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Numerical Simulation of Dissolved Oxygen and Reaeration Coefficients in the Hilla River at Saddat Al-Hindiyah Reservoir, Iraq

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ABSTRACT

Dissolved Oxygen (DO) reaeration rate amount is an important indicator for measuring water quality and ecosystem health in water bodies. In this study, a model was developed to simulate the DO reaeration rate coefficient (Ka) temporal distribution for the Hilla River headwater at the Saddat Al-Hindiyah Reservoir, Iraq. The DO transfer rate at the reservoir water surface was determined uniquely by implementing the explicit forward time numerical scheme to simulate the Ka variation along with DO based on monthly field measurements of DO and temperature during the study years (2021 and 2022). With low statistic errors, the results showed that there is good agreement between the DO numerical determination, field data and the analytical solution, giving headwater reaeration coefficient value of 0.1 day^{-1} at 20℃ and temporal values of (0.091- 0.128) day^{-1} and (0.086 - 0.128) day^{-1} during 2021 and 2022, respectively. The Ka temperature dependency, which is a direct relationship, led to high DO levels during winter and low during summer. Thus, it is necessary to vary Ka based on temperature for DO modeling applications, especially for water quality management purposes in rivers, lakes and reservoirs where Ka is variable during the year.

1. INTRODUCTION

Reaeration is a crucial process that controls the water body DO content by allowing oxygen to permeate the interface between the atmosphere and the water surface. The reaeration rate of surface water resources depends on the gas transfer mechanism at the water-air interface [1]. This rate decides the DO levels in waterbodies, impacting the natural aquatic habitats due to the interaction of DO with other water quality constituents. For this reason, DO monitoring by different modeling approaches are necessary [2-5]. Hence, the oxygen reaeration rate coefficient (Ka) is required for the numerical determination of DO in surface waterbodies. Different ways of different accuracies have been used to determine Ka in order to use it for DO predictions in surface waters. The determination process can be conducted empirically, experimentally, analytically, numerically, and combination of different approaches. As a result, the good choice of Ka determination method leads to proper model predictions of DO [6, 7].

Many studies have been performed to determine Ka in waterbodies. Chimezie et al. [8] predicted the reaeration coefficient empirically based on the flow characteristics (water depth and flow velocity) and known reaeration coefficient value for three different rivers. Using the available data, a new model was developed, called N-Model. Its results were compared with some existing empirical models to evaluate its suitability for use without vigorous laboratory work. It was found that the values of the reaeration coefficient for the N-Model were very close to the other models with very low error. In addition, the reaeration coefficient has a direct and opposite relationship with the stream velocity and water depth, respectively. Results showed that all the values of the reaeration coefficient that were obtained were low. This means highly polluted and unsafe water for drinking without being treated for human consumption. As a result, Ka values reflect the waterbody state of health. This empirical approach depends on the mean waterbody characteristics only and ignores other water quality constituents' interactions, giving a one single value of Ka. Akatah et al. [9] used the regression analysis method to model the reaeration coefficient for the Mmubete River, Nigeria. The regression analysis method is used with a focus on predicting the stream reaeration. The reaeration coefficient was determined using empirical models that were developed using the regression analytical approach. To calibrate the model, performance evaluation statistics, the root mean square error and the coefficient of determination were used. When conducting statistical analysis for the developed models results, it was found that the surface area, kinematic viscosity, dispersion coefficient, flow depth and velocity are hydrodynamic data that have a significant impact on the reaeration coefficient. The results revealed that three equations cab be used to calculate the reaeration coefficient based on the hydrodynamic data. The values of the reaeration coefficient were (2.4432 - 3.7568) day^{-1} in the wet season and (0.96 - 2.712) day^{-1} in the dry season. Where the value of the reaeration coefficient was from 1.983 to 3.088 day^{-1} depending on velocity and flow depth, 1.983 to 3.5065 day^{-1} depending on velocity, flow depth, dispersion coefficient, surface area, and kinematic viscosity, and 3.0221 to 4.1817 day^{-1} depending on velocity, flow depth, dispersion coefficient, and kinematic viscosity. This method needs an expensive machine learning effort with many samples to get good statistic errors. However, any sudden event related to the waterbody conditions might impact the model performance since it was built depending on train and test data of different conditions. Wu and Yu [10] simulated the dissolved oxygen transport numerically through the coupled Shallow Water Equation (SWEs) and Streeter Phelps model. The SWEs were adopted to calculate the waterbody level and velocity to be used to evaluate the DO distribution by the modified Streeter-Phelps model. In this technique, the two-film theory was implemented to simplify aeration process based on experimental data and small eddy concepts. This results in a reaeration coefficient equation following the small eddy and stationary reaeration model. The accuracy of the proposed model was verified by predicting the distribution of DO and comparing with the analytical results. Results showed that this numerical modeling can be used to investigate the DO distribution in the water body and helps decision-makers improve their self-purification and risk reduction plans. In this numerical calculation, it is required to solve the shallow water governing equations in order to determine Ka values from the two-film theory analytical formula. Hence, the determination approach is computationally expensive and hard to calibrate with real field data due to the hydrodynamic link existence. Ta Bui and Thi Nguyen [11] built an applied machine learning algorithm to determine the reaeration coefficient in the Ohio River, USA. This study relies mainly on water quality monitoring time series data to make predictions of water quality at fixed monitoring points. Streeter-Phelps model was conducted for monitoring the BOD/DO in the river to determine the water quality variation along the river, where the value of the reaeration coefficient was 0.12 day^{-1} according to the study area. To create a machine learning data set, the MIKE package is used in this study and then three different sets of data were created using reaeration coefficients of 0.1, 0.2, and 0.3 day^{-1} to be used in a separated python code. These groups gave three reaeration coefficients of 0.112089, 0.172470, and 0.31098 day^{-1}. The results showed the reaeration coefficients were calculated with an error of about 15%. Accordingly, this machine learning method results in an algorithm which can be applied to make predictions in similar conditions to the data used to train and test the model without taking into account the waterbody parameters variability such as during the extreme events. Nuruzzaman et al. [12] investigated the Pusu River's reaeration coefficient in Malaysia by using a novel laboratory technique. The chemical method by the conventional sampling and graphing technique was used to determine the reaeration rate. Samples were taken from the upstream and downstream points, and the dissolved oxygen concentration was subsequently measured. A nonlinear regression analysis was carried out using Excel environment in order to obtain an empirical equation for the reaeration coefficient. The Water Quality Analysis Simulation Program (WASP) was used to model the river dissolved oxygen, taking into account the appropriate reaeration coefficient for the river. The performance of the reaeration equations was evaluated during the calibration and validation process based on statistics errors, where the RMSE value was (0.083-0.067) mg/L and MAE value was (0.05-0.06) mg/L between the observed and predicted data. The results demonstrate that the most effective method for predicting DO exchange rate for the Puso River is the reaeration equation that combines velocity and depth with a reduction factor. Furthermore, the findings will support the simulation of DO concentrations in the dry season precisely in the river for various scenarios. However, an empirical model was developed based on a laboratory experiment designed for a specific study area of a specific waterbody characteristics.

Regarding the above reaeration rate calculation methods, these methods determined the Ka value once during the model simulation period rather than taking into account its temporal variability effects. However, it is necessary to determine the reaeration coefficient during the study simulation period in surface water quality modeling and mainly for dissolved oxygen modeling efficiently and simply. Therefore, the main objective of this research is to simulate the dissolved oxygen of the Hilla River headwater at Saddat Al-Hindiyah in Iraq by calculating the reaeration coefficient numerically based on a unique approach easy to apply and by considering its temporal variability. In addition, this reaeration rate determination way helps evaluate the ecosystem health level since DO is considered one of the main indicators in surface water quality.

2. MATERIALS AND METHODS

2.1 Study area and sampling

Saddat Al-Hindiyah is a reservoir located on the Euphrates River, south of the city of Al-Musayib, within the Babylon Governorate, Iraq (Figure 1). It is situated between, longitude (44°16′ 05.7") E and latitude (32°43' 55.5") N with an elevation of 31.4 m above sea level. It is considered the most important irrigation project and the oldest in Iraq. It nourishes agricultural lands in the governorates downstream the river. In addition, fish and other species grow within this headwater and transport to the river too. The reservoir is the only water resource that feeds the Hilla River and is considered its headwater. It was noticed that the reservoir has been receiving a considerable amount of sediments and floating plants coming with the reservoir inflows. The presence of these constituents has different drawbacks on the waterbody aquatic ecosystem health and the reservoir mountainous activity. As a result, any dissolved oxygen impact due to these constituents can be harmful to the river watershed ecosystem downstream and the reservoir itself.

Three sampling locations (S1, S2, and S3) at the Saddat AI-Hindiyah Reservoir as shown in Figure 1 were used to collect water temperature and DO dataset for the study period, during 2021 and 2022. This location is covering the entire study area. The first location (S1) is close to the dam, the second location (S2) is in the middle of the reservoir, and the third location (S3) is close to the inflow location. The collection process included taking three samples per month for each sampling location during the study period. All samples were tested by the Iraqi Ministry of Environment - Babylon Environment Directorate. Table 1 shows the monthly average water temperature and DO concentrations during the study period. It is clear that the relationship is inverse between DO and temperature. As the DO concentration increased from 5.85 to 10.15 mg/L in 2022 and from 7.05 to 11.3 mg/L in 2021, the temperature decreased from 30.5 to 13.9℃ in 2022 and from 30.5 to 16.057℃ in 2021. This dataset was used to calibrate and validate the numerical model.

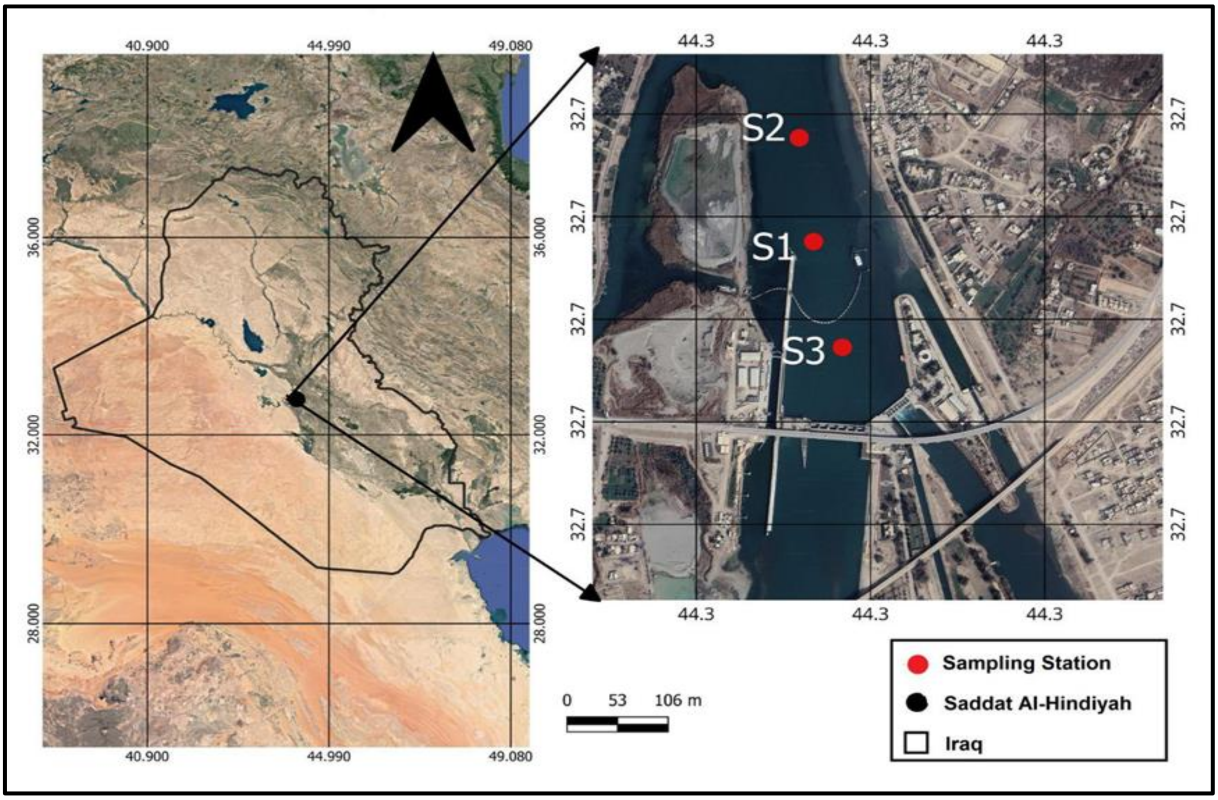

Figure 1. The location of study area and sampling stations

Table 1. Water temperature and DO levels at the Saddat Al-Hindiyah Reservoir

	2021		2022	
Month	DO, mg/L	T, °C	DO, mg/L	T, °C
January	8.8	17.1	10.15	13.9
February	8.125	19.4	9.75	17.45
March	9.3	17.75	9.42	22.8
April	9.125	23.1	7.45	24.7
May	8.95	28.9	8.2	25.7
June	7.65	26.4	7.15	28.05
July	7.1	30.5	5.85	30.5
August	8.125	30	6	30
September	7.05	29	6.65	29.5
October	7.2	24.68	7.9	26.75
November	7.9	20.37	6.8	21.5
December	8.7	16.057	6.85	18.2

2.2 Reaeration process modeling

A model was written within the Matlab environment in order to solve the governing and auxiliary equations numerically. Figure 2 depicts the numerical modeling approach toward calculating the reaeration coefficient of the Hilla River headwater. In this model, the DO governing equation was solved based on an assumed Ka value to be calibrated based on field data until getting the best matching between the predicted and measured DO values with less statistical errors. In addition, a comparison between the numerical solution and the analytical solution was performed for the model robustness assessment.

The general one-dimensional advection diffusion equation (Eq. (1)) that governs the DO transport in surface water bodies is as follows [13]:

$$\frac{\mathrm{dDO}}{\mathrm{dt}} + \mathrm{u}\frac{\mathrm{dDO}}{\mathrm{dx}} = \mathrm{D}\frac{\mathrm{d^2DO}}{\mathrm{dx^2}} + \mathrm{S} \tag{1}$$

where, DO is the dissolved oxygen concentration at any time at any distance (mg/L), t is time (sec), x is the distance (m), u is the velocity along x-axis (m/sec), D is the diffusion coefficient (m^2/sec), and S is the dissolved oxygen source-sink term (mg/L/sec).

Assuming a well-mixed water body, zero advection and diffusion, and reaeration source-sink only for DO, and

$$S = Ka(DO_s - DO) \tag{2}$$

where, DO_s is the saturated dissolved oxygen concentration (mg/L), DO is concentration of dissolved oxygen in water (mg/L), and Ka is the reaeration coefficient for oxygen at any temperature (sec^{-1}).

The explicit forward time numerical solution of Eq. (1) will be as follows:

$$\frac{DO^{n+1} - DO^{n}}{\Delta t} = Ka\,(DO_s - DO^{n}) \tag{3}$$

$$DO^{n+1} = DO^{n} + [Ka\,(DO_s - DO^{n})]\Delta t \tag{4}$$

where, DO^{n+1} and DO^{n} are DO values at the new and old time level (n), respectively, and Δt is the time step (sec).

Usually, Ka is measured at 20°C. Therefore, Ka can be calculated based on 20°C using Arrhenius equation specifications $Ka = Ka_{(20)}\,(1.024)^{(T-20)}$ [1-14].

In addition, DO_s can be calculated using the following [15]:

$$DO_s = A \cdot e^{[7.7117-1.31403\,ln(T+45\cdot 93)]} \tag{5}$$

$$A = B\left[1 - \frac{h}{44.3}\right]^{5.25} \tag{6}$$

where, B is a calibration factor by which DO measured and calculated values can be validated if necessary, and A is a correction factor for the elevation of the water body above sea level (h), h must be in Kilometers.

Furthermore, the numerical model was verified by performing comparisons with the analytical solution as follows:

$$DO = DO.e^{-Ka.t} + DO_s(1 - e^{-ka.t}) \quad (7)$$

Lastly, the root mean squared error (RMSE) and the mean absolute error (MAE) were used to compare the predicted results (P) with field or analytical values (M) for the total number of comparisons (N) to make choice for the appropriate Ka value [16, 17].

$$RMSE = \sqrt{\frac{\sum_1^N (P - M)^2}{N}} \quad (8)$$

$$MAE = \frac{\sum_1^N |P - M|}{N} \quad (9)$$

Accordingly, the model solution starts by entering a suitable Ka value to simulate DO model, see Eq. (4), along with reading the field data (Table 1). Different values of Ka are used until the model matches the field data with less statistic error (Eqs. (8) and (9)).

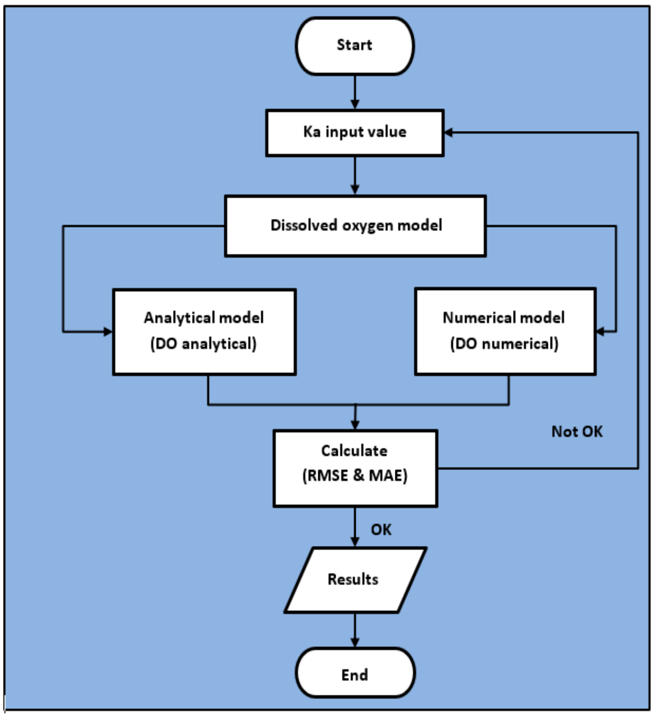

Figure 2. The numerical modeling framework of the study

3. RESULTS AND DISCUSSION

3.1 Reaeration coefficient numerical determination

Using field measurements of DO and T, the governing equation numerical solution was coded and run in Matlab environment. The model calibration was performed by varying the $Ka_{(20)}$ value until the best match with field data is reached with less statistical error. The modeling results indicated that the value of $Ka_{(20)}$ was 0.1 day^{-1} during the study period. Figures 3 and 4 show the DO numerical modeling performance compared to field data during 2021 and 2022, respectively. Noticeably, the DO model was very robust and it was validated with very low MAEs and RMSEs. Hence, the DO values calculated by the model agree with the values obtained from the measurements (the MAE value was 0.4987 mg/L in 2021 and 0.7880 mg/L in 2022, and the RMSE value was 0.1176 mg/L in 2021 and 0.3841 mg/L in 2022).

Figures 5 and 6 show the model performance results against the analytical solution results at the Hilla River headwater during 2021 and 2022, respectively. This process helps verify the numerical model at the early stage of its development in which the model predictions follow the DO analytical distribution of the considered waterbody. Using the estimated $Ka_{(20)}$ value, the numerical predictions revealed more accurate results compared to the analytical values (the MAE value was 0.1248 mg/L in 2021 and 0.1276 mg/L in 2022, and the RMSE value was 0.0113 mg/L in 2022 and 0.0384 mg/L in 2021).

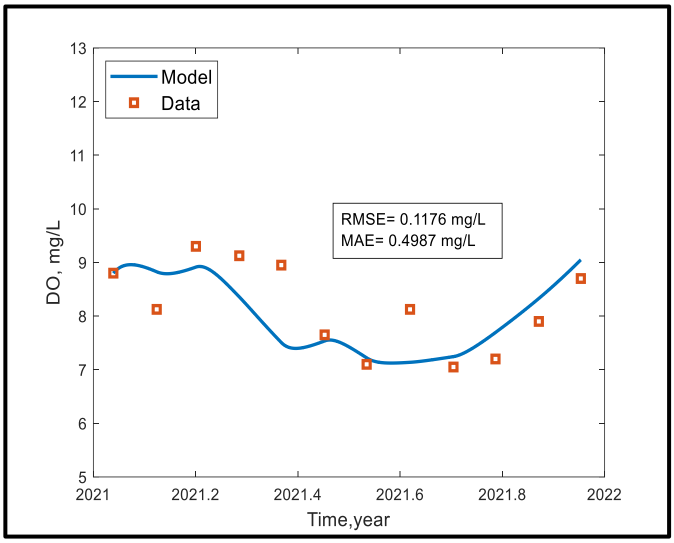

Figure 3. Numerical simulation of DO at the Hilla River headwater during 2021

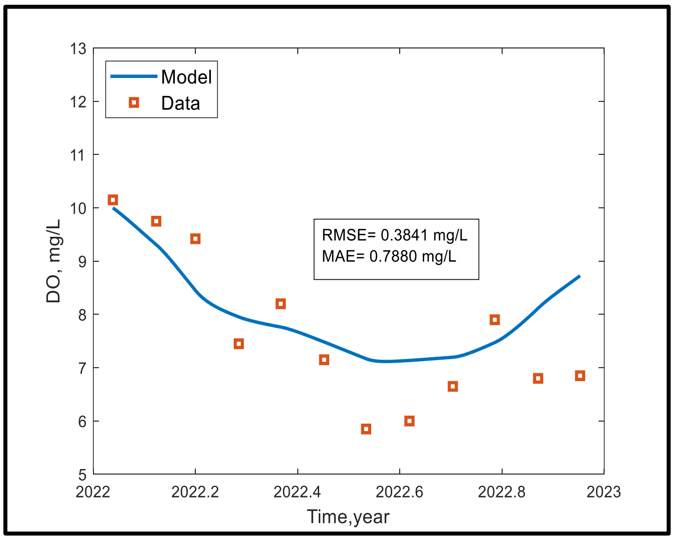

Figure 4. Numerical simulation of DO at the Hilla River headwater during 2022

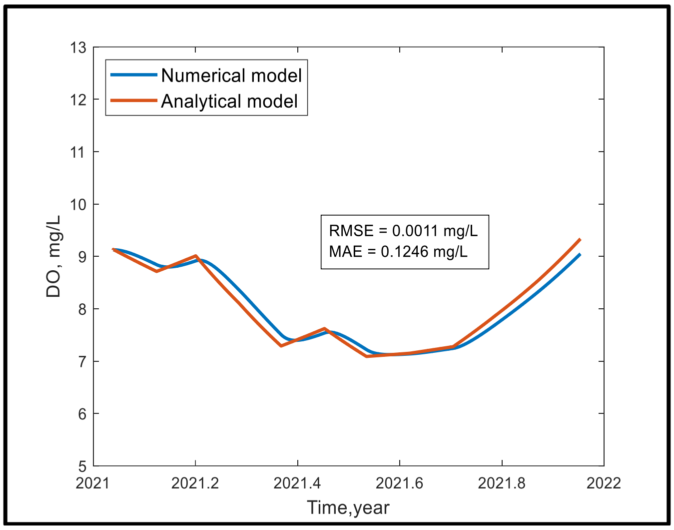

Figure 5. Comparison between the numerical modeling of DO and the analytical solution results at the Hilla River headwater during 2021

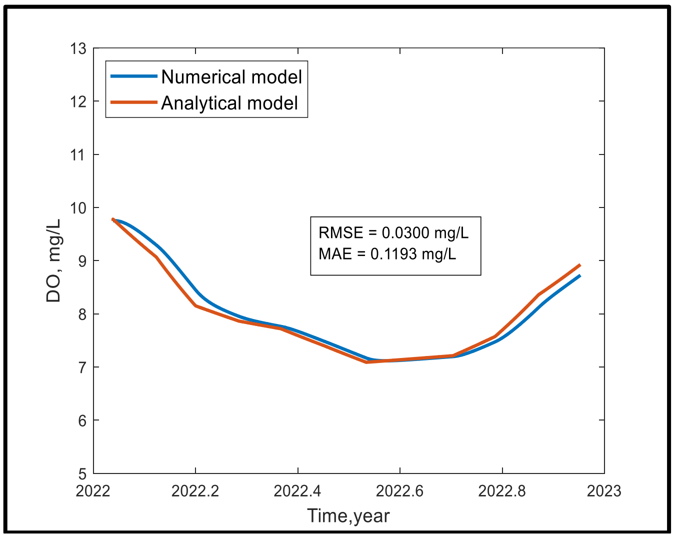

Figure 6. Comparison between the numerical modeling of DO and the analytical solution results at the Hilla River headwater during 2022

In water quality concepts, Ka$_{(20)}$ values differ depending on the water body system whether it is a river, lake, or reservoir. Chin [13] reported that the values of Ka$_{(20)}$ range from 0.1 day^{-1} to greater than 1.15 day^{-1}. Since the Hilla River headwater is from the Saddat Al-Hindiyah Reservoir that suffers from low inflows during the year and noticeable extra algae growth, minimum Ka$_{(20)}$ value was predicted in this study. It was reported that Ka$_{(20)}$ value (0.1-0.23) day^{-1} for small ponds and bake waters, (0.23-0.35) day^{-1} for large lakes and sluggish streams, (0.35-0.46) day^{-1} for large streams of low velocity, (0.46-0.69) day^{-1} for large streams of normal velocity, (0.69-1.15) day^{-1} for swift streams, and greater than 1.15 day^{-1} for rapids and waterfalls [13]. Hence, low water velocity conditions impacted Ka$_{(20)}$ of the headwater too. As a result, matching the general impacts of dissolved oxygen sources and sinks on the Ka determination in the present numerical modeling confirms the calculation accuracy and must be taken into account when estimating the value of Ka because it affects the reliability of dissolved oxygen concentrations distribution in water bodies.

3.2 The temperature dependency of DO reaeration rate

Since the DO is important for respiration and other metabolic processes in aquatic organisms, the predicted reaeration coefficient value is an essential parameter to model the dissolved oxygen concentration in different aquatic ecosystems. The DO values at the study area increase in the winter season when temperature values are low, and opposite behavior occurs in summer season when temperature values become higher. In addition, Figure 7(A) and Figure 8(A) depict the saturated dissolved oxygen distribution at the study area during the study period. the saturated value of DO is a temperature dependent. The highest saturated values of dissolved oxygen were during winter season and the lowest values were during the summer season. This is due to the effect of water temperature on the reaeration process, as shown in Figure 7(B) and Figure 8(B), such that the highest temperature values are during the hot season and the lowest values are during the cold season. Water temperature is the main factor that controls reaeration rates. Because the amount of oxygen that can be dissolved in water is directly proportional to the temperature of the water [18]. Thus, water temperature varies with Ka directly and exponentially. The higher the water temperature is, the higher the reaeration rate that increases Ka values becomes (Figure 9). As a result, the high reaeration rate values occur during summer with lower values during winter.

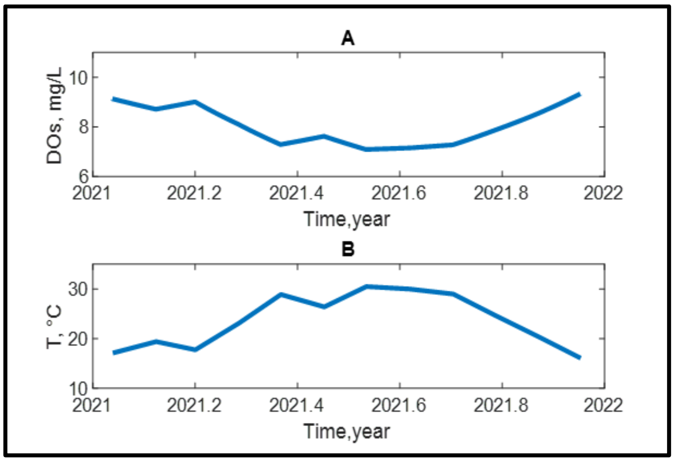

Figure 7. The temperature and saturation dissolved oxygen distribution at the Hilla River headwater during 2021

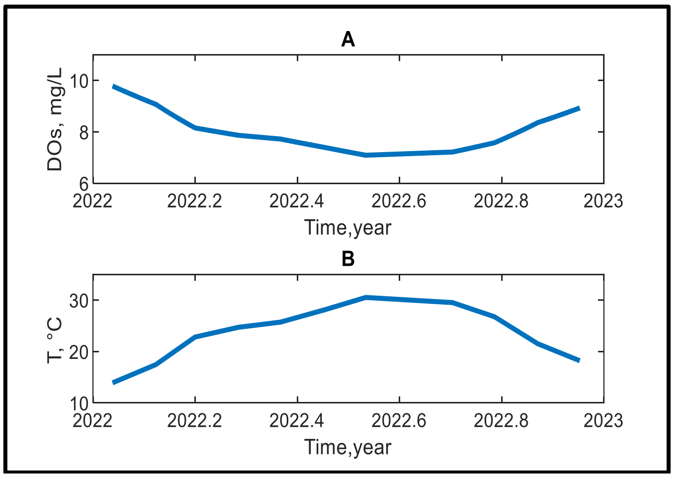

Figure 8. The temperature and saturation dissolved oxygen distribution at the Hilla River headwater during 2022

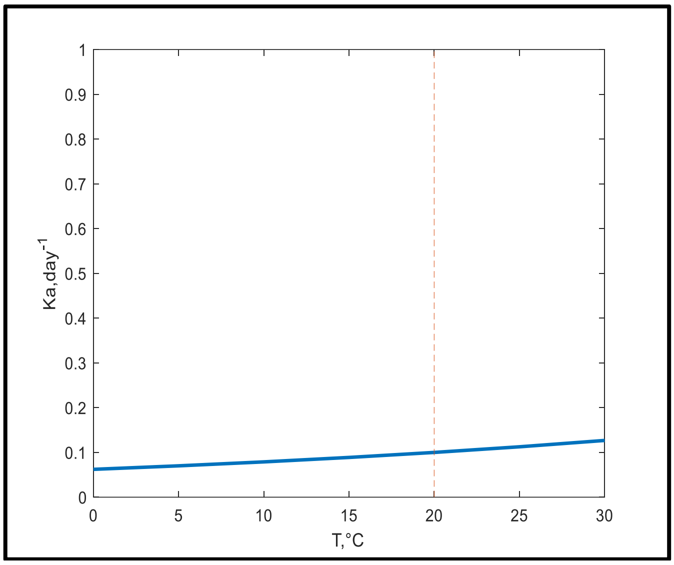

Figure 9. Reaeration coefficient temperature dependency at the Hilla River headwater

3.3 The temporal variation of reaeration coefficient

The temporal values of Hilla River headwater reaeration coefficient were (0.091- 0.128) day^{-1} and (0.086 - 0.128) day^{-1} during 2021 and 2022, respectively. Following the main conclusion of Figure 9, it was found that the highest rate of reaeration in the reservoir was during the summer season, in the dry season, while the lowest rate was during cold weather conditions. The temporal variation of reaeration coefficient can be more emphasized as shown in Figures 10 and 11, which shows the Ka values at the Hilla River headwater during the study period. This disparity reduces the presence of dissolved oxygen during summer due to high water temperatures and oxygen transfer rate, impacting the water quality in water [18]. It is clear that there is a considerable temperature impact on the dissolved oxygen levels in the reservoir, recall the model predictions of Figures 3 and 4. This could be worse as additional sediments and plants reach the reservoir with inflows, particularly during summer. Different managing strategies might be used reduce this impact [19]. Mechanical and diffused aerators can enhance reservoir DO levels. Shading and reservoir habitat restoration play a major role in water quality management too. Implementing such strategies needs comprehensive water quality monitoring and making predictions by modeling the dissolved oxygen for the right reason with less complexity and resources.

Ugbebor et al. [20] determined the reaeration coefficient for a stagnant waterbody during the dry season with flowing water during the rainy season using empirical equations. The reaeration coefficient values ranged between 0.01 and 0.19 day^{-1} during the dry and rainy period. Similarly, the Hilla River headwater is stable in the reservoir during the year. This forces the reaeration coefficient values to be low because the increase in the water flow velocity leads to an increase in the reaeration coefficient [18, 20].

Accordingly, there is an indirect relationship between the headwater dissolved oxygen and temperature variation in the reservoir. Zhong et al. [21] confirmed the presence of this indirect association between saturated DO and temperature. Hence, the determination of Ka must be performed along with water temperature simultaneously for any water quality modeling application related to dissolved oxygen prediction and evaluation. Consequently, constant dissolved reaeration coefficient must not be applied to determine the DO yearly cycle distribution.

Furthermore, this seasonal variability of dissolved oxygen in the reservoir may be impacted by many other water quality parameters significantly [22, 23]. Algae blooms occurrence is the most water quality problem, especially during the warm seasons. The high temperature and sunlight associated with low flow conditions at this area during summer and spring seasons increase the algae growth, providing suitable conditions for decomposing organic matters and lowering DO eventually (Figures 3, 4, 7 and 8). Another factor that can impact the seasonal variation of dissolved oxygen is the increasing inflow and precipitation at the Iraq water resources lately, transporting sediments and organic matters into the reservoir waterbody. Hence, modeling the dissolved oxygen in the Hilla River at Saddat Al-Hindiyah Reservoir should account for water quality seasonality due to its impact on dissolved oxygen. Thereby, the present model performance succeeded in holding the water quality seasonality without the need to collect information about other factors.

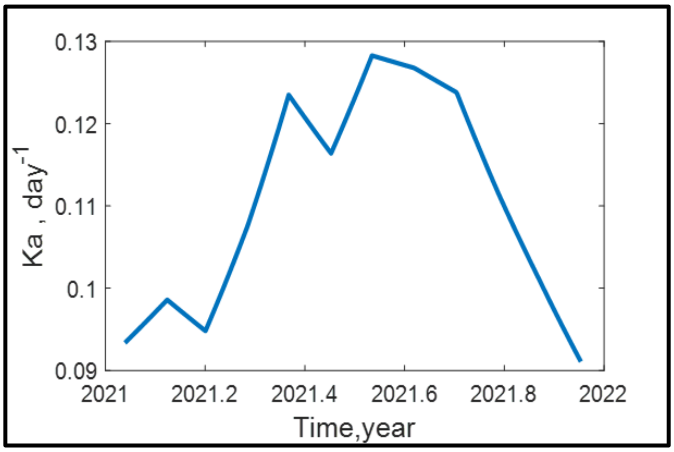

Figure 10. The reaeration coefficient distribution at the Hilla River headwater during 2021

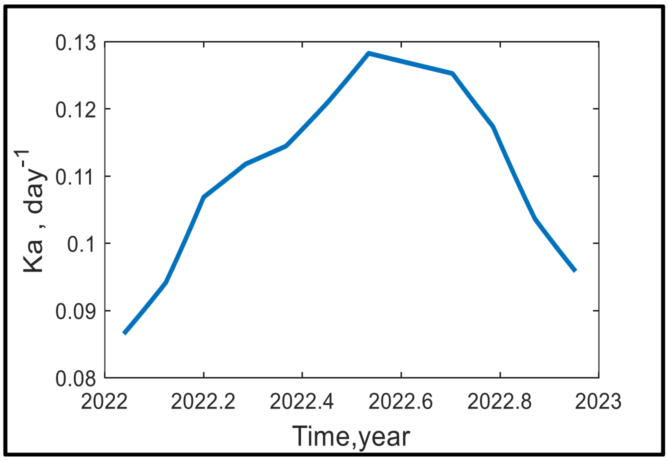

Figure 11. The reaeration coefficient distribution at the Hilla River headwater during 2022

4. CONCLUSIONS

The temporal variation of DO reaeration coefficient was simulated for the Hilla River headwater at the Saddat Al-

Hindiyah Reservoir, Iraq, based on field data of DO and temperature. The simulation process emphasized that that the correct and accurate choice of the reaeration coefficient value is one of the most important factors affecting the accuracy of the DO predictions. It was found that the headwater reaeration coefficient was low during the entire study period (0.1 day^{-1} at 20°C with temporal ranges of (0.091- 0.128) day^{-1} and (0.086 - 0.128) day^{-1} during 2021 and 2022, respectively). The stagnant water at the reservoir was the main reason of low Ka values, forcing the water body to be a well-mixed system. In addition, the DO reaeration coefficient is a function of temperature. This plays a major role in the seasonal variability of DO in the reservoir. Therefore, high Ka and low DO was predicted in summer due to the high temperature, while low Ka and high DO was in winter. Hence, the temporal variation of Ka, DO, and temperature must be taken into account while performing water quality modeling since the sources and sinks impact of dissolved oxygen must be met by the model predictions with less statistic errors. Applying these findings in real world-setting helps decision-makers address the challenges of dissolved oxygen fluctuation with temperature effectively. By running the model with real-time data, DO predictions will be available, and forecasting high algae growth period and DO depletion can be optimized by aeration strategies during the critical events. Furthermore, using the Ka model prediction values for other numerical or analytical water quality models as an input rather than using the empirical formulas can improve the robustness of these models.

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NOMENCLATURE

A	Correction factor, units depend on the context
B	Calibration factor (dimensionless)
D	Diffusion coefficient (m^2/sec)
DO	Dissolved oxygen concentration at any time at any distance (mg/L)
DO_s	Saturated dissolved oxygen concentration (mg/L)
DO^n	DO values at the current time level (n) (mg/L)
DO^{n+1}	DO values at the next time level (n+1) (mg/L)
h	Elevation of the water body above sea level (Kilometers)
Ka	DO reaeration coefficient at any temperature (sec^{-1})
$Ka_{(20)}$	DO reaeration coefficient at 20°C (sec^{-1})
M	Field or analytical values, units depend on the context, for example, DO concentrations (mg/L)
MAE	Mean absolute error, units depend on the context, for example, (mg/L)
N	Total number of comparisons (dimensionless)
P	The model predicted values, units depend on the context, for example, DO concentrations (mg/L)
RMSE	Root mean squared error, units depend on the context, for example, (mg/L)
S	Dissolved oxygen source-sink term (mg/L/sec)
t	Time unit (sec)
T	Temperature (°C)
u	Velocity along x-axis (m/sec)
x	X-axis direction

Superscripts

n	Time level (dimensionless)

Greek symbols

Δt	Time step (sec)