

Numerical Modeling of Reaeration Coefficient for Lakes – A Case Study of Sawa Lake, Iraq

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ABSTRACT

Accurate determination of reaeration coefficient in lakes is a key factor for accurate modeling of dissolved oxygen. This study developed a new numerical model to determine the lake reaeration coefficient of Sawa lake, Iraq based on solving the transform mechanisms of dissolved oxygen without the using the empirical and laboratory methods. The model solved the gas transport at the water-air surface numerically to predict the dissolved oxygen and the reaeration coefficient simultaneously. Results showed that the lake reaeration coefficient was 0.001 day^{-1} at 20°C with low root mean squared errors (0.138, 0.137, and 0.168 mg/L for the three years of simulation 2007, 2012, and 2017, respectively) and absolute mean errors (0.121, 0.114, and 0.145 mg/L in 2007, 2012, and 2017, respectively). It was noticed that the lake habitat was impacted causing unhealthy conditions (low reaeration rate), and there was upward dissolved oxygen movement due to the presence of positive trend in the yearly cycle of temperature. In addition, including this numerical approach along with other water quality models can improve the predictions of other water quality parameters.

Keywords: dissolved oxygen modeling, lake ecosystems, numerical modeling, oxygen reaeration, reaeration coefficient, Sawa Lake, water quality modeling.

INTRODUCTION

Dissolved oxygen concentration (DO) is considered as an indicator for the health of lakes. The dominant reaeration in lakes is by wind shear, rather than boundary shear in rivers (Cole and Wells, 2006). Many models have been developed for calculating the reaeration in lakes in addition to those developed for calculating river reaeration (Al-Zubaidi and Wells 2020; Al Mamun and Nuruzzaman 2023). These models were developed based on the data collected at the model study location and have been used for other locations widely. In addition, wind speed data at a specific height

is required in order to determine the reaeration coefficient in lakes using such models. Ranjith et al. (2019) used many empirical equations to calculate the reaeration rate coefficient of the Tungabhadra River, India, in order to evaluate the river dissolved oxygen. These equations are all related to stream variables, such as river slop, depth, and velocity. The evaluation method was based on solving the biochemical oxygen demand decay model as well as Streeter and Phelps model simultaneously at specified points along the river. It was found that one of the empirical equations was best in demonstrating this river reaeration case based on statistical errors, and it was recommended to use this

equation for other rivers of similar conditions. Hence, this method requires solving analytical two models at many field points and trying to calculate the reaeration rate coefficient from many equations at each point. Peña-Guzmán et al. (2021) evaluated many well-known reaeration coefficient equations for the rivers located in Colombia. The evaluation method was based on calculating the reaeration directly from the equations after collecting the river conditions, and then the statistical frequency as well as principal component analysis were performed to group the consistence equations, since each equation gives a different coefficient value from the other. The analyses revealed that the reaeration rates are influenced by the river depth and velocity. The fact that the water velocity decreases more quickly as the water depth increases suggests that reaeration rates are highly sensitive to these two hydraulic variables, particularly the depth of the water. Ashok and Keshari (2018) used a statistical approach to estimate the re-aeration coefficient of the Yamuna River by employing the multivariate linear regression (MLR) based on both hydraulic and water quality parameters. Field data of five years were used to develop five models. To determine the best fit model, the model performance was assessed using root mean squared error (RMSE) and R-squared. The most accurate correlation between the observed and predicted re-aeration coefficient was produced, according to the results, by the MLR model that was developed using the river hydraulics and water quality parameters. The results indicated that MLR may be a useful tool for reaeration coefficient modeling. In this study, the best fit model yielded a correlation coefficient of 0.896 1/day. However, none of the previously developed equations are able to calculate the reaeration coefficient accurately, and it was indicated that extra parameters should be taken into account to improve the modeling predictions. Thus, it is necessary to find a simple way to determine an accurate reaeration coefficient values depending on the dissolved oxygen transport mechanisms itself, instead of using the empirical equations. Therefore, this paper developed a new numerical approach to determine the reaeration coefficient along with the predicted dissolved oxygen concentration in lakes without using the empirical equations or laboratory methods.

MATERIALS AND METHOD

Study location and data

This study was carried out on Sawa Lake, Iraq (N 31°18' and E 45°00'). Sawa Lake is a natural salt lake with an approximate area of 5.1 km², water depth of about 3.0–5.5 m, and bottom elevation of about 3.0–5.5 m above sea level. Detailed descriptions of the lake can be found in Ziyadi et al. (2015). Figure 1 shows the Sawa Lake map, downloaded from Landsat 8 OLI/TIRS Level-2 Data Products (WRS path/row: 168/038; acquired on 3rd June 2021). The lake is located within a salty region and has an approximate total dissolved solids (TDS) of 35000 mg/L (Boschetti et al., 2018). No inflows or outflows exist except by rainfall, evaporation, or ground water. Because the lake location is close to the Euphrates River (about 22 km to the east of the lake), the river is considered a source for the ground water that feeds the lake (Al-Handal et al., 2014). A few kinds of fish exist, in addition to some algae species and phytoplankton (Awadh and Muslim 2014; Hassan et al., 2006; Mohammad 2005). The lake serves as a recreation area used by the visitors (mainly from the surroundings) for hunting, fishing, and other human activities, making the lake under environmental concerns that have recently been highlighted and pushed the researchers to study the lake ecosystem deeply. The monthly time series of dissolved oxygen concentration (DO) and temperature (T) were measured and recorded for the sampling locations (Fig. 1)

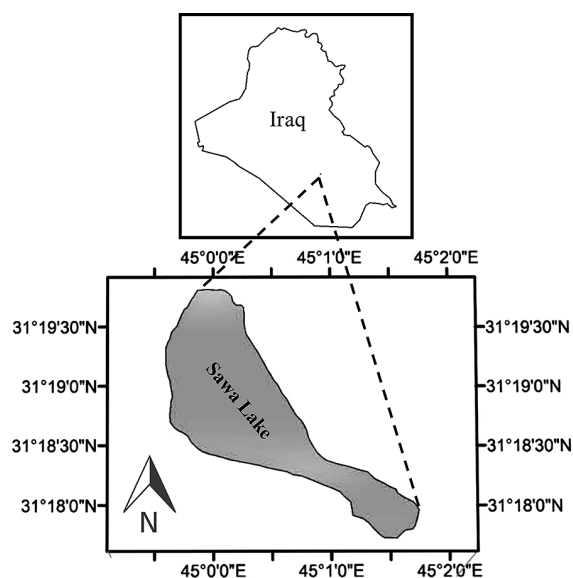


Fig. 1. Sawa Lake map

by the Iraqi Ministry of Health and Environment. Three datasets during 2007, 2012, and 2017 were available for this study. The data was collected from many locations throughout the lake on the fifteenth of each month and averaged. Figures 2 and 3 show the dissolved oxygen concentrations and water temperature time series datasets used to determine the reaeration coefficient for the considered period of time.

Development of the dissolved oxygen numerical model

The reaeration coefficient for the Sawa Lake was determined numerically by using the available time series of dissolved oxygen and temperature. Before illustrating the determination procedure, the following assumptions were made in order to simplify the problem. The only source-sink of dissolved oxygen is due to reaeration through the lake waterbody surface. The lake is well-mixed (the mass transport by advection and diffusion is neglected anywhere in the lake). On the basis of on the assumptions above, the dissolved oxygen concentration varies temporally, as shown below:

$$\frac{dC}{dt} = R_{DO} \tag{1}$$

where: C is the dissolved oxygen concentration in mg/L, t is the time in days, and R_{DO} is the dissolved oxygen source-sink term in mg/L/Day.

Chapra (2008) expressed the dissolved oxygen source-sink for the reaeration process between water surface and air as:

$$R_{DO} = ka_{(T)}(C_s - C) \tag{2}$$

where: $ka_{(T)}$ is the reaeration coefficient for oxygen in Day⁻¹ at any temperature (T), and C_s is the saturated dissolved oxygen concentration in mg/L.

Following Mortimer (1981), Cole and Wells (2006), and Al-Zubaidi (2018), the saturation dissolved oxygen was determined using the following formula:

$$C_s = P \cdot e^{[7.7117 - 1.31403 \ln(T + 45.93)]} \tag{3}$$

where: P is a correction factor for the waterbody elevation (ELV).

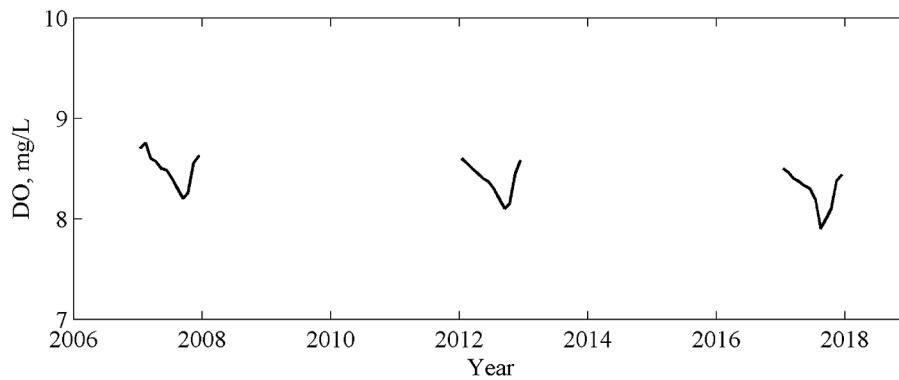


Fig. 2. Dissolved oxygen time series data of Sawa Lake

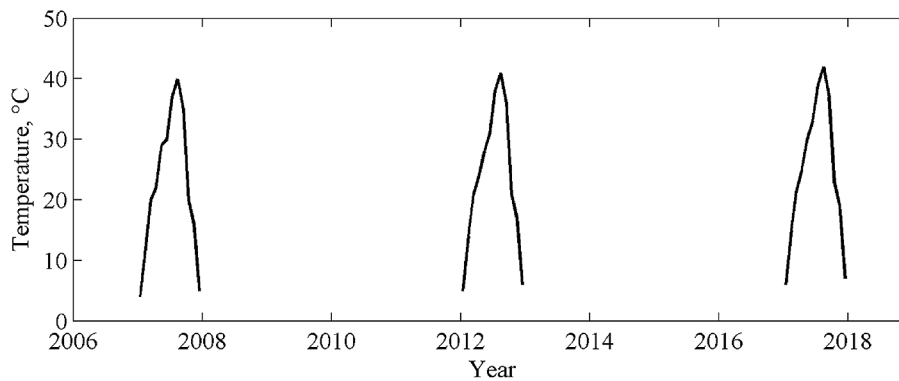


Fig. 3. Water temperature time series data of Sawa Lake

$$P = \left[1 - \frac{ELV}{44.3} \right]^{5.25} \quad (4)$$

ELV presents the waterbody height above sea level in kilometers. Temperature impacts the reaction rates in natural waters and also impacts the molecular diffusivity of oxygen. To include the effect of water temperature change on the lake reaeration process and to improve the numerical calculations, since both dissolved oxygen and temperature are time dependent variables according to lake raw dataset, the reaeration coefficient was modified based on the Arrhenius equation by using a temperature rate multiplier (Chapra 2008). This approach provides a linkage between the two variables in the model, reflecting the real situation of the lake. Because most reactions in water quality modeling are reported at 20 °C, the temperature rate multiplier equation is usually described as follows:

$$ka_{(T)} = ka_{(20)}\theta^{(T-20)} \quad (5)$$

where: $ka_{(T)}$ is the reaeration coefficient at any temperature (T), $ka_{(20)}$ is the reaeration coefficient at 20 °C, and θ is a coefficient (1.024 for oxygen reaeration).

Thus, by combining Eq. 1 through (5), the final governing equation of dissolved oxygen for the Lake can be written as:

$$\frac{dC}{dt} = ka_{(20)}\theta^{(T-20)}(C_s - C) \quad (6)$$

Or simplified further to show that the temporal variation of dissolved oxygen in the lake at any time (t) is a function of dissolved concentration C(t) itself and temperature T(t) at that time (t):

$$\frac{dC}{dt} = f(C, T) \quad (7)$$

where: $f(C, T)$ is the right-hand side of Eq. 6.

Numerically, Eq. 7 can be discretized as

$$C(t + \Delta t) = C(t) + \Delta t f(C(t), T(t)) \quad (8)$$

where: Δt is the numerical computations time step.

Equation 8 is the final dissolved oxygen numerical model that was used to determine the lake reaeration coefficient at 20 °C based on DO and T temporal dataset. A code was written within the Matlab environment to apply Eq. 8 and fit the final model among the available dataset using different

ka values to determine the appropriate one for the Sawa Lake case study.

The model performance was measured through the root mean squared error (RMSE) and the absolute mean error (AME), Eq. 9 and Eq. 10, respectively (Al-Dalimy and Al-Zubaidi, 2023).

$$RMSE = \sqrt{\frac{\sum_1^N (DO_{model} - DO_{data})^2}{N}} \quad (9)$$

$$AME = \frac{\sum_1^N |DO_{model} - DO_{data}|}{N} \quad (10)$$

where: N is the number of observations, DO_{model} is the calculated dissolved oxygen by the model, and DO_{data} is the measured values of dissolved oxygen.

The former gives an idea of how the data points spread around the model. Zero value means the model passes through all data points (no error). As *RMSE* goes higher, the model predictions agree less with data, see Wagner et al. (2011). The latter gives an indication to the model performance since it interprets the model directly (Cole and Wells 2006).

RESULTS AND DISCUSSION

The numerical determinations of reaeration coefficient

The monthly water temperature and dissolved oxygen time series plots show strong yearly cycles, as well as monthly and yearly trend in which the dissolved oxygen goes down as the water temperature goes up. The correlation plot in Figure 4 displays the strong negative correlation (a Pearson correlation coefficient of 0.73) between temperature and dissolved oxygen in Sawa Lake during the three years of recorded data. In addition, no outliers exist, see the graphical summary (boxplots) of the two variables in Figure 5. Thus, choosing ka values must satisfy the periodic behavior of dissolved oxygen dynamics including the water temperature influence.

The dissolved oxygen model in Eq. 8 was run using a high resolution time step of 0.01 day to improve the numerical determinations. Figures 6, 7, and 8 present the calibration results of the dissolved oxygen model during 2007, 2012, and 2017, respectively. In the plots, the dissolved

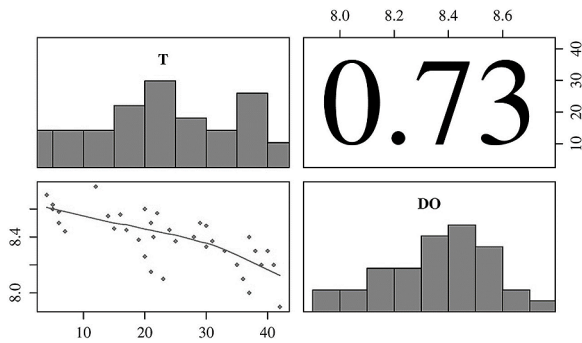


Fig. 4. Temperature and dissolved oxygen correlation in Sawa Lake during 2012, 2012, and 2017

oxygen datasets were temperature scaled during the annual cycles. Different values of k_a were used to calibrate the model. It was found that a k_a value of 0.001 Day^{-1} at 20°C simulates the three years with well-predicted dissolved oxygen concentrations. Clearly, the model captured the annual cycles of the dependent variable. As

temperature goes higher during the hot season in summer (large size circles in Figures 6, 7, and 8), the dissolved oxygen goes down. The model performance was very robust with low RMSEs (0.138 , 0.137 , and 0.168 mg/L for the three years 2007, 2012, and 2017, respectively). This shows the model prediction magnitudes were robust. Furthermore, the model accounts for lake stratification during the simulation periods, following the observed trend in datasets (an absolute mean error of 0.121 , 0.114 , and 0.145 mg/L in 2007, 2012, and 2017, respectively).

The yearly cycles of reaeration coefficient and dissolved oxygen mass transfer

Because the lake is almost a closed system, the effect of dynamics (except the dissolved oxygen exchange with air at the lake surface) was not included in the model. This is a major concern in water quality numerical models due to the

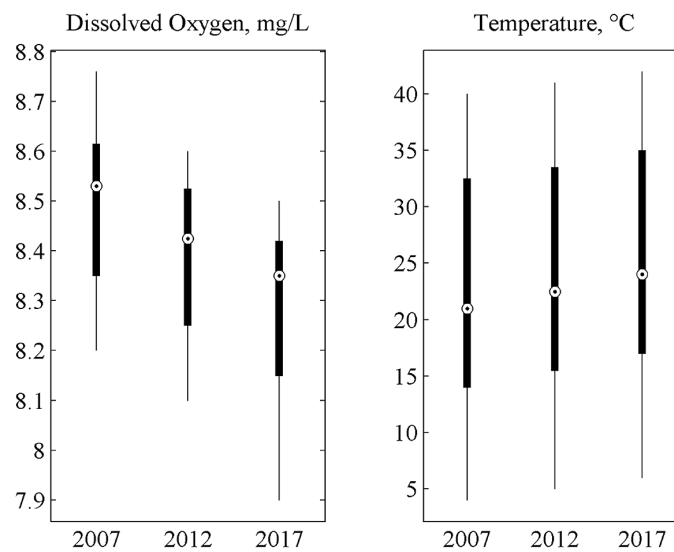


Fig. 5. Dissolved oxygen and water temperature graphical summarization of Sawa Lake

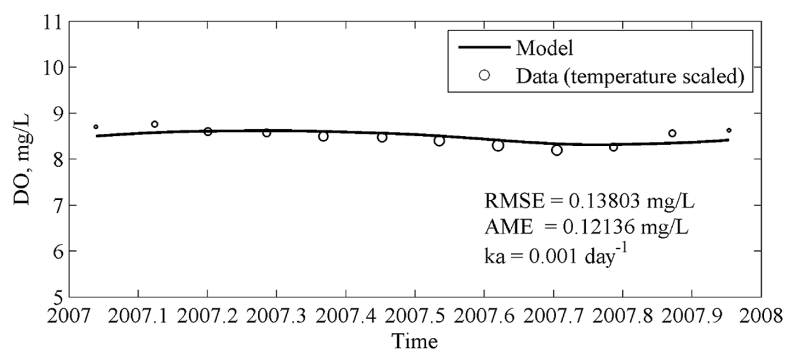


Fig. 6. Numerical results of k_a in 2007

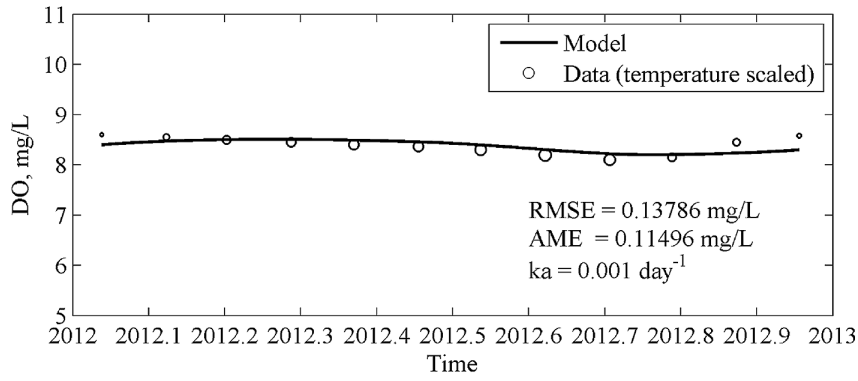


Fig. 7. Numerical results of ka in 2012

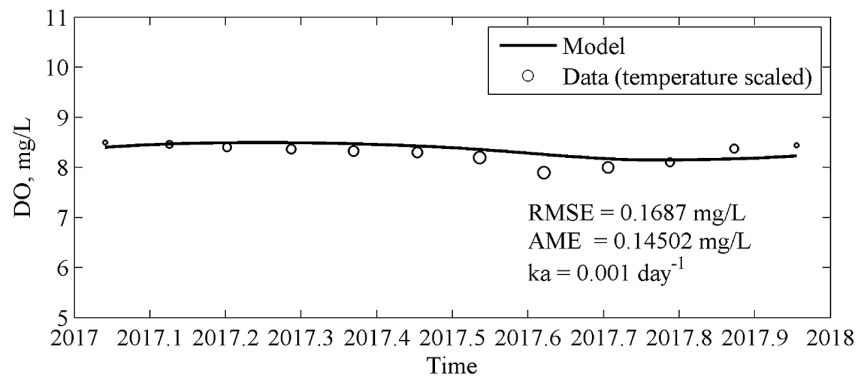


Fig. 8. Numerical results of ka in 2017

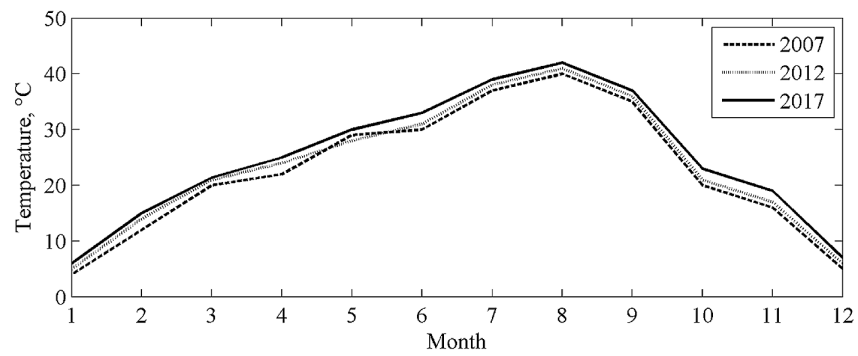


Fig. 9. Yearly cycles of water temperature at Sawa Lake

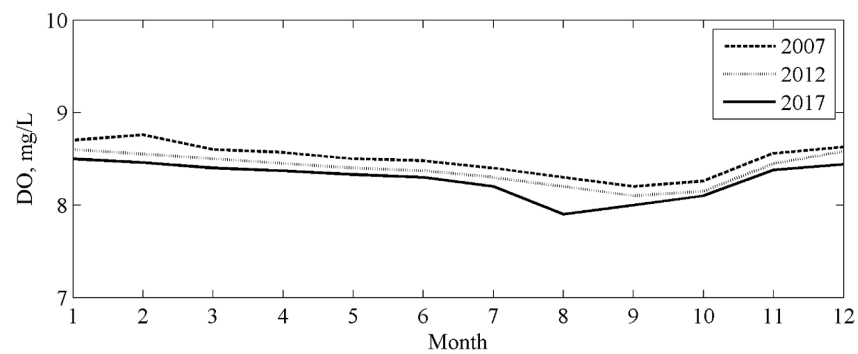


Fig. 10. Yearly cycles of dissolved oxygen at Sawa Lake

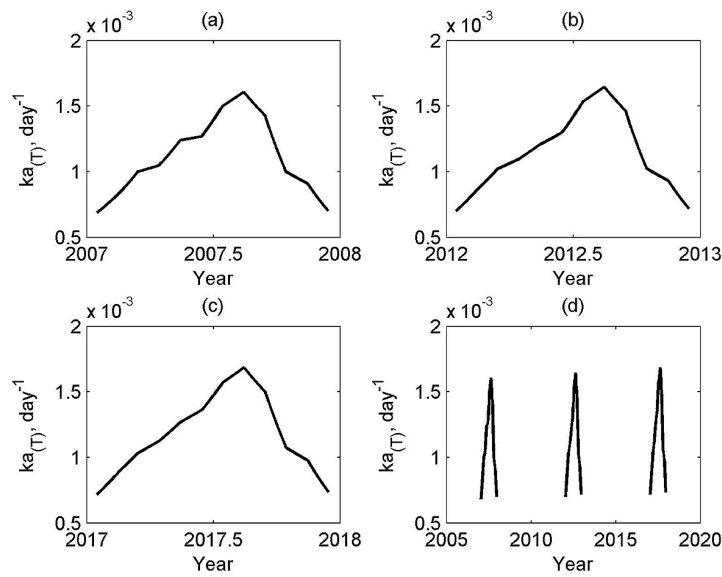


Fig. 11. Model yearly cycles of reaeration coefficient in Sawa Lake: a – during 2007, b – during 2012, c – during 2017, and d – during 2007, 2012, and 2017

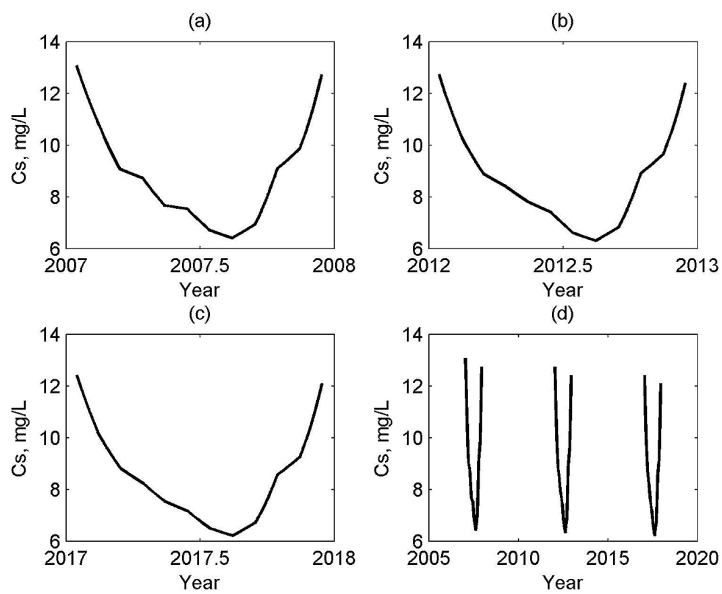


Fig. 12. Model yearly cycles of saturated dissolved oxygen in Sawa Lake: a – during 2007, b – during 2012, c – during 2017, and d – during 2007, 2012, and 2017

difficulties in representing the inflows and outflows exactly. However, the model predicts dissolved oxygen annual cycles as well as capturing the increase in water temperatures contained in the record of Sawa Lake regime during the summer seasons. On the basis of the lake temperature record, the average lake temperature increased from 2007 to 2017 slightly (Figure 9 shows that yearly temperature cycles have the same tendency with different amplitudes). Certainly, this increase has a reverse impact on dissolved oxygen

in the lake (Figure 10). In terms of air-water exchange, the reaeration-temperature dependence applied by the model was used to retrieve the lake reaeration coefficient as a function of temperature. The model results in Figure 11 is the yearly cycles of reaeration coefficient in the lake. The coefficient increased positively from 2007 to 2017 due to an equivalent increase in water temperature. The maximum coefficient occurred during the hot season in summer, while the minimum was in winter season. This made the oxygen

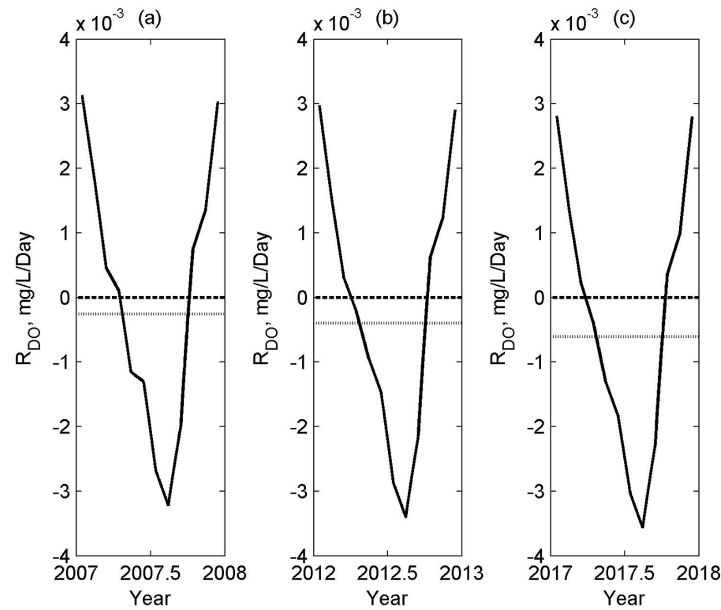


Fig. 13. Model yearly cycles of dissolved oxygen source-sink in Sawa Lake: the dashed line represents the dissolved oxygen source-sink under equilibrium conditions, while the dotted line represents the mean amount of dissolved oxygen source-sink

transfer rate higher during summer (loss) and lower during winter (gain), reducing the presence of dissolved oxygen during summer and increasing the dissolved oxygen during winter.

The dissolved oxygen mass transfer analysis

Beside the model's ability to retrieve the temporal variation of reaeration coefficient numerically, the model can predict the saturation value of dissolved oxygen as a function of time. Figure 12 shows the model predictions of oxygen saturated values. The values vary negatively with years. This behavior has an influence on the mass transfer magnitude and direction, see Eq. 2. In other words, the mass transfer magnitude and direction depend on the saturated and actual dissolved oxygen value in the water at a given temperature. For the unsaturated conditions ($C_s > C$), oxygen moves outside the lake through the air-water interface. On the other hand, oxygen transfers into water during the saturated conditions ($C_s < C$). Since temperature yearly cycle increased from 2007 to 2017 (Fig. 10), the oxygen transfer direction was upward (Fig. 11). This was confirmed by the model, as shown in Figure 13 in terms of mass transfer rate per unit volume. The positive y-axis represents the dissolved oxygen source, whereas the negative y-axis is its sink. In the model, the source-sink balance was controlled

by temperature and dissolved oxygen saturation conditions. As a result, the oxygen mass transfer rate increased from 2007 to 2017, see the dotted line in Figure 13. Thus, the health of the Sawa Lake aquatic ecosystem has a decreasing trend with time due to oxygen loss in the lake system.

CONCLUSIONS

A novel simplified numerical model was developed to determine the reaeration coefficient in lakes using temporal datasets of dissolved oxygen and temperature from the Sawa lake, Iraq, taking into account the effect of water temperature variation over time. Running the model based on the highly correlated dissolved oxygen and temperature datasets showed that the reaeration coefficient has a value of 0.001 day^{-1} at 20°C in the lake. This low value is compatible with the dissolved oxygen levels over time since the dissolved oxygen yearly cycles are under the saturated level during the simulation years. The low water-air exchange in the lake forces the unhealthy dominant conditions that impact the lake habitat. In addition, the model is capable of displaying the dissolved oxygen transfer rate and direction graphically. As the temperature trend in the lake is positive, upward dissolved oxygen movement exists, confirming the unhealthy situation of the lake. Finally, linking

the developed model with other water quality and dynamic models provides robust prediction of the reaeration coefficient based on real data instead of using the reaeration coefficient empirical models.

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