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Evaluating the performance of CE-QUAL-W2 version 4.5 sediment diagenesis model

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Abstract. This study set out to assess the performance of the state-of-the-art CE-QUAL-W2 v4.5 sediment diagenesis model. The model was applied to a reservoir in Portugal using observed sediment particulate organic carbon values corresponding to a six-year period (2016-2021). The model was calibrated by comparing its results with 35 observed dissolved oxygen and water temperature profiles, as well as annual total nitrogen, total phosphorus, biochemical oxygen demand, and chlorophyll-a measurements corresponding to three different depths. In addition to model calibration, a sensitivity analysis was also conducted by varying the input particulate organic carbon values and applying a user-specified sediment oxygen model (zero-order model). The results demonstrated the overall effectiveness of the sediment diagenesis model, which accurately simulated dissolved oxygen profiles, nutrient concentrations, and organic matter levels (Dissolved oxygen profiles: NSE = 0.41 ± 0.67; RMSE = 1.73 mg/L ± 0.69), highlighting its potential as an effective tool for simulating lakes and reservoirs and supporting water management processes. The study further suggests that the zero-order model is able to serve as an effective starting point for implementing the sediment diagenesis model, providing an initial estimate for mean reservoir sediment oxygen demand (SOD) values.

1 Introduction

Modeling water quality plays a crucial role in managing lakes and reservoirs, providing essential insights into the dynamics of nutrients, organic matter, and phytoplankton within aquatic systems (Abbaspour et al., 2015; Whitehead et al., 2009). These models simulate the physical, chemical, and biological processes that influence water quality, with examples including widely-used tools like CE-QUAL-W2 (Wells, 2021), MIKE21 (Chapman, 1996), and DYRESM (Hamilton and Schladow, 1997). The value of such modeling lies in its capacity to aid researchers and policymakers in understanding the complex interactions between various factors that impact the ecological health of water bodies (Varis et al., 1994; Loucks and Beek, 2017). However, the intricacy of these systems, combined with the substantial data requirements, often presents significant challenges for those developing and applying water quality models.Effective inflow data characterization (quantity and quality) is hard to obtain, both for major river branches and small tributaries, as is waterbody sediment characterization related to carbon and nutrients due to the significant cost associated with the sampling and laboratorial analysis process and the fact that water management stakeholders are still more focused on the classification of waterbody water quality rather than the collection of water quality forcing data. The absence of sediment initial particulate organic carbon (POC),

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particulate organic nitrogen (PON) and particulate organic phosphorus (POP) data can be decisive to the overall performance of a water quality model, in essence generating an imbalance right from the start of the simulation with regard to the sediment concentration of POC, PON and POP, which then has a considerable impact on the SOD and, consequently, the waterbody dissolved oxygen (DO). When calibrating the model, water quality modelers therefore need to plug this gap by evaluating the model performance considering: i) different initial sediment oxygen demand (SOD) where a zero-order model is applied, ii) different POC, PON and POP values where a predictive diagenesis model is considered.

The main problem with these solutions is that the source of DO decay can also be driven by the inflow of organic matter or algae mortality. In other words, the final baseline model results are able to fit the observed DO profiles with reasonable accuracy but the model prediction capability may be unbalanced if the DO sinks/sources are not well defined. For example, the model's response to a reduction of inflow phosphorous is a function of the phosphorus released from the sediments during anoxia periods and, therefore, if the SOD is not accurately computed the waterbody phosphorous balance will, in turn, be incorrect. The calibration of other constituents, such as nutrients can help to minimize this uncertainty. For example, orthophosphates ($P\text{-}PO_4$) are released from the sediments under anaerobic conditions and therefore the calibration of this nutrient can help with the overall calibration of the water body DO concentration. The release of $P\text{-}PO_4$ from the sediments is, however, a function of several variables, for example, the initial $P\text{-}PO_4$ dissolved concentration and the $P\text{-}PO_4$ release rate (zero-order approach), or a diagenesis rate for POP (diagenesis model). In other words, the modeling uncertainty may diminish but will persist without observed POC, PON and POP. Of the three variables (POC, PON, and POP), POC has the most significant impact on SOD. Consequently, access to sediment POC values is crucial for ensuring accurate modeling even where PON and POP concentrations are unavailable.

The CE-QUAL-W2 model has been widely used to simulate various water bodies and water quality scenarios, including reservoir physical and biochemical dynamics in response to warming projections (Mi et al., 2020; Mi et al., 2023). This model has also been used to predict DO in a number of water bodies worldwide, although the SOD has always been modeled with a zero-order and/or 1-order model (e.g. Park et al., 2014; Zouabi- Zouabi-Aloui et al., 2015; Terry et al., 2017; Sadeghian et al., 2018; Lindenschmidt et al., 2019). The bibliographic research conducted before and during this study suggests that the CE-QUAL-W2 sediment diagenesis model has not been applied to any waterbodies other than the Wahiawa Reservoir in central Oahu (Berger and Wells, 2014). Moreover, no scientific publications on the evaluation of this model in other contexts have been identified, further highlighting the importance of the primary motivation for this study, namely, to evaluate the performance of the CE-QUAL-W2 model with its new sediment diagenesis component. This study benefited from having access to observed reservoir sediment total organic carbon (TOC) values, which are rare. Although, in theory, these values are typically higher than particulate organic carbon (POC) values, they provided an excellent starting point for this study. The methodological approach was, therefore, defined to evaluate the performance of the CE-QUAL-W2 model considering the new state-of the art sediment diagenesis model in modeling a reservoir, DO, Total Phosphorus (Total P); Total Nitrogen (Total N), Biochemical Oxygen Demand (BOD_5), Chlorophyll -a and SOD.

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To achieve this, the water quality of a highly productive reservoir was simulated using the CE-QUAL-W2 v4.5 model, incorporating both a zero-order sediment model and the sediment diagenesis model over a six-year period, spanning 2016 to 2021. It should be noted that the zero-model was included in this study to back-calculate the DO uptake rate in the reservoir water column as a function of the reservoir boundary conditions. The zero-order model is not a predictive model, as it fails to include the accumulation of particulate organic matter and algae in the sediments and rates do not vary over time, except as a result of decay rate temperature dependence. Nevertheless, the consideration of this model proved useful for addressing potential issues related to the calibration quality of the sediment diagenesis model. If the predicted zero-order model DO profiles in the water column are exactly matched, then the values for SOD used in calibration are very close to the actual dissolved oxygen uptake rates in the water column (Wells, 2011). Therefore, if the W2 model with the sediment diagenesis function performs in the same way under the same boundary conditions as the zero-order model in terms of DO in the water column we can conclude that the performance of the sediment diagenesis function is accurate. In the case of water temperature and DO, the modeling results were compared with 35 water column profiles observed near the dam. The remaining parameters were calibrated against time series data sets observed at different depths. A sensitivity analysis was performed to evaluate the reservoir water quality response, namely DO, to the variation of POC, PON and POP concentration in the reservoir sediments. The results of this study will hopefully prove useful by helping to improve lake and reservoir water quality modeling and, therefore, the water management process from a practical perspective.

2 Methods

2.1 Site Location and Main Characteristics

Portugal experiences a temperate maritime climate characterized by a wet, cool season and a dry summer. Despite most of the precipitation occurring during the winter months, there is significant inter-annual variability. Precipitation patterns are spatially and temporally heterogeneous, with annual maxima exceeding 2500 mm in the rugged highlands of the northwest, while the low-lying plains of the southeast receive around 400 mm per year (Cardoso et al., 2013; Soares et al., 2015) (Fig.1). The Torrão dam, located in the northern region of mainland Portugal in the Tâmega River, is a significant hydraulic structure designed for multiple purposes, including water supply, irrigation, and hydroelectric power generation. The reservoir has a substantial storage capacity, contributing to regional water management and flood control. This infrastructure plays a crucial role in the socio-economic development of the region, balancing resource management and environmental preservation. However, it is also important to note that the reservoir was classified as eutrophic for all the simulated years, a condition that can lead to persistent water quality issues.

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Table 1: Main features of Torrão dam and reservoir

Full supply volume (hm^3)	Mean inflow (m^3/s)	Average annual inflow (local basin)	Active storage volume (hm^3)	Surface area at FLV (km^2)	Structural height (m)	Max depth (m)	Turbine number/power	Hydraulic residence time (days)	Watershed area (km^2)	Trophic state (2016 - 2021)(1)
123.9	76.98	2 147	40.4	6.5	70	58	2 reversible pump-turbines/146 (MW)	13.59	3 252	Eutrophic

(1) Classification according to OECD Trophic State limits (OECD, 1982)

2.2 Modeling approach

The bathymetry of the Torrão reservoir was initially defined using a Digital Elevation Model (DEM) provided by Energies of Portugal, S.A. (EDP) and structured according to the methodology outlined in Wells (2021). The reservoir comprises one main branch (the Tâmega River), three tributaries and one distributed tributary (Fig. 1). Tributaries 1 and 2 are depicted in Fig 1. Tributary 3 represents the inflow from the Douro River into the pump-back system of the Torrão Reservoir. The bathymetric map includes 27 segments, each measuring 1000 meters in length, and a maximum number of 58 layers, each with a depth of 1 meter. Following this preliminary step, the reservoir boundary conditions (including water quality, hydrology, meteorology, and sediment characterization) were defined according to the methods described in Section 1.2.3. Due to the lack of available information, the model structure only includes a single algae group (Diatoms). Subsequently, two different CE-QUAL-W2 model versions (see section 2.3) were calibrated for the 2016-2021 period (vide section 1.2.4): a) incorporating the sediment diagenesis model (W2_SD), and b) considering a user-specified sediment oxygen model (zero-order model) that was not coupled with the water column (W2_zero-order). The zero-order model was selected for the analysis because it typically provides an accurate approximation of the sediment oxygen demand (SOD) in a reservoir without relying on sediment concentrations or requiring a separate sediment compartment and was thus a useful tool for establishing a SOD benchmark for the reservoir. This is not, however, a predictive approach, as, other than variations resulting from the temperature dependence of the decay rate, the rates remain constant over time (Wells, 2021).

The models were calibrated by adjusting their parameters to improve the fit between the model output and observed data. Please refer to Wells (2021) for a detailed account of the model calibration parameters and default values. Water temperature was the first constituent to be calibrated. The wind sheltering coefficient (WSC) was manually adjusted to achieve the best fit between the modeled and observed water temperature profiles, resulting in a final value of 1. A value of 1 implies that the WSC has no effect over the wind velocity forcing the model. The zero-order model for sediment oxygen demand (SOD) was then manually adjusted to improve dissolved oxygen (DO) predictions based on 35 DO profiles. The optimal result was achieved with a constant SOD value of 2.5 g O_2/m^2/day. Following this calibration, the phosphorus sediment release rate (PO4R) in the zero-order model was modified from its default value of 0.001 to 0.015. All other parameters were kept at

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their relevant default values and the default settings for the sediment diagenesis model were also maintained. The observed data included water temperature (WT), dissolved oxygen (DO), Total P, Total N, BOD5, and chlorophyll-a. These two runs were named: W2_SD_baseline and W2_zero-order_baseline. A sensitivity analysis was conducted after the calibration process to evaluate the model's response: a) to different POC, PON and POP values in the case of the W2_SD model; and b) to different SOD values in the case of the W2_zero-order model. Section 1.2.5 details the methodological approach employed for the sensitivity analysis. The evaluation of the model's performance, along with the results obtained from the sensitivity analysis, provided deeper insights into modeling SOD using the diagenesis model.

2.3. CE-QUAL-W2 v4.5 model

This study employed the latest version of CE-QUAL-W2 (Version 4.5), a model originally developed in 1975 by the US Army Corps of Engineers and written in Fortran. Since its inception, the model has undergone regular updates and enhancements, primarily by researchers at Portland State University (Cole and Wells, 2006). CE-QUAL-W2 is a two-dimensional, laterally averaged hydrodynamic and water quality model capable of simulating free surface elevation, hydrostatic pressure, density, horizontal and vertical velocities, as well as constituent concentrations. The model uses the finite difference method to solve key equations, including mean transverse momentum in the x- and z-directions, the continuity equation, state equations, and water surface elevation equations (Adelena et al., 2015; Tavera-Quiroz et al., 2024; Wells, 2021). A sediment diagenesis module, originally tailored for oil sand pit lakes, has been adapted for application in other aquatic environments and integrated into version 4.0 (Vandenberg et al., 2015). The conceptual framework of the model has been elaborated in works by Prakash et al. (2014), Berg and Wells (2014), and Vandenberg et al. (2015). CE-QUAL-W2 has demonstrated its utility in simulating hydrodynamic and ecological processes—such as stratification, internal waves, oxygen dynamics, and phytoplankton blooms—in lakes and reservoirs worldwide (Zhang et al., 2015; Chuo et al., 2019; Kobler et al., 2018; Uhlmann, 2017; Terry et al., 2017; Mi et al., 2020). Additional details about the model's structure, algorithms, and historical applications can be found in the user manual (Wells, 2021).

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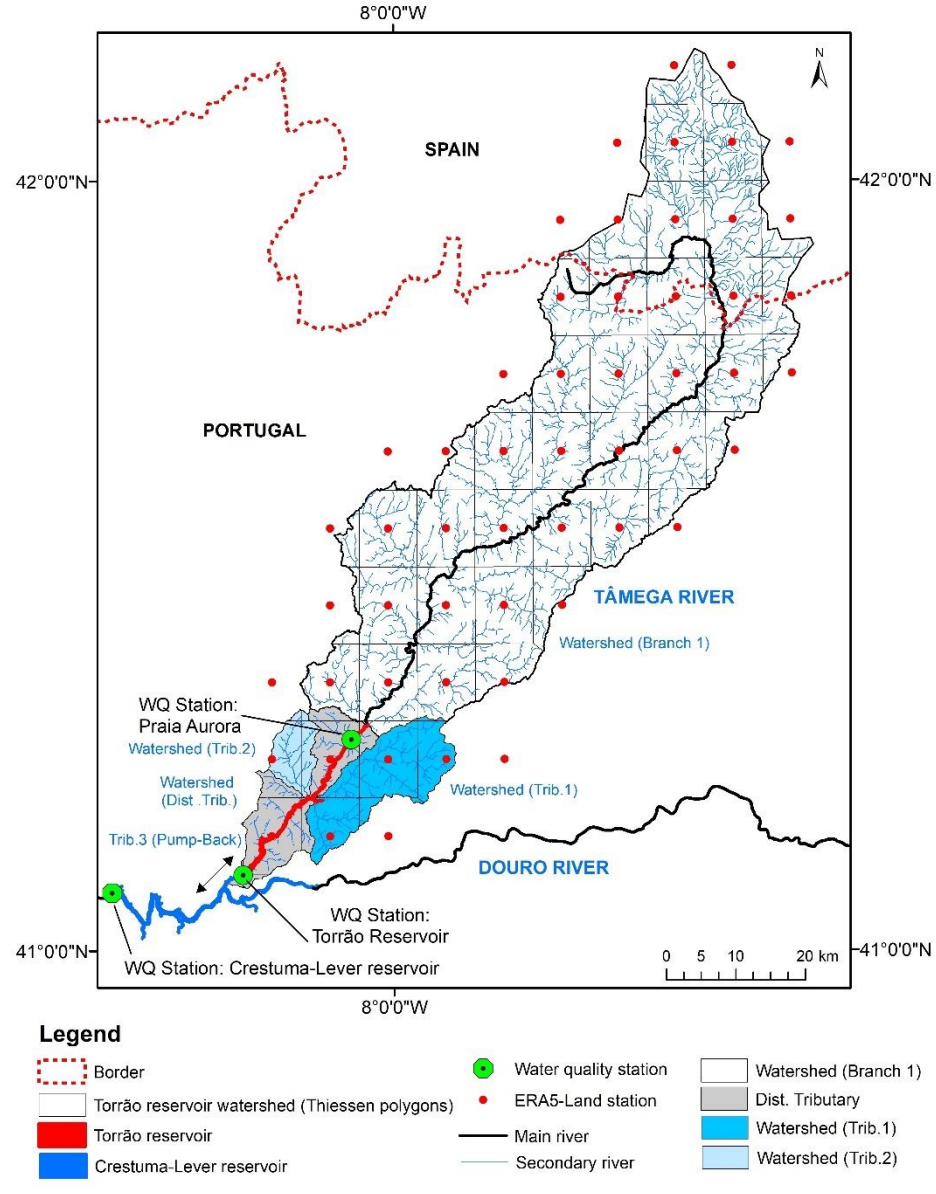

Figure 1: Torrão reservoir watershed. Thiessen polygons. Water quality stations

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2.4 Model Forcing Datasets

The meteorological data used to drive the model, including hourly air temperature, dew point, solar radiation, cloud cover, and wind characteristics, were sourced from ERA5-Land, a high-resolution reanalysis dataset optimized for land applications. Reservoir data, such as daily inflow/outflow, water levels, and water quality, covering the years 2016–2021, were provided by EDP. Water quality data specific to Branch 1 originated from the Praia Aurora Station, accessed via the Portuguese National Water Resources Information System (SNIRH, 2024). With only 21 recorded measurements for Branch 1 during this period, three modeling methods were employed to address the 99.04% of missing data. The variables include: water temperature; DO; Total P; Ammonium ($N\text{-}NH_4$); Nitrate+Nitrite ($N\text{-}NO_X$; BOD_5); Chlorophyll-a; Alkalinity; Conductivity and Total Suspended Solids (SST).

The first method employed regression models implemented through the LOADEST package (Runkel et al., 2004) developed by the USGS. The second method utilized the Extreme Gradient Boosting (XGBoost) machine learning algorithm, implemented using the Chen and Guestrin (2016) open-source library, a method proven effective in various environmental studies (Feigl et al., 2021; Adedeji et al., 2022; Xu et al., 2022). For additional details on the algorithm, refer to Almeida and Coelho (2023). The third approach relied on Support Vector Regression (SVR), implemented via the scikit-learn library (Pedregosa et al., 2011), which has also demonstrated strong performance in environmental modeling applications (Adedeji et al., 2022; Ji and Lu, 2018). For machine learning approaches, datasets were split into training (80%) and testing (20%) sets. Hyperparameters for these models were optimized using the Tree-structured Parzen Estimators (TPE) algorithm, executed with the Hyperopt library (Bergstra et al., 2013) and 100 iterations. The Nash-Sutcliffe Efficiency (NSE) was used to determine the best model. Table A1 describes the input features of each model. Correlations derived from Branch 1 informed data extrapolation to other tributaries using flow as the predictor. Observed data for Tributary 3 was retrieved from the Crestuma-Lever reservoir monitoring station.

Water quality variables used for model inputs included water temperature, DO, orthophosphates ($P\text{-}PO_4$), $N\text{-}NH_4$, N-NOx, labile and refractory dissolved and particulate organic matter (LDOM, RDOM, LPOM, RPOM), alkalinity, inorganic suspended solids (ISS), total dissolved solids (TDS), total inorganic carbon (TIC), and algal biomass (diatoms). For non-monitored variables, estimations were made based on available data: i) $P\text{-}PO_4$: Derived from total phosphorus, assuming inorganic phosphorus represents 70% of the total; ii) Organic matter: BOD_5 was converted to organic matter using a stoichiometric ratio of 1.4 g O_2/1.0 g organic matter, with 60% assumed refractory and 40% labile; iii) ISS: Estimated as 97.4% of TSS; iv) TDS: Calculated from electrical conductivity (Eq.1); v) TIC: Estimated from alkalinity (Eq. 2); vi) Algae biomass: Chlorophyll-a was converted to biomass using the following ratio: Algal Biomass (mg/L)/Chlorophyll-a (µg/L) = 0.05

$$\text{TDS (mg/L)} = 0.65 \times \text{Electrical Conductivity}(\mu\text{S/cm}) \quad (1)$$

$$\text{TIC (mg/L)} = 0.2782 \times \text{Alkalinity (mg/L)}0.9706 \quad (2)$$

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This equation was derived from the relationship between TIC and alkalinity values observed in four reservoirs within the United States, utilizing a dataset comprising 55232 value pairs available in the CE-QUAL-W2 v4.5 model examples (Wells, 2021). The analysis achieved an R2 value of 0.99.

Figure 2 illustrates the locations of the five sediment sampling sites used to define the W2_SD_baseline run. The spatial distribution of the sediment samples depicted in the figure were linked to specific reservoir segments to characterize the initial sediment content of particulate organic carbon (POC), particulate organic nitrogen (PON), and particulate organic phosphorus (POP), as detailed in Table 2. Sediment values were assigned as follows: site A to segments 25–28, site B to segments 20–24, site C to segments 16–19, site D to segments 11–15, and site E to segments 2–10. Several assumptions were made to establish the sediment characterization: i) A sediment density of 960 kg/m³ (Minear, 2007) was applied to convert sample values from mg/kg to mg/L; ii) POP values were set at 25 mg/L, based on established literature benchmarks (Wells, 2021); iii) The Total N value observed at site B was used to characterize sites C, D, and E; iv) TOC and Total N were assumed to exist entirely in particulate form, represented as particulate organic carbon and nitrogen. This approach ensured a consistent and representative characterization of sediment properties across the reservoir segments.

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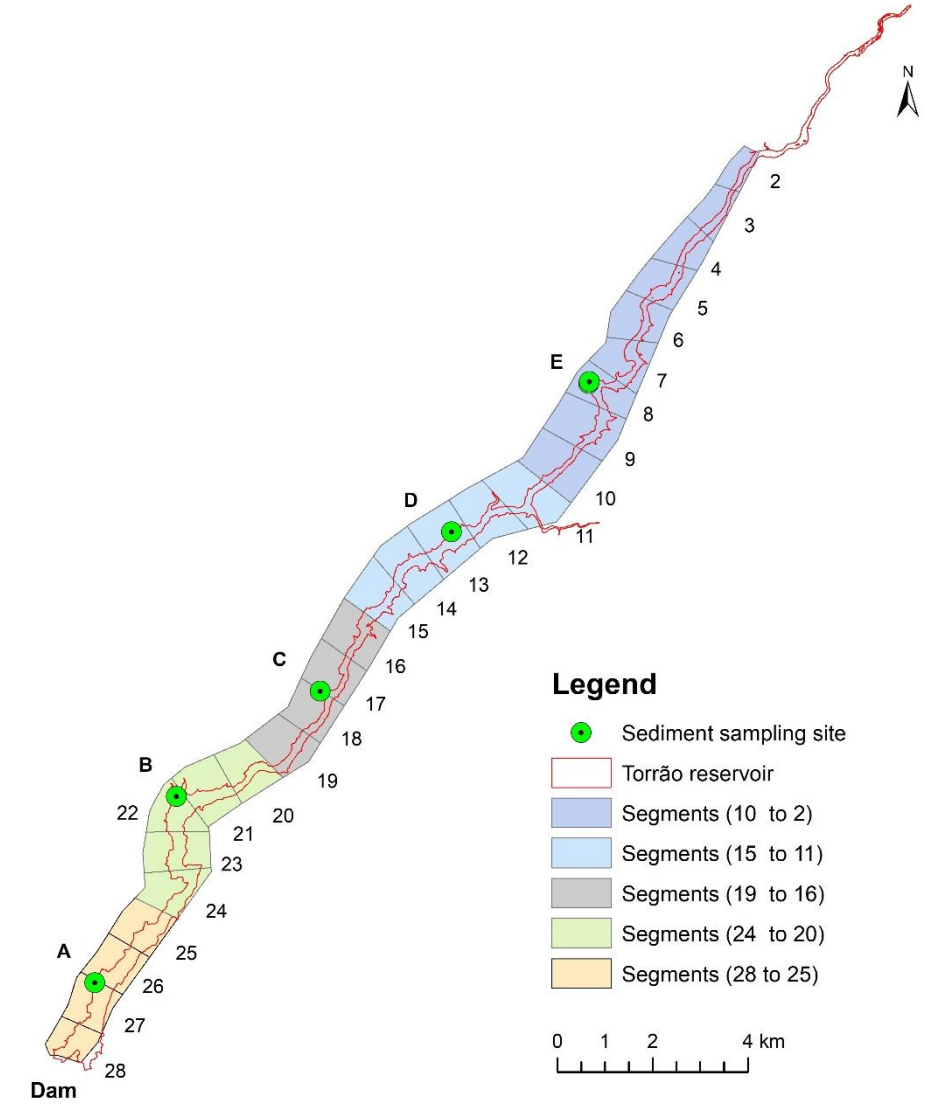

Figure 2: Sediment sampling sites. CE-QUAL-W2 model segments

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Table 2: Torrão Reservoir sediment chemical characterization obtained for each sampling site.

Observed values			
Sampling site	**TOC, mg/kg**	**Total N, mg/kg**	**POP, mg/kg**
A	25 000	6020	-
B	20 900	5990	-
C	22 300	-	-
D	20 100	-	-
E	5 600	-	-
Final values included in the sediment diagenesis model			
	POC, mg/L	**PON, mg/L**	**POP, mg/L**
A	24 000	5779	25
B	20 064	5750	25
C	21 408	5750	25
D	19 296	5750	25
E	5376	5750	25

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2.5 Water Quality Model (CE-QUAL-W2) Calibration

The simulation period considered for this study spanned 2016 to 2021. This period was selected due to the availability of flow and water quality data. The trial-and-error technique was applied to calibrate the model for the simulation period, considering the default calibration parameters described in Wells, 2021. The error between observed and predicted values of
235 six state variables was evaluated with five different metrics (vide section 1.2.6). The observed data included water temperature (WT), dissolved oxygen (DO), Total P, Total N, BOD_5, and chlorophyll-a. These time series were obtained from: (a) an integrated sample between the reservoir surface and a depth of 5.8 meters, (b) a depth of 23 meters, and (c) a depth of 43.7 meters. 35 water temperature and DO profiles, with six profiles per year from 2016 to 2021, were also considered. These profiles were observed 300 meters upstream from the Torrão Dam. The models' initial conditions,
240 parameters, constants, and the forcing datasets can be obtained from Almeida and Coelho, 2025.

2.5 Sensitivity analysis

A sensitivity analysis was conducted after the calibration process to evaluate the model's response:

i) Different initial sediment values for POC, PON, and POP were used in the W2_SD model (Table 3). It is important to note that for each of the 24 runs described in Table 2, only the corresponding parameter was modified, while the other
245 two parameters retained their default values shown in Table 1. The number of runs varying the PON and POP values is

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higher than the number of runs considered for POC, with 6 versus 9 runs, respectively. This adjustment was necessary to achieve a minimal RMSE in the predictions of dissolved oxygen in the water column.

ii) Different SOD values for the W2_zero-order model (0.5, 1.0, 1.5, 2.0, 2.5 and 3.0 g O_2/m^2/day)

In the results analysis for each run and for both scenarios (i) and (ii), the prediction error for dissolved oxygen (DO) was compared with the sediment oxygen demand (SOD) values derived from each model. Specifically, Runs 5, 8, and 20 were forced with the particulate organic carbon (POC), particulate organic nitrogen (PON), and particulate organic phosphorus (POP) values defined in the W2_SD_baseline run.

Table 3. TOC, PON, and POP initial sediment values for the W2_SD model sensitivity analyses.

Parameter	Sampling site/Model segments					W2_SD model run
	A	B	C	D	E	
	28-25	24-20	19-16	15-11	10-2	
POC	4 800	4 013	4 282	3 859	1 075	1
	9 600	8 026	8 563	7 718	2 150	2
	14 400	12 038	12 845	11 578	3 226	3
	19 200	16 051	17 126	15 437	4 301	4
	24 000	20 064	21 408	19 296	5 376	5 (W2_SD_baseline)
	28 800	24 077	25 690	23 155	6 451	6
PON	8 669	8 625	8 625	8 625	8 625	7
	5 779	5 750	5 750	5 750	5 750	8 (W2_SD_baseline)
	2 890	2 875	2 875	2 875	2 875	9
	1 445	1 438	1 438	1 438	1 438	10
	722	719	719	719	719	11
	361	359	359	359	359	12
	181	180	180	180	180	13
	90	90	90	90	90	14
	45	45	45	45	45	15
POP	128	128	128	128	128	16
	85	85	85	85	85	17
	57	57	57	57	57	18
	38	38	38	38	38	19
	25	25	25	25	25	20 (W2_SD_baseline)
	13	13	13	13	13	21
	6	6	6	6	6	22
	3	3	3	3	3	23
	2	2	2	2	2	24

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2.6 Metrics

The evaluation of model calibration and the analysis of quantitative differences across simulation scenarios utilized various performance metrics. These included the root mean square error (RMSE), mean absolute error (MAE), Nash-Sutcliffe efficiency (NSE) (Nash and Sutcliffe, 1970), percent bias (PBIAS), and the coefficient of determination (R^2). The calculations were carried out using equations where m_i and o_i represent the simulated and observed values, respectively, and $\bar{o}_i$ the observed values mean.

$$\text{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(m_i - o_i)^2} \quad (3)$$

$$\text{MAE} = \frac{1}{N}\sum_{i=1}^{N}|m_i - o_i| \quad (4)$$

$$NSE = 1 - \left[\frac{\sum_{i=1}^{N}(o_i - m_i)^2}{\sum_{i=1}^{N}(o_i - \bar{o}_i)^2}\right] \quad (5)$$

$$PBIAS = \frac{\sum_{i=1}^{N}(o_i - m_i)}{\sum_{i=1}^{N}(o_i)} \times 100 \quad (6)$$

$$R^2 = \frac{\sum_{i=1}^{N}(m_i - \bar{o})^2}{\sum_{i=1}^{N}(o_i - \bar{o})^2} \times 100 \quad (7)$$

3 Results

3.1 Observed Inflow Water Quality Characterization

The SVR algorithm was more effective at predicting the inflow water temperature compared to the other models. The R^2 and PBIAS values achieved with the SVR were 0.87, and 3.77%, respectively, indicating that the water temperature trends and average magnitudes are well described (Table A1). Additionally, the RMSE and MAE values of 2.1ºC and 1.6ºC, respectively, demonstrate an accurate approximation of the observed datasets. The SVR algorithm was also the best model in predicting DO. The R^2, PBIAS, RMSE, and MAE values reached, 0.91, 0.92%, 0.40 mg/L and 0.26 mg/L, respectively, indicating that the model performed well. This was not the case for the remaining parameters. In fact, the Loadest regression outperformed the other models for the remaining water quality variables. This was primarily due to the limited number of training samples. Simpler models like regressions can have lower variance (i.e., be less susceptible to overfitting) compared to SVR and XBOOST algorithms. Overall, the PBIAS obtained for NH_4, N-NOx, and Chlorophyll-a (10.88%, 43.64%, and 30.00%) suggests that the average magnitude was reasonably well represented.

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3.2 CE-QUAL-W2 calibration

The results of the calibration process for both models are presented in Table 4 and illustrated in Fig. 3. Table 3 displays the metrics obtained during calibration, while Fig. 3 depicts the evolution of the predicted constituent time series throughout the simulation period. Fig. 3 shows that both models predicted the reservoir water temperature reasonably well, a conclusion confirmed by the metrics obtained for this constituent (Table 4). The water column DO was accurately predicted by both models, however, the W2_zero-order model performed slightly better according to all metrics, with the exception of PBIAS. According to Fig.3, the remaining parameters were also well simulated by both models. The only exception to this were the Total N and Total P concentration values predicted by the W2_zero-order model for the reservoir bottom, which were overestimated (Table A2).

Based on the analysis of Fig. 3 and the values obtained for RMSE, MAE, and PBIAS, it is reasonable to conclude that both models performed equally well in predicting reservoir water quality. However, the W2_zero-order model was slightly better at predicting reservoir DO. Despite this, the model overestimated Chlorophyll-a concentrations from the surface down to a depth of 5.8 meters, and the concentrations of Total P and Total N at the reservoir bottom were also overestimated. During anoxic periods, the model exaggerated the release of $P\text{-}PO_4$ and $N\text{-}NH_4$, an issue that was not mitigated by tuning the release rates of $P\text{-}PO_4$ and $N\text{-}NH_4$ from the sediments, which suggests that the problem was driven by excessive anoxia in the bottom layers. Conversely, the W2_SD model provided a more balanced response, predicting the mean evolution of all constituents reasonably well.

Table 4: Metrics between observed and predicted values for both models. Water temperature and DO metrics were obtained from 36 observed and predicted profiles.

Constituent	**W2_SD model (run 5 - baseline)**				
	NSE	**R^2**	**PBIAS**	**RMSE**	**MAE**
Water temperature	0.56±0.19	0.56±0.13	-0.11±0.71	3.51±0.32	1.56±0.10
DO	0.34±0.69	0.55±0.31	-8.26±14.70	1.79±0.63	1.34±0.47
Constituent	**W2_zero-order model (SOD = 2.5 g O_2/m^2/day - baseline)**				
	NSE	**R^2**	**PBIAS**	**RMSE**	**MAE**
Water temperature	0.56±0.19	0.56±0.13	-0.12±0.80	3.51±0.32	1.57±0.10
DO	0.50±0.59	0.54±0.31	-4.77±15.52	1.62±0.73	1.20±0.55

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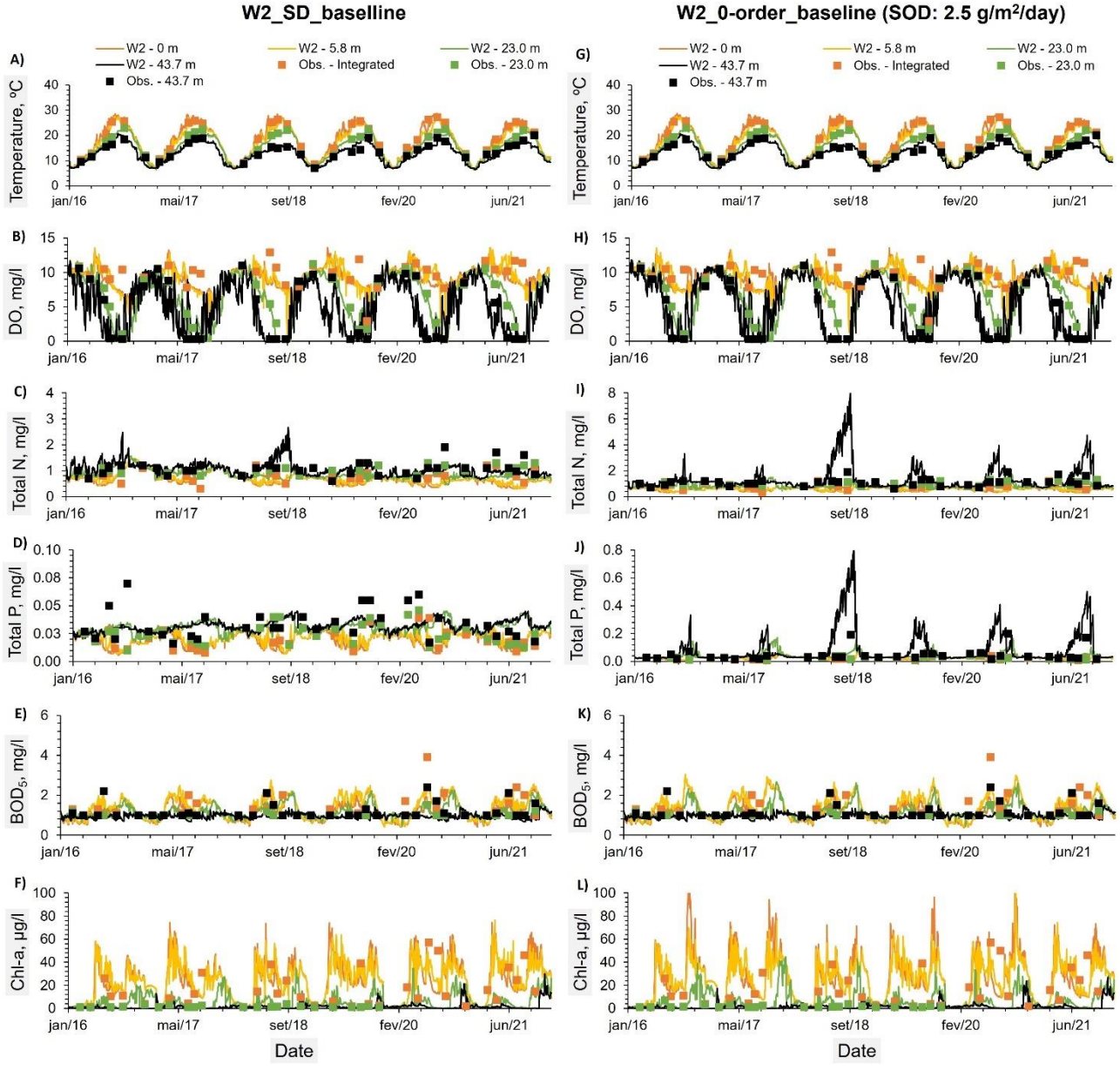

Figure 3: Constituents observed values at three different depths: (a) an integrated sample between the reservoir surface and an average depth of 5.8 meters, (b) an average depth of 23 meters, and (c) an average depth of 43.7 meters. These observed values were compared with the predicted time series from the W2_SD_baseline (A to F) and W2_zero-order_baseline (SOD: 2.5 g/m²/day) (G to L) for the same depths.

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3.3 Sensitivity analysis

The SOD values strongly influence the water column DO; therefore, this parameter was considered to support this analysis. Figure 4 shows the SOD values from the reservoir bottom layer, predicted by the W2_SD_model for Runs 1 to 6, compared with the RMSE (Fig4A) and the NSE (Fig4A) values obtained between the predicted water column DO profiles and the mean initial POC values (across all sites values) for each run. These results suggest that Run 2 was the best modeling solution. Considering the results obtained for Run 5 (baseline), Run 2 reduced the RMSE from 1.79 mg/L to 1.73 mg/L and increased the NSE from 0.34 to 0.41. The average SOD value in the bottom layer of the reservoir (across all model segments) decreased from 1.2 g O_2/m_2/day (Run 5) to 0.81 g O_2/m^2/day (Run 2). Although not a significant reduction, it suggests an initial overestimation of POC values. This outcome was expected, given the initial assumption in Run 5 that all TOC existed in the form of POC. Based on the initial POC values of both runs, it can be concluded that the particulate fraction of organic carbon constitutes 40% of the TOC. Table A4 presents the metrics for water temperature, DO, Total N, Total P, BOD_5, and Chlorophyll-a obtained for Run 2. Although this run improved the reservoir DO prediction, the results for the other constituents are very similar to those obtained for Run 5 (baseline).

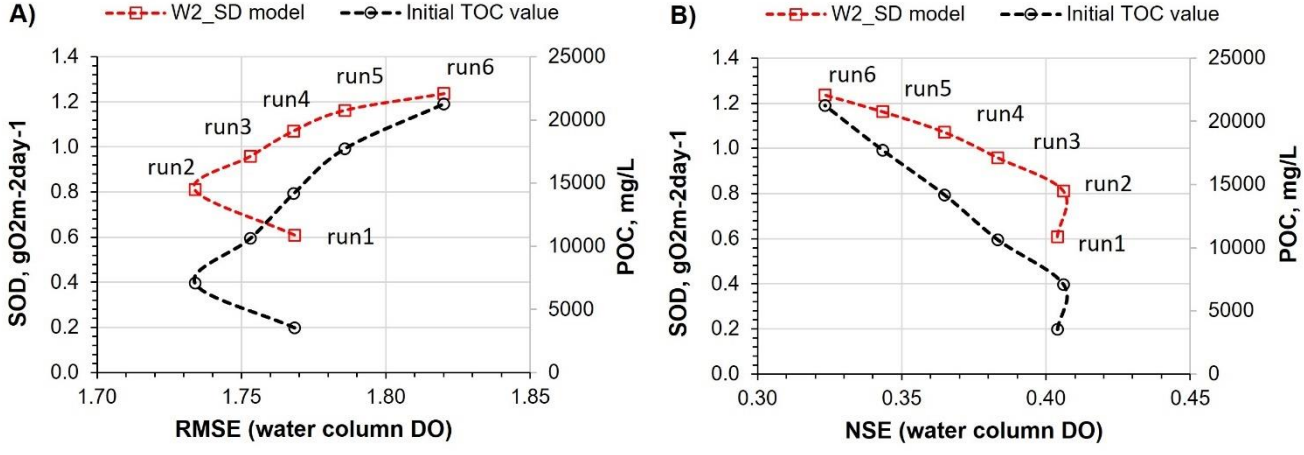

Figure 4: A) SOD values from the reservoir bottom layer, predicted by the W2_SD_model for Runs 1 to 6, compared with the RMSE obtained between the predicted water column DO profiles and the mean initial POC values (across all sites values) for each run of the W2_SD_model. B) Similar to A but considering the NSE metric.

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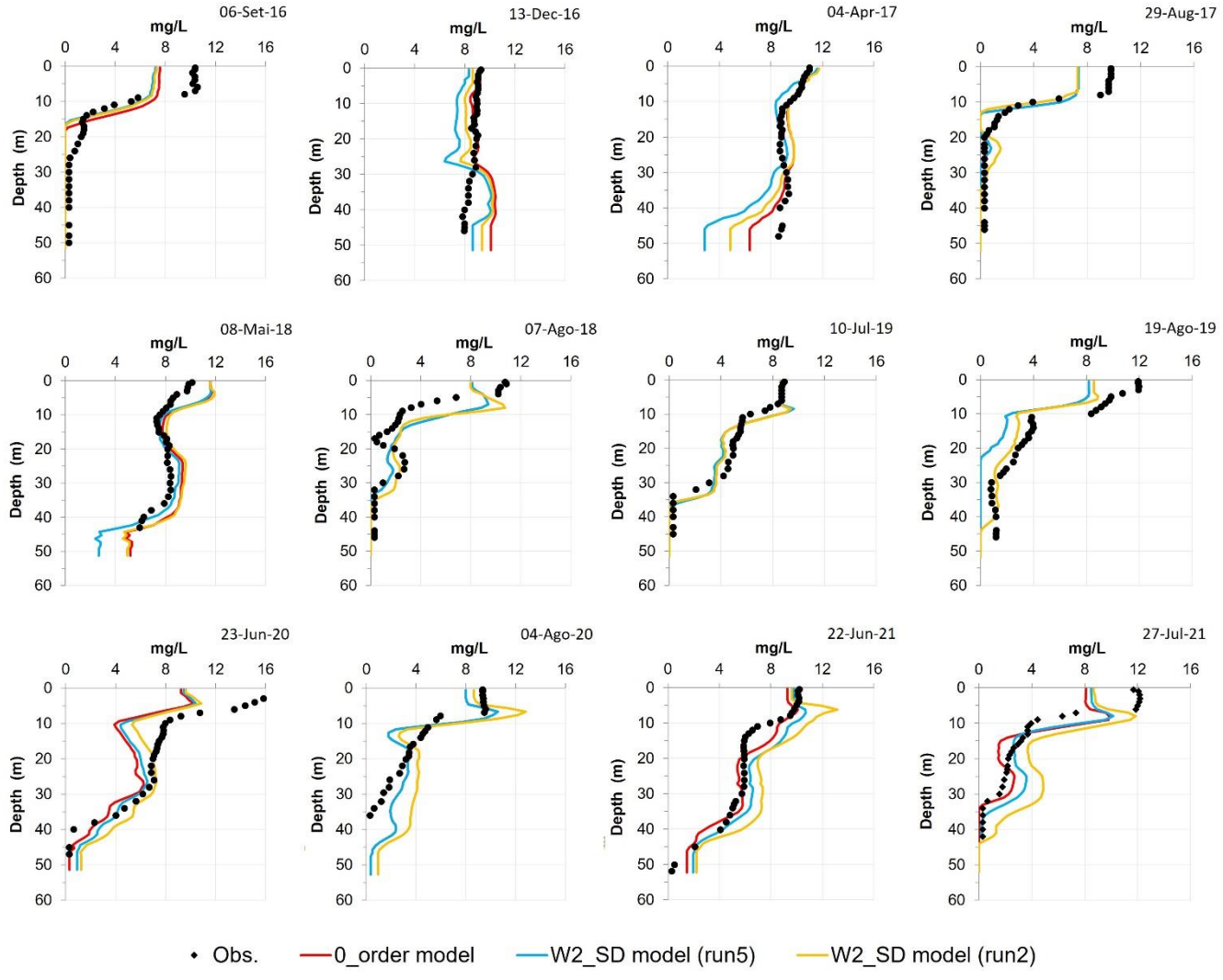

Figure 5: Observed DO profiles (300 m from the dam) compared to predicted profiles using the W2_zero-order model (baseline), W2_SD model (Run 2) and (Run 5; baseline).

The sensitivity analysis also involved varying the initial values of PON and POP for each run. The results indicate that mean reservoir SOD values remained nearly constant, as depicted in Fig. 6, suggesting that the W2_SD model was not significantly affected by variations in the initial PON and POP values in the sediments. However, in Runs 7, 8, and 9, where PON values were higher, there was a significant increase in the release of $N\text{-}NH_4$ and $N\text{-}NO_X$ from the reservoir sediments, leading to an impact on water column DO. This is evidenced by the notable increase in RMSE and the reduction of NSE values, as shown in Fig. 6A and 6B.

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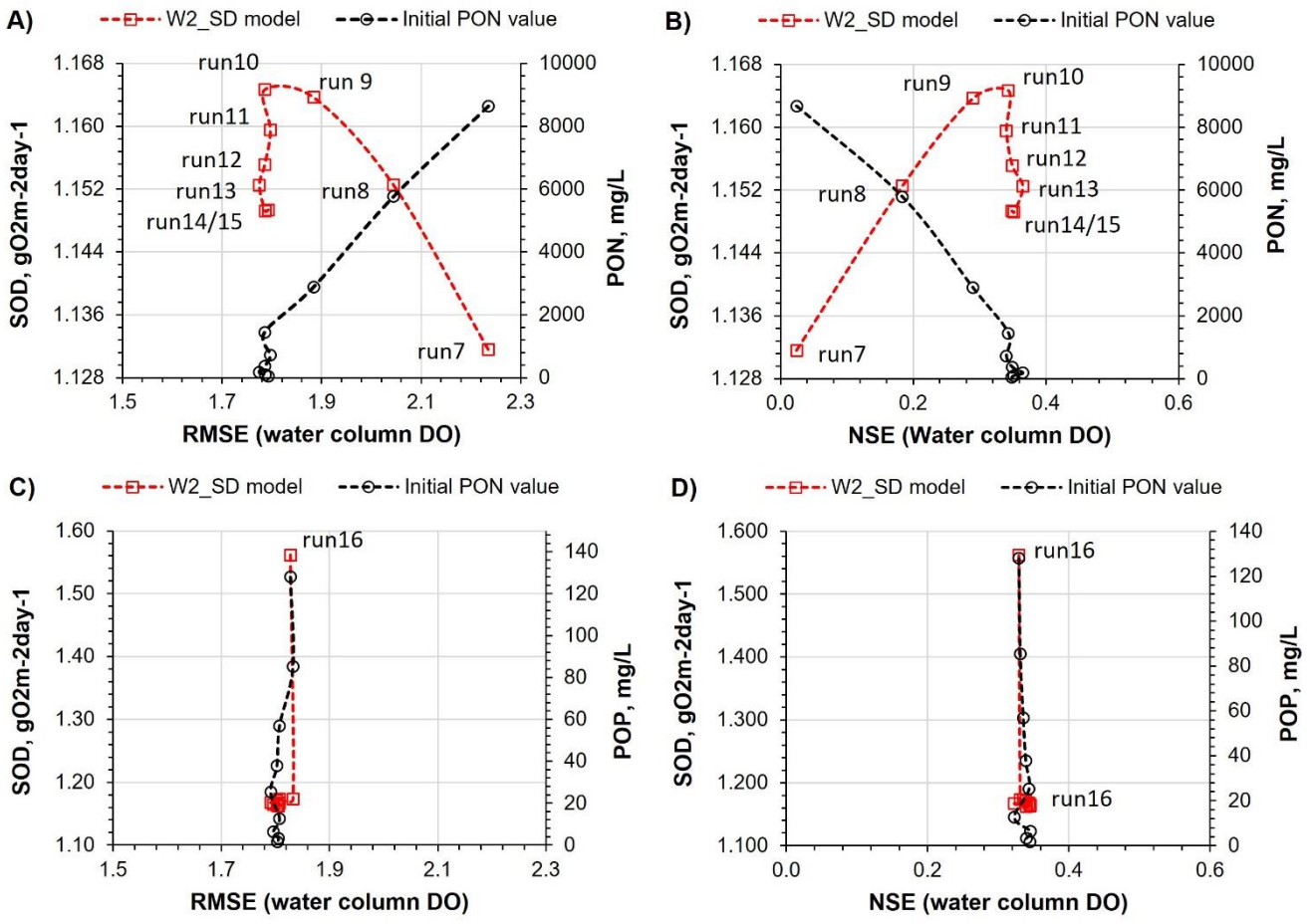

Figure 6: A) SOD values from the reservoir bottom layer, predicted by the W2_SD_model for Runs 7 to 15, compared with the RMSE obtained between the predicted water column DO profiles and the mean initial PON values (across all sites) for each run B) Similar to A) but considering the NSE metric. C) SOD values from the reservoir bottom layer, predicted by the W2_SD_model for Runs 16 to 24, compared with the RMSE obtained between the predicted water column DO profiles and the mean initial POP values (across all sites) for each run. D) Similar to C) but considering the NSE metric.

Figure 7 shows the RMSE (Fig. 7A) and the NSE (Fig. 7B) values between observed and predicted water column DO profiles for both models: W2_SD model (Runs 1 to 6) and the W2_zero-order model, each with six different SOD values ranging from 0.5 to 3.0 g/m²/day, along with the corresponding reservoir SOD values. Overall, these results show that the zero-order model with a constant SOD of 2.5 g O_2/m²/day was better than the W2_SD model at predicting reservoir DO. The analysis of this figure also indicates that varying the SOD in the zero-order model from 0.5 to 3.0 g O_2/m²/day resulted in changes in DO prediction, with RMSE values ranging from 2.27 to 1.62 g O_2/m²/day and NSE values ranging from 0.14 to 0.50. The reservoir SOD obtained with the W2_SD model was less sensitive to changes in the initial sediment POC value,

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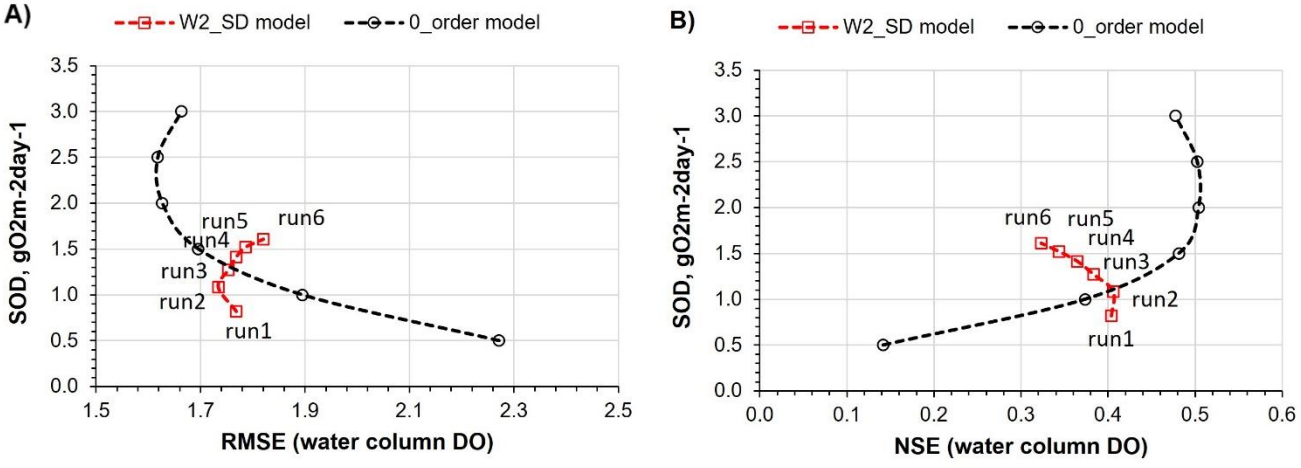
355 suggesting that the initial POC value must be significantly higher than 20 000 mg/L to achieve SOD values of more than 2.0 g O_2/m²/day.



360 **Figure 7. A) RMSE values between observed and predicted water column DO profiles predicted by both models (W2_SD model Runs 1 to 6 and 0_order model with six different SOD values ranging from 0.5 to 3.0 g/m²/day) compared with the reservoir SOD values. B) Similar to A) but considering the NSE metric.**

4 Discussion

Overall, the temperature and DO predictions for the reservoir boundary conditions (Tâmega river) were quite good: PBIAS: 365 0.76% and 0.92%, respectively. When a significant number of samples and forcing variables are available the accuracy of machine learning algorithms can be greatly enhanced. This was demonstrated in the studies by Lu et al. (2020), Rajesh and Rehana (2021), and Feigl et al. (2021), where the RMSE for river water temperature prediction reached 1.04ºC, 1.03ºC, and 0.58ºC, respectively. The results obtained for alkalinity, conductivity and TSS were also good: Alkalinity-PBIAS: 17.44%; Conductivity - PBIAS: 8.23%; TSS- 0.73; PBIAS: 11.86%. However, as expected, the PBIAS values obtained for the 370 remaining constituents were not as favorable (Total P- PBIAS: 7.11%; N-NO_X- PBIAS: 3.92%; BOD_5- PBIAS: 6.93%; Chla-PBIAS: 30%). The modeling of these constituents involves complex biological, chemical, and physical processes that are harder to model accurately. However, except for Chla, the PBIAS values were generally less than 10%, reflecting acceptable levels of bias. Ammonium (N-NH_4) was the only parameter for which performance was significantly lower, generating a PBIAS of 28.27%. Moriasi et al. (2015) suggest that $\pm 10 \leq PBIAS \leq \pm 25$ is indicative of a satisfactory model performance.

375 Based on the RMSE, the overall calibration results obtained for all constituents with both models for the 2016-2021 period were consistent with the results seen in other studies (see Table A3). The mean RMSE values for Chlorophyll-a obtained

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with both models (W2_SD model: 13.43 µg/L; W2_zero-order model: 15.84 µg/L) are aligned with the results of other modeling studies (Brito et al., 2018: 62.9 µg/L; Kim et al., 2019: 6.7 to 13.2 µg/L; Tasnim et al., 2021: 0.6 to 27.6 µg/L; Almeida et al., 2023: 19.36 to 25.57 µg/L). This can also be said of Total P, with the mean RMSE values obtained with both models (W2_SD model: 0.02 mg/L; W2_zero-order model: 0.06 mg/L) corresponding to those of other studies (Brett et al., 2016: 0.012 mg/L; Kim et al., 2019: 0.014 to 0.068 mg/L; Tasnim et al., 2021: 0.005 to 0.036 mg/L; Almeida et al., 2023: 0.07 to 0.09 mg/L). The mean RMSE values obtained with both models (W2_SD model: 0.37 mg/L; W2_zero-order model: 0.64 mg/L) for Total N were, however, lower than the only reference found for this constituent, which was recorded as 0.77 mg/L (Deliman et al., 2002).

The RMSE obtained with the W2_SD model and the zero-order model for DO (1.79 mg/L and 1.62 mg/L, respectively) are also in line with the results obtained in other studies (e.g., Deliman et al., 2002: 1.34 mg/L; Brett et al., 2016: 1.2 mg/L; Brito et al., 2018: 7.6 mg/L; Luo et al., 2018: 1.78 mg/L; Tasnim et al., 2021: 2.33 mg/L). In general terms, the metrics obtained for both models and visual analysis of the predicted time series suggest that the CE-QUAL-W2 diagenesis model performed well and produced a more balanced response than the W2_zero-order model. It is also important to evaluate the magnitude of the SOD value associated with each model. Both models performed similarly well with regard to modeling the water column dissolved oxygen (DO). The SOD considered for the W2_zero-order model (2.50 $gO_2/m^2/day$) was significantly higher than the mean SOD computed with the best W2_SD model (Run 2) (0.810 $gO_2/m^2/day$). This can be explained by the fact that the W2_zero-order model SOD represents all of the reservoir's DO uptake rate in the water column and not just the sediment uptake. Overall, despite their limitations and assumptions, both models are capable of adequately reproducing the hydrodynamic and water quality dynamics of the reservoir. While not perfect, they effectively capture the main water quality trends given the current boundary conditions. It is important to stress the fact that this study did not set out to identify the best model overall but rather to evaluate the performance of the sediment diagenesis model. Specifically, we sought to determine whether this model could replicate dissolved oxygen (DO) profiles and perform comparably to the zero-order model.

The zero-order model employs a constant SOD value that only varies with water temperature and does not account for organic matter decay or its impact on SOD values. As a result, it cannot predict water quality trends since it is not integrated with the water column. Nevertheless, it can and was used to back-calculate the oxygen uptake rate in the water column. The fact that the reservoir's dissolved oxygen profiles matched the zero-order model SOD values used in calibration indicated that these values were close to the actual uptake rates of dissolved oxygen (Wells, 2011). Therefore, since the W2 model with the sediment diagenesis function performs similarly to the zero-order model in reproducing dissolved oxygen profiles under the same boundary conditions, it can be concluded that the sediment diagenesis function is performing accurately. This approach proved useful when it came to compensating for the uncertainty related to boundary condition limitations and all the assumptions made for the model's definition.

The W2_SD model includes a variable SOD computed from the sediment diagenesis model. In the best W2_SD model (Run 2), the SOD ranged from 0.013 to 4.110 $gO_2/m^2/day$ ($\mu = 0.810$; $\sigma = 0.659$). The SOD remained below 1 $g/m^2/day$ from

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December to April, increasing during the remaining months and peaking in September each year. These values are consistent with the SOD values obtained in other studies, such as those of Schnoor and Fruh (1979), which concluded that the SOD values of Lake Lydon B. Johnson (located in the U.S.) ranged from 1.7 to 5.8 $gO_2/m^2/day$, and of Beutel (2015), which measured SOD values in different locations around Lake Hodges (located in the U.S.) ranging from 0.6 to 2.3 $gO_2/m^2/day$. It would, however, be useful to be able to compare these results with SOD values measured at different sites within the Torrão reservoir. Additional SOD monitoring studies need to be conducted in lakes and reservoirs and be extended to other regions, also focusing on the chemical characterization of sediments and the definition of sediment burial rates.

The results also revealed that the particulate fraction of organic carbon in the reservoir sediments corresponded to 40% of the total organic carbon (TOC). This value is small compared to the results obtained for Taihu Lake by Yu et al. (2022), where the ratio of particulate organic phosphorus (POP) to TOC varied from 97.85% to 89.53%. However, this value (40%) was obtained indirectly through the analysis of the reservoir's predicted SOD values as a function of different initial POC values and may, therefore, reflect other sources of uncertainty, such as inflow organic matter characterization. Given the fact that the magnitude of TOC in the sediment can be affected by numerous factors, including water column productivity, terrestrial inputs of organic materials, sediment properties, and microbial activity rates (Gireeshkumar et al., 2013), and that, partly due to differences in reservoir productivity and morphology, the spatial distribution and sources of organic carbon vary greatly across regions (Anderson et al., 2009), it is reasonable to assume that the only way to accurately assess the POC prediction is by monitoring the reservoir POC content.

Furthermore, this project has highlighted a need to further expand the study to include other water bodies in different regions to enhance our understanding of the performance of the CE-QUAL-W2 diagenesis model and the significant heterogeneity of water body characteristics, as well as underlining the vital importance of establishing performance measures and evaluation criteria for daily water quality simulations in reservoirs and lakes.

5 Conclusions

The primary objective of this study was to evaluate the performance of the state-of-the-art CE-QUAL-W2 sediment diagenesis model. This evaluation was conducted by applying two different approaches to conceptualize the sediment compartment in the CE-QUAL-W2 model: a) incorporating a sediment diagenesis model, and b) using a zero-order model. The models were applied to the Torrão reservoir located in northern Portugal. Overall, the study's results clearly demonstrate that the CE-QUAL-W2 water quality model performed very well when coupled with the advanced sediment diagenesis model despite the poor characterization of the reservoir inflow water quality. The mean NSE and RMSE obtained for the reservoir water column DO were 0.41±0.67 and 1.73 mg/L±0.69, respectively. The results also suggest that the zero-order model can serve as a good starting point for applying the sediment diagenesis model, as it helps to define an initial threshold for the mean reservoir SOD value.

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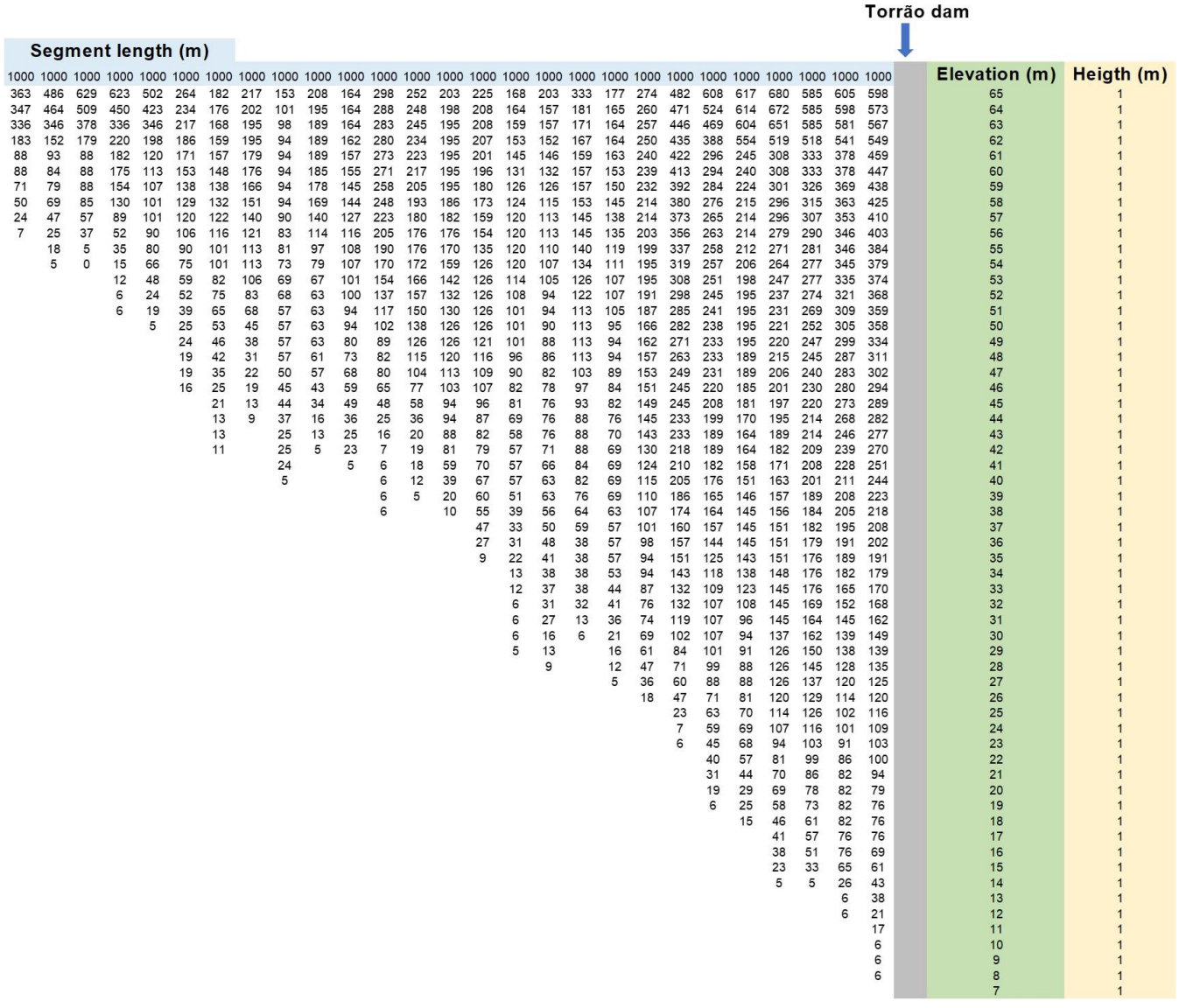
Appendix A



Segment length (m)																											Elevation (m)	Heigth (m)
1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000		
363	486	629	623	502	264	182	217	153	208	164	298	252	203	225	168	203	333	177	274	482	608	617	680	585	605	598	65	1
347	464	509	450	423	234	176	202	101	195	164	288	248	198	208	164	157	181	165	260	471	524	614	672	585	598	573	64	1
336	346	378	336	346	217	168	195	98	189	164	283	245	195	208	159	157	171	164	257	446	469	604	651	585	581	567	63	1
183	152	179	220	198	186	159	195	94	189	162	280	234	195	207	153	152	167	164	250	435	388	554	519	518	541	549	62	1
88	93	88	182	120	171	157	179	94	189	157	273	223	195	201	145	146	159	163	240	422	296	245	308	333	378	459	61	1
88	84	88	175	113	153	148	176	94	185	155	271	217	195	196	131	132	157	153	239	413	294	240	308	333	378	447	60	1
71	79	88	154	107	138	138	166	94	178	145	258	205	195	180	126	126	157	150	232	392	284	224	301	326	369	438	59	1
50	69	85	130	101	129	132	151	94	169	144	248	193	186	173	124	115	153	145	214	380	276	215	296	315	363	425	58	1
24	47	57	89	101	120	122	140	90	140	127	223	180	182	159	120	113	145	138	214	373	265	214	296	307	353	410	57	1
7	25	37	52	90	106	116	121	83	114	116	205	176	176	154	120	113	145	135	203	356	263	214	279	290	346	403	56	1
	18	5	35	80	90	101	113	81	97	108	190	176	170	135	120	110	140	119	199	337	258	212	271	281	346	384	55	1
	5	0	15	66	75	101	113	73	79	107	170	172	159	126	120	107	134	111	195	319	257	206	264	277	345	379	54	1
			12	48	59	82	106	69	67	101	154	166	142	126	114	105	126	107	195	308	251	198	247	277	335	374	53	1
			6	24	52	75	83	68	63	100	137	157	132	126	108	94	122	107	191	298	245	195	237	274	321	368	52	1
			6	19	39	65	68	57	63	94	117	150	130	126	101	94	113	105	187	285	241	195	231	269	309	359	51	1
				5	25	53	45	57	63	94	102	138	126	126	101	90	113	95	166	282	238	195	221	252	305	358	50	1
					24	46	38	57	63	80	89	126	126	121	101	88	113	94	162	271	233	195	220	247	299	334	49	1
					19	42	31	57	61	73	82	115	120	116	96	86	113	94	157	263	233	189	215	245	287	311	48	1
					19	35	22	50	57	68	80	104	113	109	90	82	103	89	153	249	231	189	206	240	283	302	47	1
					16	25	19	45	43	59	65	77	103	107	82	78	97	84	151	245	220	185	201	230	280	294	46	1
						21	13	44	34	49	48	58	94	96	81	76	93	82	149	245	208	181	197	220	273	289	45	1
						13	9	37	16	36	25	36	94	87	69	76	88	76	145	233	199	170	195	214	268	282	44	1
						13		25	13	25	16	20	88	82	58	76	88	70	143	233	189	164	189	214	246	277	43	1
						11		25	5	23	7	19	81	79	57	71	88	69	130	218	189	164	182	209	239	270	42	1
								24		5	6	18	59	70	57	66	84	69	124	210	182	158	171	208	228	251	41	1
								5			6	12	39	67	57	63	82	69	115	205	176	151	163	201	211	244	40	1
											6	5	20	60	51	63	76	69	110	186	165	146	157	189	208	223	39	1
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														47	33	50	59	57	101	160	157	145	151	182	195	208	37	1
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															12	37	38	44	87	132	109	123	145	176	165	170	33	1
															6	31	32	41	76	132	107	108	145	169	152	168	32	1
															6	27	13	36	74	119	107	96	145	164	145	162	31	1
															6	16	6	21	69	102	107	94	137	162	139	149	30	1
															5	13		16	61	84	101	91	126	150	138	139	29	1
																9		12	47	71	99	88	126	145	128	135	28	1
																		5	36	60	88	88	126	137	120	125	27	1
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																				23	63	70	114	126	102	116	25	1
																				7	59	69	107	116	101	109	24	1
																				6	45	68	94	103	91	103	23	1
																					40	57	81	99	86	100	22	1
																					31	44	70	86	82	94	21	1
																					19	29	69	78	82	79	20	1
																					6	25	58	73	82	76	19	1
																						15	46	61	82	76	18	1
																							41	57	76	76	17	1
																							38	51	76	69	16	1
																							23	33	65	61	15	1
																							5	5	26	43	14	1
																									6	38	13	1
																									6	21	12	1
																										17	11	1
																										6	10	1
																										6	9	1
																										6	8	1
																											7	1

Figure A1: CE-QUAL-W2 bathymetry - Cross section of the Tâmega River with the average segment width

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Table A1. Model metrics. Characterization of Tâmega river inflow

Constituent	Model	R^2	PBIAS	RMSE	MAE	Input features	Input sample number	Sample Time period
Water temperature	LOADEST	0.81	5.14	2.61	1.86	Flow; AirT; WT	21	2016-2021
	XGBOOST	0.85	0.76	2.19	1.76	Air T; WT		
	SVR	0.87	3.77	2.07	1.60	Air T; WT		
DO	LOADEST	0.11	5.02	1.32	1.03	Flow, DO	78	2010-2021
	XGBOOST	0.83	1.50	0.56	0.33	WT; DO; Month		
	SVR	0.91	0.92	0.40	0.26	WT; DO; Month		
Total P	LOADEST	0.21	7.11	0.02	0.01	Flow, Total P	47	2010-2021
	XGBOOST	0.12	-	45.72	32.73	WT; Total P; Month		
	SVR	-	-	38.74	38.74	WT; Total P; Month		
$N\text{-}NH_4$	LOADEST	0.11	43.64	0.02	0.02	Flow; $N\text{-}NH_4$	46	2010-2021
	XGBOOST	0.26	32.20	0.02	0.02	WT; $N\text{-}NH_4$; Month		
	SVR	0.03	28.27	0.02	0.02	WT; $N\text{-}NH_4$; Month		
$N\text{-}NO_X$	LOADEST	0.11	10.88	0.18	0.14	Flow; $N\text{-}NO_X$	63	2010-2021
	XGBOOST	0.15	3.92	0.16	0.12	WT; $N\text{-}NO_X$;Month		
	SVR	0.26	7.48	0.16	0.13	WT; $N\text{-}NO_X$;Month		
BOD_5	LOADEST	0.19	6.93	0.98	0.83	Flow; BOD_5	77	2010-2021
	XGBOOST	-	782.16	16.31	16.28	WT; BOD_5; Month		
	SVR	0.14	1438.34	30.64	29.93	WT; BOD_5; Month		
Chlorophyll-a	LOADEST	0.65	30.00	6.27	4.96	Flow; Chl-a	49	2010-2021
	XGBOOST	0.12	774.02	39.12	29.36	WT; Chl-a; Month		
	SVR	0.02	345.72	15.05	13.25	WT; Chl-a; Month		
Alkalinity	LOADEST	0.26	17.44	6.59	6.30	WT; Chl-a; Month	31	2013-2021
	XGBOOST	0.26	471.67	88.57	57.64	WT; Alkalinity;		
	SVR	0.20	242.35	37.97	30.52	WT; Alkalinity;		
Conductivity	LOADEST	0.80	8.23	8.81	7.69	Flow; Conductivity	77	2010-2021
	XGBOOST	0.32	184.79	133.16	120.16	WT; Conductivity;		
	SVR	0.02	17.67	21.96	17.32	WT; Conductivity;		
TSS	LOADEST	0.00	11.86	1.83	1.45	Flow; SST	78	2010-2021
	XGBOOST	0.19	7.06	1.96	1.38	WT; SST; Month		
	SVR	0.24	8.44	1.62	1.24	WT; SST; Month		

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Table A2. Metrics between observed and predicted values for both models. The predicted values were compared with observed values at three different depths: (a) an integrated sample between the reservoir surface and an average depth of 5.8 meters, (b) an average depth of 23 meters, and (c) an average depth of 43.7 meters. The values shown in this table represent the mean value of the metrics obtained for each date and the corresponding standard deviation.

Constituent	W2_SD model (run 5 - baseline)			
	R^2	PBIAS	RMSE	MAE
Water temperature	0.56±0.13	-0.11±0.71	3.51±0.32	1.56±0.10
DO	0.55±0.31	-8.26±14.70	1.79±0.63	1.34±0.47
Total N	0.03±0.03	-13.46±14.10	0.37±0.03	0.29±0.03
Total P	0.16±0.08	-3.98±34.11	0.02±0.02	0.01±0.01
BOD5	0.03±0.01	-1.46±20.17	0.52±0.17	19.58±0.14
Chl-a	0.01±0.01	87.44±43.14	13.43±12.81	11.16±9.69
Constituent	**W2_zero-order model (SOD = 2.5 g O2/m2/day - baseline)**			
	R^2	PBIAS	RMSE	MAE
Water temperature	0.56±0.13	-0.12±0.80	3.51±0.32	1.57±0.10
DO	0.54±0.31	-4.77±15.52	1.62±0.73	1.20±0.55
Total N	0.30±0.07	-4.19±44.37	0.64±0.45	0.45±0.22
Total P	0.18±0.07	74.68±89.24	0.06±0.07	0.04±0.04
BOD5	0.01±0.01	-0.73±18.73	0.55±0.22	19.73±0.17
Chl-a	0.00±0.00	190.46±183.89	15.84±12.80	12.11±10.90

Table A3. Root mean square error values obtained with different models and across different time frames

Constituent	Model	Simulation	RMSE	Author
Water temperature	CE-QUAL-W2		2.95 ºC	Deliman et al., 2002
	CE-QUAL-W2		1.93 ºC	Kim and Kim, 2006
	CE-QUAL-W2		0.56 ºC	Zhang et al., 2015
	CE-QUAL-W2		< 2.0 ºC	Lindenschmidt et al., 2019
	Delft3D-FLOW	2015-2017	0.96 to 1.0ºC	Piccioni, et al. 2020
	CE-QUAL-W2	2001-2011	1.80 ºC	Brito et al., 2018
	CE-QUAL-W2	2010	2.36 ºC	Liu et al., 2019
	MINLAKE2020	2-4 years	1.51 ºC	Tasnim et al., 2021
	CE-QUAL-W2	2000-2019	3.01-3.17 ºC	Almeida et al., 2023
DO	CE-QUAL-W2		1.34 mg/l	Deliman et al., 2002
	CE-QUAL-W2		0.61 mg/l	Zhang et al., 2015

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	CE-QUAL-W2	2001	1.2 mg/l	Brett et al., 2016
	CE-QUAL-W2	2001-2011	7.6 mg/l	Brito et al., 2018
	DYRESM 4.0	2009-2011	1.78 mg/l	Luo et al., 2018
	MINLAKE2020	2-4 years	2.33 mg/l	Tasnim et al., 2021
	CE-QUAL-W2	2000-2019	2.22-3.46 mg/l	Almeida et al., 2023
Total P	CE-QUAL-W2	2001	0.012 mg/l	Brett et al., 2016
	CE-QUAL-W2	2005-2010	0.014 to 0.068 mg/l	Kim et al., 2019
	MINLAKE2020	2-4 years	0.005 to 0.036 mg/l	Tasnim et al., 2021
	CE-QUAL-W2	2000-2019	0.07-0.09 mg/l	Almeida et al., 2023
Total N	CE-QUAL-W2		0.77 mg/L	Deliman et al., 2002
BOD_5	CE-QUAL-W2	2000-2019	3.06-4.83 mg/l	Almeida et al., 2023
	CE-QUAL-W2		1.08 µg/l	Zhang et al., 2015
Chl-a	CE-QUAL-W2	2001	4.6 µg/l	Brett et al., 2016
	CE-QUAL-W2	2005-2010	6.7 to 13.2 µg/l	Kim et al., 2019
	CE-QUAL-W2	2001-2011	62.9 µg/l	Brito et al., 2018
	MINLAKE2020	2-4 years	0.6 - 27.6 µg/l	Tasnim et al., 2021
	CE-QUAL-W2	2000-2019	19.36-25.57 µg/l	Almeida et al., 2023

Table A4. Metrics between observed and predicted values for W2_SD model (Run 2). Water temperature and DO metrics were obtained from 36 observed and predicted profiles. The predicted values for the remaining constituents were compared with observed values at three different depths: (a) an integrated sample between the reservoir surface and an average depth of 5.8 meters, (b) an average depth of 23 meters and (c) an average depth of 43.7 meters. The values in this table represent the mean value of the metrics obtained at each date and the corresponding standard deviation or, in the case of water temperature and DO, the mean value of the metrics obtained for each profile and the standard deviation.

Constituent	**W2_SD model (Run 2)**			
	R^2	**PBIAS**	**RMSE**	**MAE**
Water temperature	0.56±0.13	-0.22±0.87	3.51±0.32	1.58±0.08
DO	0.53±0.30	0.93±16.44	1.73±0.69	1.33±0.56
Total N	0.03±0.03	-13.64±15.67	0.37±0.03	0.29±0.04
Total P	0.17±0.08	-3.98±34.46	0.02±0.02	0.01±0.01
BOD5	0.03±0.01	-3.61±19.35	0.51±0.18	19.70±0.15
Chl-a	0.01±0.01	85.06±42.15	13.26±12.65	11.11±9.77

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Code availability

The exact version of the models' source code is archived on Zenodo at https://doi.org/10.5281/zenodo.14606105 (Almeida and Coelho 2025). The current version of the open-source CEQUAL-W2 model (version 4.5) used in this study is also available from the project website (http://www.ce.pdx.edu/w2/, last access 24 January 2024).

Data availability

Input files needed to run the models' and the hydrometric water quality and meteorological datasets used to force and validate each model are freely available and are archive on Zenodo at https://doi.org/10.5281/zenodo.14606105 (Almeida and Coelho 2025).

Competing interests

The contact author has declared that none of the authors has any competing interests.

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Author contribution: MA conceptualized the study, developed the methodology, and handled software and data curation, as well as writing the original draft. PC administered the project and contributed to reviewing and editing the manuscript

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