg/L)	1.88	0.58	0.57
Chl_a (ug/L)	0.3	0.54	0.55
TN (mg/L)	0.24	0.58	0.59
TP (mg/L)	0.01	0.55	0.55
NH_3-N (mg/L)	0.015	0.52	0.52

3.2 Results analysis: seedbed，evolution and driving forces of MOM

Stratification is the primary prerequisite for MOM, shaping the vertical oxygen profiles. Further details can be obtained from the modelling results. The depth profiles of oxygen concentration in 2017and 2020 at site 5 and site 1, respectively, are shown in Fig. 8(b, c, e, f). As a relative comparison, the depth profiles of temperature in 2017 and 2020 at site 1 are plotted, and the thermocline depth is specified by the $\Delta T / \Delta x > 1$°C m^{-1} from bottom to surface, which are also shown in Fig. 8(a, d).

[Insert Figure 8 about here]

Oxygen depletion in the metalimnion was much more pronounced in 2017 than in 2020. In 2017, the MOM started in mid-July and ended after turnover in November, and the oxygen depletion at site 1 was more pronounced than that at site 5. In 2020, the oxygen minima at site 5 were more intense than those at site 1 in mid-July, and the metalimnetic depth corresponded to the bottom of the upstream site 8, where the oxygen concentration was almost zero in Fig. 5.

Several types of images are combined to provide a comprehensive analysis of oxygen changes. The 2D the magnitude contours of temperature, oxygen and velocities, with streamlines are plotted in Fig. 9 (a, b, c). The velocities were calculated using $\mathrm{UW} = \sqrt{u^2 + w^2}$. The TP, TN, Chl_a, and DOM concentrations in the surface layer in the longitudinal direction on Jul 23, 2020 are shown in Fig. 9 (d). The Chl_a concentration at the surface by remote sensing interpretation is exhibited in Fig. 9 (e).

[Insert Figure 9 about here]

The vertical thermal gradient in the metalimnion has a high temperature at the top and a low temperature at the bottom (Fig. 9(a)), similar to the "stratosphere" where horizontal flow dominates with a low value of the vertical diffusion. The relatively high-speed horizontal currents indicated in Fig. 9(c), transport the oxygen depletion and the reduced compounds from the tail to the head of the reservoir in the metalimnion. The upwelling against the bathymetric slope can be seen, which may be a kind of similar phenomena observed and mentioned in stratified estuaries related to shelf bed hypoxia (Wei et al., 2021). In addition, the vertical flow in front of the dam region can be seen. Upstream river inflow caused concentration changes in the reservoir, particulate deposition, algal growth and sedimentation, together with the upwelling, account for the high oxygen consumption sedimentary zone (HOCSZ). In July 2020, hypoxia developed at the bottom of site 8 first, where the metalimnion is at the same level, as shown in Fig. 9(a) and (b).

In terms of the evolutionary process, the MOM at site 1 lags behind that at site 5, and the oxygen minima become less pronounced in Fig. 9(b). The intensity and depth of advection in the metalimnion can shape the MOM differently. The stratification disappears with the strong vertical mixing of the autumn turnover at site 8 and the benthic hypoxia disappears, as seen in Fig. 5. The turnover characteristics and DO responses in PJKR can be seen in Du et al. (2023).

In addition, 2D oxygen concentration and velocity distribution in Fig. 10 (a, b), are shown in conjunction with the oxygen and temperature profiles at site 1 in Fig. 10 (c) on 11 September 2017.

[Insert Figure 10 about here]

It can be clearly seen in Fig. 10 (a) that the oxygenated water was wedged into the upper metalimnion and inserted into the formed MOM. The front of the oxygenated water reached site 3. By presenting the oxygen and current distributions, we can easily explain the peculiar oxygen profile patterns at the upstream sites in Fig. 4. The oxygen profile at site 4 was similar to that at site 1, although the water depth was different. The influence of the intruding current was attenuated in the wing area (Fig. 1) and near the dam area. The relatively high velocity in the metalimnion can also be seen in the velocity magnitude contour in Fig. 10(b). Again, we found upwelling in the hypolimnion along the bathymetric slope in Fig. 10(b) through the streamlines. According to the 2-year modelling results, the benthic anoxic zone occurred around the lower edge of the metalimnion at the end of the reservoir. Sediment oxygen consumption on the reservoir tail shelf is the seedbed of MOM, and horizontal oxygen advection in the metalimnion, is the driving force that develops MOM throughout the reservoir. It can explain the conclusions of Williams (2007) that the withdrawal at the metalimnion accelerated the horizontal flow intensity in the metalimnion, thereby intensifying the MOM.

3.3 Scenarios Results

The results of the designed scenarios in 2.4 are used for further analysis, and the 2017 results in Fig. 6 are taken as the control. The computed depth profiles of oxygen concentration at site 5 and site 1 of S-A, S-B, and S-C are plotted and shown in Fig 11.

[Insert Figure 11 about here]

The thermocline depths are shallow in summer when the water is essentially stationary in the reservoir in Scenario A in Fig 11(a). The convective transport term by currents becomes very small and the dispersion by the concentration gradient dominates the distribution of temperature and dissolved matter. MOM was not observed throughout the reservoir, although oxygen depletion in the hypolimnion was evident. The disappearance of advection in the metalimnion leads to the disappearance of MOM in Fig. 11(a) and (d). The results of Scenario A again show the crucial role of hydrodynamic forces and explain the MOM in 2020.

When the upstream SOD was set in Scenario B, MOM was still produced throughout the reservoir, but the intensities of oxygen depletion became subtle, especially in the head of the reservoir, shown in Fig. 11 (b) and (e). In Scenario C with the downstream SOD setting, MOM was evident in the downstream region but disappeared in the upstream region, as shown in Fig. 11 (c) and (f). High inflow and outflow rates lead to short HRT, and strong mixing effects vertically in the hypolimnion and advection in the metalimnion, likewise to generate MOM. The strong MOM in 2017 was the comprehensive function of advection in stratified reservoirs, upstream and downstream SOD.

4. Discussions

4.1 Relationship between HOCSZ distribution and upwelling in the hypolimnion

In the reservoir, HOCSZs on the bed are embodied in the larger sediment oxygen demand (SOD), and the SOD distribution settings are based on the Wang et al. (2021). The fieldwork for the study was carried out in May 2020. Although benthic water temperature was not provided, DO concentrations at the sediment-water interface were measured at several sites and reported to range from 9.64 to 11.8. According to the modelling results shown in Fig. 5, the thermal stratification started. At the same time, the DO concentration profiles were basically unstratified with high benthic DO, which is consistent with the measurements in other studies. Hypoxia in the benthic zone is a gradual process that was not fully synchronised with thermal stratification (Du et al., 2023).

The modelling results for 2017 and 2020 show that there was upwelling against the bed slope in the hypolimnion. Due to the long-term influence of upwelling during the stratification periods, the flux of reducing substances from the sediment decreased, resulting in relatively lower SOD on the deep slopes. At the same time, upwelling and inflow meet at the height of the metalimnion, causing strong sedimentation, altering nutrient transport, and forming a high oxygen-consuming sedimentary zone at the reservoir tail. The distributions of SOD in reservoirs are therefore shaped by the specific hydrodynamics in stratified reservoirs. Once thermal stratification has started, oxygen depletion usually occurs first at the bottom below the metalimnion due to shallow depth and high sediment oxygen consumption at HOCSZ. During the stratification, HOCSZs become the seebeds of the low-oxygen in the metalimnion.

4.2 Hydrological processes, trophic states and MOM displays

In Section 2.1, we mentioned that the variation of the vertical water temperature and oxygen profiles in September were different in 2017, 2019, and 2020. Since the oxygen depletions in the metalimnion were most obvious in September, the temperature and oxygen profiles in September 2017, 2019 and 2020 at sites 1, 5, and 8 were selected for comparison, as shown in Fig. 12. The depth of the metalimnion determined the depth of MOM. The oxygen minimum at S1 was more pronounced in the metalimnion in 2017 and 2019 than in 2020, and an oxygen protrusion occurred in the middle of MOM at S5 in 2017. Compared to the temperature profiles, the spatial variability of MOM profiles is more pronounced.

[Insert Figure 12 about here]

We were confused when we saw the zigzag oxygen profiles measured from S5 to S8 in Sep. 2017 as our first monitoring campaign, which were difficult to interpret using previous theories before we received the hydrological data and ran the model. Based on the modeling results, hydrological processes are used to further understand the inter-annual MOM variations. The water level and total inflow rates of the reservoir in 2017, 2019, and 2020 are shown in Fig. 13.

[Insert Figure 13 about here]

Hydrodynamics determine the characteristics of the sediments, and long HRT enhance sedimentation (Lindström and Bergström, 2004). Controlled by the average operating water levels of the reservoir, the HOCSZs at the tail bed are considered at the specific elevation zone, and the corresponding water surface elevation zone during stratification was briefly denoted as WL-HOCSZ. The water levels and inflow rates in 2017, 2019, and 2020 are exhibited in Fig. 11, and the elevations of WL-HOCSZ in the stratified period are also indicated in Fig 11. In order to clearly illustrate the hydrological differences in these three years, the characteristic parameters such as averaged water levels, inflow rates, and HRT during the stratified period of 2017, 2019, and 2020 were 334.7d, 396.1d and 412.8d respectively. HRT in 2019 and 2020 were over 1 year.

Combined with the analysis in 3.1 and 3.2, the formation of oxygen profiles in these three years was reviewed. In 2017, the operating water levels ranged from 210.01m to 221.31m during the stratification period. In early July, the water level reached the annual minimum, then rose significantly, and passed over WL- HOCSZ, with two flood events in early and late August. Nix (1981) thought that the invasions of high-concentration organic matter from the stormwater was a likely contributor to MOM. In PJKR, an August flood contained high oxygen with high temperature, passed through the high oxygen consumption zone, flowed along the upper edge of the metalimnion, and reformed the MOM, as shown in Fig. 10. The oxygen-rich water was transported horizontally from upstream to site 3, where there were two wings, and the longitudinal movement was distributed, resulting in different oxygen profiles throughout the reservoir. Therefore, inflow may be the destroyer rather than the contributor of MOM. During the stratification period in 2019, the inflow rates were low and the water levels varied between 213.08 and 219.27 m, which were consistent with WL- HOCSZ, and the remarkable MOM profiles were observed throughout the reservoir.

In 2020, the water levels during stratification were about 10~20m lower than those in 2017 and 2019, and also lower than WL-HOCSZ. The inflow rates remained as low as in 2019, with no flooding events during the wet season. Referring to Fig. 5, the MOM was pronounced near the tail region (S5), then gradually weakened along the longitudinal direction (S3), and was almost invisible in the head of PJKR (S1) on 28 Aug 2020. The currents in the metalimnion in 2020 were assumed to be similar to those in 2019, and the water levels may be one of the key reasons for the MOM differences. The low water levels did not correspond to the HOCSZ at the tail, which weakened the intensity of the metalimnetic oxygen depletion, while the remarkable hypolimnetic oxygen depletion remained in contrast.

The oxygen depletion in the metalimnion was the most intense in 2017, secondary in 2019, and subtle in 2020 in the head of the reservoir (Fig. 11). In addition to the hydrodynamic process, the trophic states are considered to be an influential factor for MOM. According to the measurements in Fig. 2, Chl_a and TP concentrations decreased significantly after 2017 with a decreasing trend from 2015 to 2020. The eutrophication conditions and the high algal biomass induced heavy algal deposition and consequently increased oxygen consumption, probably in the year and following years. The benthic sediments are aerated by limnic turnover in winter in the seasonal stratified reservoir(Du et al., 2023). The agitated turnover and long vertical mixing periods result in sufficient sediment oxygenation and lower SOD. The lakes and reservoirs have become significantly more stratified over the last half century as the climate has warmed, reducing turnover and inhibiting the vertical mixing (Posch et al., 2012). Oxygen consumption is not only related to trophic status, but is also influenced by several other factors. MOM profiles in PJKR in three years have illustrated the trophic influences that may be represented by the observed MOM in Lake Constance (Rhodes et al., 2017). Based on the observed and simulated results over three years, the drivers of the formation of metalimnetic dissolved oxygen minima in a stratified reservoir are well interpreted in terms of hydrological processes, hydrodynamics, and sediment oxygen consumption.

4.3 Summary of crucial impact factors on MOM

The metalimnetic dissolved oxygen minima are the result of comprehensive effects of reservoir regulation and hydrodynamics, sedimentation patterns, and trophic status. We have tentatively classified three types of flow intensity, combined the sedimentation patterns, and summarized the corresponding MOM exhibitions, as shown in Table 3.

Table 3. MOM exhibitions in stratified reservoirs under different conditions

Flow intensity	Tail HOCSZ	Downstream HOCSZ	MOM exhibitions	Corresponding cases
NO	+	+	Disappeared	Scenario A
Weak	+	+	Pronounced	2019
	-	+	Not obvious	2020

Modest	+	+	Pronounced	2017
	+	-	Appeared upsteam	Scenario B
	-	+	Appeared downstream	Scenario C

The cases summarized in Table 3 would be helpful in extending the theory to other reservoirs or lakes to interpret the MOM formation. Many deep reservoirs (>100m) have been constructed for hydropower generation in the upper reaches of Changjiang Rivers in China. The inflow and outflow discharges of the reservoirs are larger, and the depth of the metalimnion varies greatly in stratification seasons, with low nutrient loads and oligotrophic conditions. The HOCSZ at the tail bed was not significant, while HOCSZ at the head of the reservoir was distinct due to the dam interception. Scenario C well explained the MOM in the large deep cascade hydropower reservoirs (Chen et al., 2021). The results also reveal the synchrony of DO depletions in the metalimnion and hypolimnion in some lakes(McDonald et al., 2022). Furthermore, the top-layer water withdrawal facilities, designed to solve the problems of low-temperature water release in stratified reservoirs, further reduce the DO concentration in the hypolimnion (Weber et al., 2017), and consequently decrease the DO in then metalimnion, which can bring a certain negative effect.

5. Conclusions

- We have recorded the evolution of the metalimnetic oxygen minimum in Panjiakou Reservoir over the years through field measurements. The numerical modeling and scenario simulations reveal the mechanism of MOM formation, the crucial factors and their effects. In general, the comprehensive functions of hydrodynamics and benthic oxygen consumption, and trophic status generate MOM in the stratified reservoirs.
- In the interfaces between the epilimnion and hypolimnion in stratified reservoirs, there is very little vertical diffusion, which inhibits water exchange between the epilimnion and hypolimnion, whereas there are relatively strong advections. Circulation and mixing occur in the epilimnion and hypolimnion respectively. The upwelling along the benthic slopes in the hypolimnion together with other features, creates the High Oxygen Consuming Sedimentation Zones (HOCSZ) mainly on the deepest bed and at the bottom of the metalimnetic elevation, where hypoxia first appears after stratification. The HOCSZ are the seedbeds and the metalimnetic advections become the drivers of the metalimnetic dissolved oxygen minima.
- By analyzing different scenarios, the intensities of oxygen depletion in the metalimnion are related to the flow intensity during the stratification period. Weak flow intensity attenuate the degree of oxygen depletion. Moderate flow intensity not only maintain stable thermal stratification, but also enhance horizontal flow and advection in the metalimnion, which tends to produce significant oxygen depletion.

Currently, upper-layer water withdrawals, which are common in stratified reservoirs, have the potential to increase oxygen depletion in the metalimnion.

- The total oxygen consumption in reservoirs mainly originally comes from algae, input of organic matter and reductants, which are decomposed and sedimented. Eutrophication has a tendency to cause intense benthic HOCSZ in subsequent years. Sediments can be aerated by the winter turnover and reduce the oxygen demand. Although the climate, reservoir regulations can influence the sediment oxygen consumption, reducing the trophic levels and algal biomass help to promote the oxygen concentrations in the metalimnion.
- A better understanding of MOM will help us unravel the complex and variable environmental problems of the limnic system in relation to pollution control and reservoir regulation. With the increasing construction of reservoirs to cope with extreme climates and clean energy demands in the future, the study provides ideas for improving water management.

List of abbreviations

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Conflicts of Interest:

No

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