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RESEARCH ARTICLE

Determination of degradation/reaction rate for surface water quality of recycled water using Lake2K model for large-scale water recycling

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Abstract

The depletion of groundwater resources in the water-stressed regions has led to the overuse of surface water reservoirs. Recharging groundwater by rejuvenating dried surface reservoirs using recycled water is a new sustainable solution. To ensure the prevention of groundwater contamination and associated health risks (as recycled water is used), it is crucial to assess the surface reservoir water quality. The study for the first time suggests the Lake2K model, a one-dimensional mechanistic mass-balance model, to simulate the changes in water quality in a series of man-made surface water reservoirs where recycled water flows under an indirect groundwater recharge scheme (soil aquifer treatment system). The model was developed, calibrated, and validated using field observations to estimate degradation/reaction rate constants for various water quality parameters. The observed average degradation/reaction rate constants for parameters including ammonia-N, nitrate–N, total nitrogen, total organic carbon, and organic phosphorous were 0.043 day^{-1}, 0.04 day^{-1}, 0.043 day^{-1}, 0.055 day^{-1}, and 0.056 day^{-1}, respectively, which were found to be relatively high compared to existing literature, indicating a greater degradation of these parameters in warmer climates. The results showed that the water quality improved significantly as the water progressed through the reservoirs, aligning with field observations. Additionally, the simulated seasonal variations revealed that the maximum growth rate of phytoplankton occurred during July, August, and September for each reservoir, while the nutrient pool (nitrate–N and orthophosphates) experienced the greatest depletion during this growth period. These findings shed light on the dynamics of surface water quality in regions facing water scarcity and contribute to the development of sustainable groundwater management strategies.

Keywords Degradation/reaction rate · Lake2K model · Surface reservoir water quality · Reservoirs in series · Recycled water

Abbreviations

ANOVA	Analysis of variance
BOD	Biochemical oxygen demand
CGWB	Central Ground Water Board
CZ	Carnivorous zooplankton
DO	Dissolved oxygen
DOC	Dissolved organic carbon
DOM	Dissolved organic matter
DOP	Dissolved organic phosphate
GLEC	Great Lakes Environmental Center
GUI	Graphical user interface
GW	Groundwater
HZ	Herbivorous zooplankton
IP	Inorganic phosphorous
ISS	Inorganic suspended solids
K&C	Koramangala–Challaghatta
LSD	Least significant difference
Mcft	Million cubic feet
MLD	Millions of liter per day
NGT	National Green Tribunal
NH_4^+-N	Ammoniacal nitrogen

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Kavita Verma and Reshma Mohan Thattaramppilly contributed equally to this work.

The terminology "degradation rate" is used interchangeably with "reaction rate" depending on the context throughout the manuscript.

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NO_2-N	Nitrite nitrogen
NO_3-N	Nitrate nitrogen
ON	Organic nitrogen
OP	Organic phosphorous
Phy	Phytoplankton
PJK	Panjiakou
POC	Particulate organic carbon
SAT	Soil aquifer treatment
SDG	Sustainable development goals
SOD	Sediment oxygen demand
SRP	Soluble reactive phosphorus
STP/STPs	Sewage treatment plant/plants
TKN	Total Kjeldahl nitrogen
TN	Total nitrogen
TOC	Total organic carbon
TP	Total phosphorous
UV	Ultraviolet
VBA	Visual Basic for Applications

Introduction

Water scarcity is a major obstacle to the economic and social progress of countries, particularly in arid and semi-arid regions (Fernandes et al. 2023; Tariq et al. 2022; Dolan et al. 2021; Marangon et al. 2020; Verma et al. 2017). Groundwater accounts for approximately 50% of the total water extracted worldwide for household purposes, and roughly 25% of the total water withdrawn is dedicated to irrigation (UNESCO 2023). However, the over-exploitation of water resources without sufficient natural replenishment has led to an irreversible shortage of this vital natural resource (Agathokleous et al. 2023; Al-Hazmi et al. 2023; Chi et al. 2022; Dangar et al. 2021). Consequently, there is an urgent need for sustainable groundwater management strategies (Xia et al. 2023; Sunyer-Caldú et al. 2022; Rock et al. 2019).

Kolar District in Karnataka, India, is a water-stressed semi-arid region affected by erratic rainfall, leading to a significant decline in groundwater levels (Verma et al. 2023a; Manisha et al. 2023a, b; CGWB 2012). The depletion of groundwater has resulted in the overuse of surface water reservoirs for agricultural irrigation, ultimately causing them to dry up. In response to the escalating water demand, the Government of Karnataka initiated the Koramangala–Challaghatta (K&C) Valley project. This innovative scheme aims to recharge groundwater by reviving dried surface reservoirs using recycled water from urban areas (Verma et al. 2023a; Manisha et al. 2023a; Rock et al. 2019; Dillon and Arshad 2016). The concept behind the scheme is based on soil aquifer treatment (SAT), where the quality of the treated water improves naturally through flow in open channels and residence time in surface reservoirs before reaching the groundwater table (Al-Hazmi et al. 2023; Xia et al. 2023; Verma et al. 2023a, b; Panagiotou et al. 2023; Singh 2020; Grinshpan et al. 2021; Alslaibi et al. 2017; Sharma and Kennedy 2017; Levantesi et al. 2010). Thus, it is crucial to monitor the water quality of the surface reservoirs critically and assess the changes in recycled water quality during its flow from one reservoir to another and residence time in each surface reservoir to prevent further groundwater contamination and associated health risks.

Various techniques exist in the literature for evaluating the quality of surface water bodies and internal nutrient loadings, including site-specific studies, laboratory experiments, and mass-balance methods (Qin et al. 2016). However, most of these studies have focused on determining the reaction rate constants of specific parameters, primarily conducted in colder-climate lakes (Abdelwahab et al. 2021; Xia et al. 2021). Since reaction rates vary geographically across different temperature ranges, it is essential to determine site-specific temperature-dependent reaction rate constants for a precise analysis of lake dynamics. A summary of the literature studies that focus on determining reaction rate constants is given in Table 1.

Field experiments provide insights into specific measurement points but often fail to capture the dynamic and transient processes occurring in a lake system (Doan et al. 2018; Luff and Moll 2004). Additionally, conducting field and laboratory studies to obtain spatial and temporal data for large lakes is economically challenging. In this context, mathematical models offer a valuable framework for simulating physical and biochemical processes in lakes (Liu et al. 2018). These models integrate diagnostic and ecosystem models, providing a powerful tool to represent idealized lake systems and simulate their dynamic responses to perturbations (Zhang et al. 2021). Modeling studies on environmental systems, such as lakes, typically investigate variations on specific time scales (Xia et al. 2023; Mccarthy 2016; Chapra and James 2012). These studies can be categorized into (i) long-term simulations and future projections under different climate change scenarios, (ii) daily/seasonal dynamics in the lake system, and (iii) short-term studies spanning from hours to several days and at various scales (Amadori et al. 2021). The Lake2K mathematical model is well suited for daily/seasonal and short-term studies (Chapra and James 2012). It is designed to simulate water quality trends in stratified lakes, considering geographic, physical, biochemical, geological, and anthropogenic factors. This one-dimensional mechanistic mass-balance model has been successfully used to simulate water quality and nutrient dynamics in both artificial and natural lakes (Kang et al. 2020; Henderson 2019; Mccarthy 2016; Epstein et al. 2013; GLEC 2007). A summary of these modeling studies in the literature is given in Table 1.

Thus, as per author's knowledge, the presented study for the first time quantifies and simulates the changes in water quality of the recycled water in a series of man-made surface

Table 1 Summary of field studies (for reaction rate constants) and modeling studies in literature on lake systems

Reference	Study area	Objective of the study	Methodology	Remarks
Field studies for determining reaction constants				
Islam et al. (2013)	6 rivers, South Korea	• Measure decomposition rates of organic phosphorus and organic nitrogen in rivers	• First-order reaction kinetics model (at 20 °C) by numerical integration using the Runge–Kutta method • The optimum coefficients determined by the least square method	• Reaction rate of particulate organic nitrogen: 0.093 per day • Reaction rate of dissolved organic nitrogen: 0.472 per day
Catalán et al. (2016)	Wide range of inland waters (aquatic ecosystems)	• Analyze organic carbon reaction rates with residence times	• First-order exponential reaction equation used to calculate reaction rates (at 20 °C)	• Negative relationship between the rate of organic carbon reaction and water retention time • Reaction of organic carbon: 0.0185 per day
Thompson and Cotner (2018)	27 freshwater systems, Minnesota and South Dakota	• Quantify bioavailability of dissolved organic carbon (DOC) and dissolved organic phosphate (DOP) from different aquatic ecosystems • Explore potential environmental drivers of dissolved organic matter (DOM) bioavailability	• 3 unique models used (linear, 2 component exponentials, and 3 component exponentials)	• DOC degradation was best fit by an exponential degradation model • Reaction rate of DOC: 0.003 to 0.024 per day • A 2-parameter exponential fit model best described the DOP data • Reaction rate of DOP: 0 to 0.025 per day
Guo et al. (2020)	Rivers of Taihu Lake Basin	• Study seasonal and temporal variability of the reaction rate coefficients of different nitrogen forms in river channels	• Reaction rate coefficient was calculated using first-order reaction kinetics model • 1-dimensional steady-state water quality model was used (at 7 to 34 °C) • Spatial and temporal differences were tested using ANOVA and Fisher's LSD test	• Reaction rate coefficient of total nitrogen (TN): 0.006–0.449 day^{-1} • Reaction rate coefficient of ammoniacal nitrogen (NH_4^+-N): 0.022–1.175 day^{-1} • Reaction rate coefficient of nitrate nitrogen (NO_3-N): − 0.096–2.402 day^{-1}
Tasnim et al. (2021)	6 lakes	• To use MINLAKE2020 to understand internal nutrient dynamics • To study an interaction among nutrients, phytoplankton, and stratification dynamics in lakes	• MINLAKE2020 used to develop a 1-dimensional model by using phytoplankton, zooplankton, nutrient, and biochemical oxygen demand (BOD) simulations • Temperature set at 20 °C as per general model conditions	• Mortality rate of phytoplankton: 0.03 day^{-1}

Table 1 (continued)

Reference	Study area	Objective of the study	Methodology	Remarks
Modeling studies using the Lake2K model				
Epstein et al. (2013)	Bull Trout Lake, central Idaho, USA	• Modeling nutrient dynamics in a glaciated watershed • To analyze if lakes are sources or sinks for nutrients • To evaluate the cumulative effect of multiple lakes in series	• Lake2K: model for ice-free season • Multiple lakes in series to evaluate nutrient transport through watersheds • Water chemistry & temperature data from epilimnion and hypolimnion for model calibration • Time period: mid-July through the rest of the summer	• Multiple lakes appear to have a compounding effect on the accumulation of nutrients • Each lake was observed to be a net nutrient source on a cumulative summer season time scale • But, the study did not take into account the input from the stream channels between lakes
Mccarthy (2016)	Lake Superior, MI, USA	• Model physical and biogeochemical dynamics: algal growth and phosphorus cycling • To investigate the dynamics changes between years	• Lake2K inputs: temperature, phosphorus, plankton conc., & kinetics • The model is run for the ice-free season • Time step of 0.1 day, for model runtime and calculating efficiency • Homogenous flow condition	• Multi-layered model: to accommodate changes in stored algal phosphorus • Phytoplankton in the epilimnion increase steadily following the onset of stratification • Model limitation when simulating dissolved phosphorous
Henderson (2019)	Mona Lake, Lake Michigan, USA	• Monitoring program: to characterize tributary and lake conditions • To develop a model capable of simulating both current and future water quality in Mona Lake	• Lake2K: inflow is equal to outflow, and precipitation is equal to evaporation, resulting in constant layer volumes • Phytoplankton: mass balance on algal carbon; photosynthesis as a source & respiration, death, and zooplankton • Temperature effect and oxygen transfer also modeled	• SRP accounts for ~ 68% of the mass total phosphorus to Mona Lake • Historical external loading: high loads of phosphorus, stimulating high amounts of seasonal biomass production • Model output: management control, for sediment release control
Kang et al. (2020)	Water reservoir, northern Hebei Province, China	• Identify the seasonal and long-term nutrient trends in the PJK reservoir and upstream inflow • To investigate how the accumulated fish feed in the sediment influences the water quality after the removal of the cage	• Lake2K model: simulated & calibrated for 2018 • Input data include daily hydrology data, daily meteorology, & monthly water quality • Water quality data, sampled on the water surface, and measured data were used to calibrate the model results in the epilimnion	• It was observed TP concentration of the reservoir will decline gradually, and a new equilibrium will be achieved within 10 years • Concentration of TN shows an increasing trend which requires more attention • Limitations of the models: in-depth research and verification are needed in the future

water reservoirs where recycled water flows under an indirect groundwater recharge scheme (SAT system) using the Lake2K model which is a one-dimensional mechanistic mass-balance model. Specific objectives of the study are as follows:

1. Estimating the rate constant of surface water degradation under the climatic conditions of India.
2. Evaluating the alteration in surface water quality as it passes through a series of reservoirs.
3. Development and validation of the Lake2K model.
4. Investigating the seasonal fluctuations in various parameters that affect the quality of surface water.

Methodology

Study area

Kolar and Chikkaballapur districts located to the North and East of the city of Bengaluru (Manisha et al. 2023a, b; Verma et al. 2023a, b; Singh 2020) receive around 440 million liters per day (MLD) of treated wastewater from Bengaluru District sewage treatment plants (STPs) and is distributed by gravity to over 137 irrigation reservoirs which, in turn, recharge the groundwater. Figure 1 represents the study site/stretch of three reservoirs in series which were identified to assess the change in surface water quality. This stretch of three reservoirs in series was selected as there was no sewage/surface runoff intervention in the reservoirs from nearby agricultural fields. Table 2 presents details, such as volume of water in reservoirs, flow rate of water, and its residence time, of the studied reservoirs.

Characterization of secondary treated water and surface reservoir water

Secondary treated water samples from the outlet of K&C Valley STP and water samples from three surface reservoirs (inlet and outlet) were collected in the morning hours (9 to 10 a.m.). Quality assurance/quality control measures were undertaken as all the water samples were tested in triplicates, and average values along with standard deviation are presented as avg. ± std. dev. Dissolved oxygen (DO) concentrations were assessed at each treatment point through two methods: field measurements using an optical DO

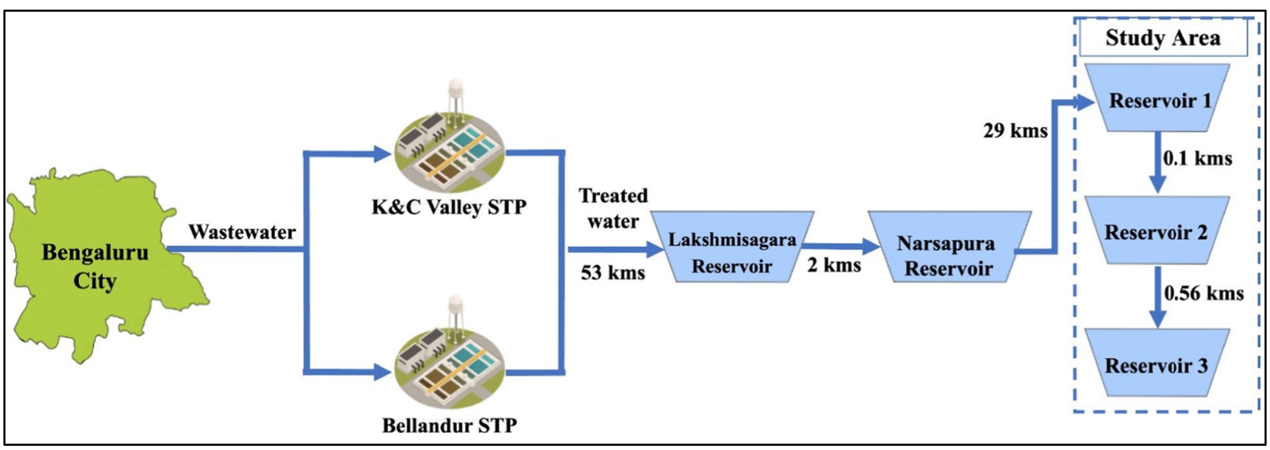


Fig. 1 Study area

Table 2 Technical information of the selected reservoirs in the study area

	Stretch of reservoirs		
	Bagalahalli reservoir (reservoir 1)	Teranahalli reservoir (reservoir 2)	Mastenahalli reservoir (reservoir 3)
Volume (Mcft)	12.55	29.28	33.22
Flow rate (MLD)	65		
Flow rate (Mcft/month)	68.86		
Residence time (months)	0.182	0.425	0.482
Residence time (days)	6	13	15

Mcft million cubic feet

probe (Lovibond 740800, featuring a luminophore-covered membrane), and laboratory measurements using the modified Winkler DO titration procedure. The latter method was employed to verify and compare the readings obtained from the probe (Mohan et al. 2022). To determine the nitrogen components, the total Kjeldahl nitrogen (TKN) and organic nitrogen (ON) in the samples were analyzed in the laboratory using the macro Kjeldahl method. This involved digesting and distilling the samples to NH_4-N. The NH_4-N content in the samples was then determined via pre-distillation and the standard titration method. The NO_3-N in the samples was determined by analyzing the difference in sample absorbances at 220 nm and 275 nm, the NO_2-N content was assessed at an absorbance of 543 nm, and orthophosphates were analyzed at 880 nm using UV spectroscopy. TOC was analyzed using a TOC analyzer (Thermo Fisher, 3100). The detailed procedure for determining all these parameters was followed from the APHA manual of standard methods for the examination of water and wastewater (APHA 2005). Phytoplankton in the reservoirs were quantified by chlorophyll *a* concentration (APHA 2005). Zooplankton in the reservoirs were identified and counted using a hemocytometer under the microscope (at × 40 in a Labomed OPTI CX UPS microscope). For representing zooplankton in terms of mg C/L, the number of zooplankton per sample was multiplied with the carbon weights of the respective zooplankton. The carbon weights were obtained from the literature review (Miron et al. 2018).

Reaction rate calculation

In this study, the reaction rate for ON, NH_4-N, TN, NO_3-N, organic phosphorous, TOC, zooplankton, and phytoplankton was calculated using the differential first-order reaction rate equation. It is a mathematical expression that describes the rate at which a substance or particle reacts over time, and is represented by the following equation (Guo et al. 2020; Thompson and Cotner 2018; Catalán et al. 2016):

$$-\frac{d[C]}{dt} = k[C] \tag{1}$$

Integrating on both sides

$$\int_{[C]_0}^{[C]} \frac{1}{[C]} d[C] = -\int_{t_0}^{t} k dt \tag{2}$$

$$\ln[C] - \ln[C]_0 = -kt \tag{3}$$

$$k = \frac{\ln \frac{[C]_0}{[C]}}{t} \tag{4}$$

where k is the first-order reaction rate constant, $[C]_0$ is the initial concentration, $[C]$ is the final concentration, and t is the residence time. This type of reaction is often observed in natural systems, such as rivers and lakes, and is used to model the removal of pollutants due to natural processes (Guo et al. 2020).

Conceptual Lake2K model

The Lake2K modeling framework developed by Chapra and James (2012) simulates the spatial (as the water passes from reservoir to reservoir) and temporal/seasonal variations of water quality in the three reservoirs. The Lake2K model is designed to compute seasonal water quality variations in stratified reservoirs. The model is programmed in the Visual Basic for Applications (VBA) macro language and uses an Excel program as the graphical user interface (GUI). The model can be applied to stratified lakes using site-specific physical or geographical conditions (temperature, inflow–outflow, altitude).

The model simulates the reservoir as a one-dimensional system with three vertical layers: the epilimnion, the metalimnion, and the hypolimnion. The volume of the upper layer (the epilimnion) was allowed to vary depending on the inflows and the outflows, while the volume of the remaining two layers (the metalimnion and the hypolimnion) was fixed. The dynamic water balance in the reservoir was computed as (Mccarthy 2016; Chapra and James 2012):

$$\frac{dV}{dt} = (Q_{in} + Q_p) - (Q_e + Q_{out}) \tag{5}$$

where V is the volume of the lake (m^3), t is the time (days), Q_{in} is the inflow (m^3/day), Q_p is the precipitation (m^3/day), Q_e is the evaporation flow (m^3/day), and Q_{out} is the outflow (m^3/day).

The inflow to the reservoir includes the inputs from all the point and non-point sources provided as a single or time-series data, while the precipitation was represented using time-series data with specific precipitation rates. The model internally computes the loss of water due to evaporation. This flow is computed as (Chapra and James 2012):

$$Q_e = \frac{J_e A_o}{\rho L_e} \times \frac{m}{100cm}$$

where J_e is the heat flux due to evaporation (cal/cm^2/day), ρ is the density of water (1 g/cm^3), and L_e is the latent heat of vaporization (cal/g). The output from the reservoir can be represented using seven output boundary conditions, depending on the flow from the different vertical layers of the reservoir. The vertical mixing of the stratified layers was incorporated into the model using a turbulent diffusion coefficient specified as a user-defined term.

A heat balance equation was solved for each vertical layer of the reservoir, and the surface heat exchange at the air–water interface was also included in the model. The surface heat exchange was as a combination of seven processes: solar short-wave radiation, atmospheric long-wave radiation, water long-wave radiation, conduction, convection, evaporation, and condensation. The first three processes contribute to net absorbed radiations, whereas the other processes were water dependent (Mccarthy 2016; Chapra and James 2012). The transfer of heat within the system was determined using a diffusion term, and the model output specified the temperature trends in the reservoir for the specified duration.

The Lake2K model included 17 state variables, including components of carbon, nitrogen, oxygen, and phosphorous along with silica, phytoplankton, and zooplankton. A mass balance was written for each vertical layer, and for the epilimnion (where the inflow and outflow pass directly), the mass balance is given as:

$$V_i \frac{dc_i}{dt} = Q_{in}c_{in} - Q_{out}c_i + E_i\prime\left(c_{(i+1)} - c_i\right) + S_i V_i \tag{6}$$

where V_i is the volume of layer (m^3), c_i is the concentration of layer (mg/L), c_{in} is the concentration of the inflow (mg/L), E_i' is the bulk turbulent diffusion coefficient across the lower boundary of layer (m^3/day), $c_{(i+1)}$ is the concentration of layer $i+1$ (mg/L), and S_i is the sources and sinks of the constituent due to reactions and mass transfer mechanisms (mg/m^3/day). The state variables and kinetic and mass transfer processes included in the model are given in Table 3. More detailed information about the processes can be found in the Lake 2 K manual (Chapra and James 2012).

As observed from Table 3, nine kinetic and four mass transfer processes were included in the model. The carbon components in the model were represented by particulate organic carbon (POC), dissolved organic carbon (DOC), phytoplankton C, and zooplankton C. The growth of phytoplankton and zooplankton was limited by the availability of nutrients (nitrogen and phosphorous) and oxygen concentrations. All the components of the nitrogen cycle (hydrolysis, nitrification, and denitrification) and the phosphorus cycle (enhanced biological phosphorous removal) were also included in the model. The reaeration of water was represented using O'Connor's model (O'Connor 1983), which was based on a set of formulas to compute gas transfer for low-solubility gases such as oxygen in the water. The sediment nutrient fluxes and sediment oxygen demand (SOD) were based on a model developed by Di Toro and Fitzpatrick (1993). The stoichiometric and kinetic default coefficients were provided in the model, but it is necessary to modify these constants based on site-specific conditions to ensure that the model output fits well with the observations.

Model inputs

The user inputs to the Lake2K model included geophysical characteristics (elevation and area of lake), flow characteristics (inflow, outflow, concentration of variables in inflow), metrological characteristics (air temperature, wind speed, precipitation rate, and average daily solar radiation), vertical mixing diffusion coefficients, initial conditions (for initiating the model run), and kinetic and stoichiometric parameters.

The study period for modeling the three reservoirs was 1 year. The inflow and outflow conditions were provided as measured in the field. It was observed that water flows from the first reservoir (Bagalahalli) to the second (Teranahalli) and from the second to the third reservoir (Mastenahalli) in series. Hence, three different model runs were performed for the three reservoirs. And, the water quality data measured at the inlet of the three reservoirs were provided as the input concentration for all the runs. The flow, hydraulic, and temperature parameters of the three reservoirs are given in Table 4. The epilimnion, metalimnion, and hypolimnion depths were set at 10.0 m, 7.5 m, and 10.0 m, respectively, and remain constant for all the model runs. The site-specific reaction rate constants of nine variables (as given in Table 4), calculated from the field observations, were used in the model. For the remaining variables, default constants were employed. The model results were generated on Lake2K worksheets, and the output variable concentration of each reservoir was compared with field measurements.

The main assumptions while developing the model were as follows:

- The reservoirs were filled with secondary treated water (from K&C Valley STP), and the water quality parameters of the treated wastewater were within the NGT discharge limit (NGT 2019).
- The three reservoirs were assumed to be in series, with outflow from one reservoir feeding as inflow to the next.
- It was assumed (according to the field observations) that there were no other sources of inflow into the reservoirs (runoff from neighboring land, sewage outlets into the reservoir).
- The subsurface runoff component was assumed to be negligible.
- The average water temperature was measured to be 26 ± 4 °C, and the reservoirs were observed to receive constant sunlight throughout the study period.
- The vertical diffusion coefficient for the reservoirs was taken from the literature (Henderson 2019).
- The meteorological data input to Lake2K including air temperature, wind speed, and precipitation rates were obtained from field observations and literature studies.

Table 3 State variables and processes included in the Lake2K model (Mccarthy 2016; Chapra and James 2012)

Variable	Unit	Processes
Dissolved oxygen (DO)	mg O_2/L	Reaeration (M) (+) Photosynthesis (K) (+) Sediment oxygen demand (M) (−) Oxidation of carbon and nitrogen components (K) (−) Growth of phytoplankton (K) (−)
Particulate organic carbon (POC)	mg C/L	Death and egestion of phytoplankton and zooplankton (K) (+) Hydrolysis to DOC (K) (−) Settling (M) (−)
Dissolved organic carbon (DOC)	mg C/L	Hydrolysis from POC (K) (+) Oxidation (K) (−) Sediment–water exchange (M) (−) Carbon for denitrification (K) (−)
Organic nitrogen (ON)	µg N/L	Death and egestion of phytoplankton and zooplankton (K) (+) Hydrolysis to NH_4-N (K) (−) Settling (M) (−)
Ammonia nitrogen (NH_4-N)	µg N/L	Hydrolysis from ON (K) (+) Respiration of phytoplankton and zooplankton (K) (+) Sediment–water exchange (M) (−) Nitrification (K) (−) Growth of phytoplankton (K) (−)
Nitrate nitrogen (NO_3-N)	µg N/L	Nitrification (K) (+) Denitrification (K) (−) Sediment–water exchange (M) (−) Growth of phytoplankton (K) (−)
Organic phosphorous (OP)	µg P/L	Death and egestion of phytoplankton and zooplankton (K) (+) Settling (M) (−) Hydrolysis to IP (K) (−)
Inorganic phosphorous	µg P/L	Hydrolysis from OP (K) (+) Respiration of phytoplankton and zooplankton (K) (+) Growth of phytoplankton (K) (−) Settling (M) (−)
Phytoplankton (Phy)	µg C/L	Growth in the presence of nutrients (nitrogen and phosphorous) and oxygen (K) (+) Death and egestion (K) (−) Respiration (K) (−) Grazing to HZ (K) (−) Settling (M) (−)
Herbivorous zooplankton (HZ)	mg C/L	Growth (K) (+) Death and egestion (K) (−) Respiration (K) (−) Grazing to CZ (K) (−)
Carnivorous zooplankton (CZ)	mg C/L	Growth (K) (+) Death and egestion (K) (−) Respiration (K) (−)
Inorganic suspended solids (ISS)	mg D/L	Settling (M) (−)

K, kinetic processes; M, mass transfer processes; +, mass input; −, mass output

Table 4 Reservoir input characteristics

Reservoirs	Latitude	Longitude	Elevation (m)	Storage capacity (Mcft)	Water spread area (ha)	Average flow (MLD)	Average temperature (°C)
Reservoir 1	13° 17′ 30.92″ N	78° 06′ 13.44″ E	837	12.55	12	65	26 ± 4
Reservoir 2	13° 17′ 17″ N	78° 06′ 47″ E	832	29.28	33	65	26 ± 4
Reservoir 3	13° 17′ 20″ N	78° 07′ 29″ E	828	33.22	12	65	26 ± 4

Model validation

The model was calibrated by adjusting the model coefficients, seeking an appropriate fit of model output to field measurements over the specified study period. The calibrated model was validated by comparing the model output with the field observations for nine major variables. The model output concentration variations from the field values were calculated as the error in the model simulation. Also, the reaction rate constants of these nine variables were back calculated from the model output values and compared with the field-measured values to ensure the robustness of the model. The validation results are given in the section "Validation of conceptual Lake2K model." Once the model was validated, the reaction rate constants of each parameter calculated from the experimental observations were compared with the model constants. The model constants were attained by back calculating the reaction rates from the simulated parameter concentrations. Finally, a transient simulation was carried out for a period of 12 months, to analyze the seasonal variations of the parameters in the three reservoirs.

Results and discussion

Characterization of surface water quality

Table 5 represents characteristics of surface water reservoir. It can be observed that when water flows from one reservoir to another in series, the water quality of the surface water body can undergo several changes. The DO improved from 3.2 to 5.7 mg/L whereas NH_4-N reduced to 91%, NO_3-N reduced to 78%, ON reduced to 67%, TN reduced by 79%, and TOC reduced by 67% with significant reduction in orthophosphate, phytoplankton, and zooplankton. These changes occurred due to various processes and factors present within each reservoir, such as (i) dilution and mixing (as water from one reservoir enters another, it undergoes dilution and mixing with the existing water in the receiving reservoir which also lead to changes in the concentration of dissolved substances), (ii) sedimentation and settling (as water flowed from one reservoir to another, the flow velocity may decrease, allowing suspended particles to settle down), (iii) biological processes (as water flowed from one reservoir to another, it carried along diverse ecosystems, including phytoplankton, zooplankton, and various aquatic organisms which resulted into different biological processes, such as photosynthesis, respiration, and decomposition, and this altered the surface water quality by influencing the levels of dissolved oxygen, nutrients, and organic matter), (iv) chemical reactions occurred (when water flowed between reservoirs and came into contact with different chemical environments, altering their composition and concentration), and (v) nutrient exchange (like phosphorous and nitrogen) occurred for biological productivity in reservoirs resulting in improved water quality. However, the biochemical reactions that reduce organic matter and nitrogen components and the nutrient exchange that aids the growth of plankton in the reservoir ecosystem are identified as the dominant factors that contribute toward the improvement of water quality.

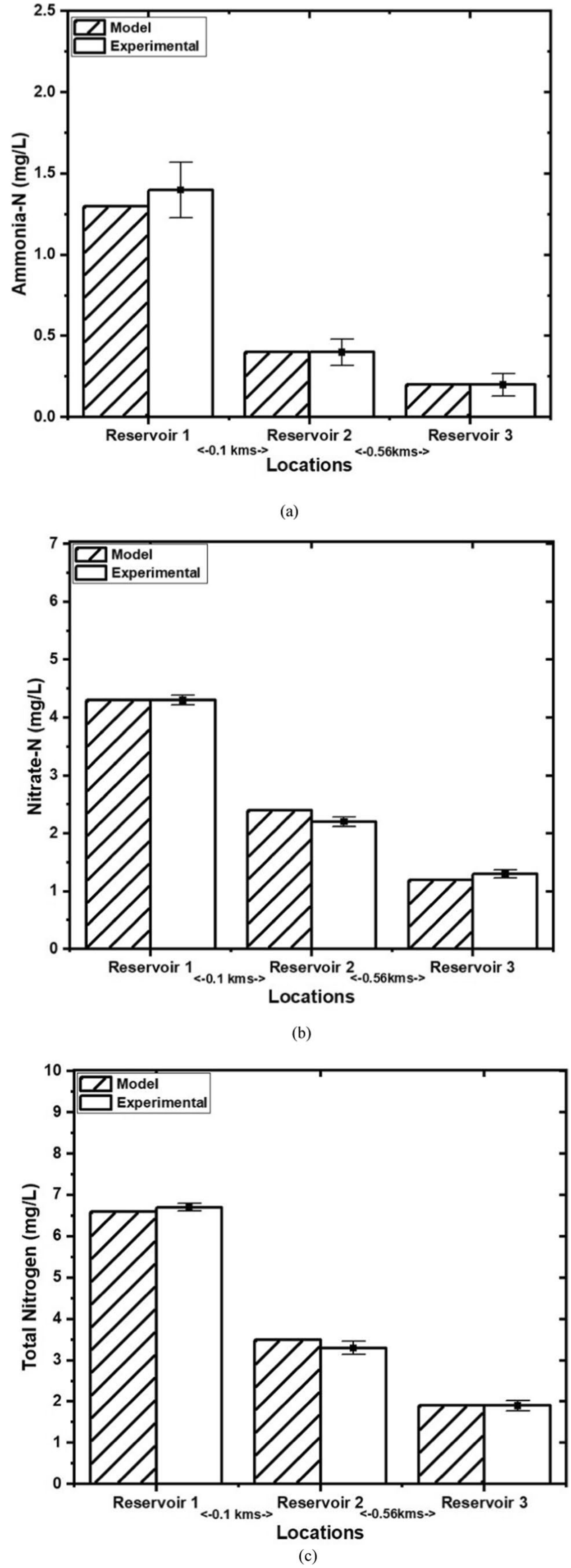
Validation of conceptual Lake2K model

The developed Lake2K model was validated by comparing the time-averaged simulated parameter concentrations with the time-averaged field observations at the outlet of the three reservoirs. Figure 2 shows the comparison of model vs. field observations (time averaged) of (a) NH_4-N, (b) NO_3-N, and (c) TN concentrations at the outlet of the three reservoirs. As seen in Table 5, the inlet NH_4-N concentration to the first reservoir was 1.83 mg/L. Eventually, it reduces to 1.36 mg/L at the outlet of the first reservoir, to 0.39 mg/L at the outlet of the second reservoir, and to 0.17 mg/L at the outlet of the third reservoir. The reduction in NH_4-N was accounted due to the nitrification reactions in the presence of high DO concentrations (given in Fig. 2). As seen from Fig. 2, a similar

Table 5 Characteristics of surface reservoir water

Parameters	Reservoir 1		Reservoir 2		Reservoir 3	
	Inlet	Outlet	Inlet	Outlet	Inlet	Outlet
DO (mg/L)	3.25 ± 0.07	3.9 ± 0.07	4.15 ± 0.12	4.76 ± 0.08	5.09 ± 0.07	5.72 ± 0.15
NH_4-N (mg/L)	1.83 ± 0.11	1.36 ± 0.17	0.44 ± 0.09	0.39 ± 0.08	0.36 ± 0.05	0.17 ± 0.07
NO_3-N (mg/L)	5.80 ± 0.06	4.26 ± 0.08	3.88 ± 0.07	2.17 ± 0.08	2.09 ± 0.07	1.28 ± 0.07
ON (mg/L)	1.45 ± 0.03	1.03 ± 0.03	.01 ± 0.02	0.72 ± 0.03	0.61 ± 0.01	0.48 ± 0.03
TN (mg/L)	9.08 ± 0.08	6.65 ± 0.09	5.32 ± 0.1	3.28 ± 0.16	3.06 ± 0.08	1.93 ± 0.1
TOC (mg/L)	242 ± 5.21	181 ± 5.02	181 ± 5.02	107 ± 5.03	103 ± 5.23	80 ± 5.02
Orthophosphates (mg/L)	0.10 ± 0.002	0.062 ± 0.002	0.05 ± 0.002	0.03 ± 0.001	0.03 ± 0.001	0.014 ± 0.001
Phytoplankton (mg Chl *a*/L)	0.013 ± 0.0003	0.005 ± 0.0003	0.004 ± 0.0002	0.001 ± 0.0001	0.001 ± 0.0001	0.0003 ± 0.0001
Zooplankton (mg C/L)	2.66 ± 0.11	2.4 ± 0.09	2.49 ± 0.1	2.18 ± 0.1	0.42 ± 0.07	0.38 ± 0.06

Fig. 2 Comparison of model vs. field observations (time averaged) of ▸ **a** NH_4-N, **b** NO_3-N, and **c** TN concentrations at the outlet of the three reservoirs



trend was observed for the simulation results too. The outflow NO_3-N concentrations were significantly lower than those in the inflow as observed for the three reservoirs. The obvious mechanism for the removal of nitrates is through denitrification, but denitrification reactions are not possible at high DO concentrations (as observed, Fig. 3). The other possible mechanism of nitrate removal is through nutrient uptake (nitrates and phosphates) mechanism by planktons, which was assumed to the attributing factor for nitrate removal. NH_4-N, NO_3-N, and the TN concentrations were also significantly reducing as water moved in series through the three reservoirs. The TN concentration at the outlet of the third reservoirs was as low as 1.93 mg/L. Also, the simulation values were matching well with the field observations, thereby validating the model.

Figure 3 shows the comparison of model vs. field observations (time averaged) of (a) TOC, (b) orthophosphate, and (c) DO at the outlet of the three reservoirs. TOC was calculated as the sum of POC and DOC. The dead biomass of planktons was represented as POC in the model. Even with this addition of concentration (from biomass) along with the POC sources from the water itself, the POC values were observed to reduce at the outflow of all the three reservoirs. This was attributed to the high hydrolysis and settling rate of POC within the reservoir. Also, the majority of POC reduction was observed in reservoir 1 and the minimum at reservoir 3.

The DOC concentrations were increasing at the outflow side of the three reservoirs. It was observed that reservoirs acted as a source and sink for DOC throughout the uptake, recycling, and growth phase of planktons. Phytoplankton consumes and produces DOC during their life cycle (Spilling and Lindström, 2008). The amino acids and peptides in DOC serve as a carbon source for phytoplankton particularly when dissolved inorganic N is scarce (Yu et al. 2023). The DOC uptake by phytoplankton generally increases with decreasing light availability. The DOC is produced by the phytoplankton by extracellular release under low nutrient and high light levels. Phytoplankton can also produce DOC under nutrient-limited conditions, while the release of DOC by zooplankton occurs through feeding and excretion (Yu et al. 2023). Hence, POC concentrations were reducing and DOC concentrations were increasing, and as a net, the TOC concentrations were reducing at the outflow. The same results were observed in the model simulation as presented in Fig. 2.

As seen in Fig. 3, the orthophosphate concentrations were reducing after each reservoir. If the mass balance of phosphorous is analyzed, the total phosphorous is the sum of its

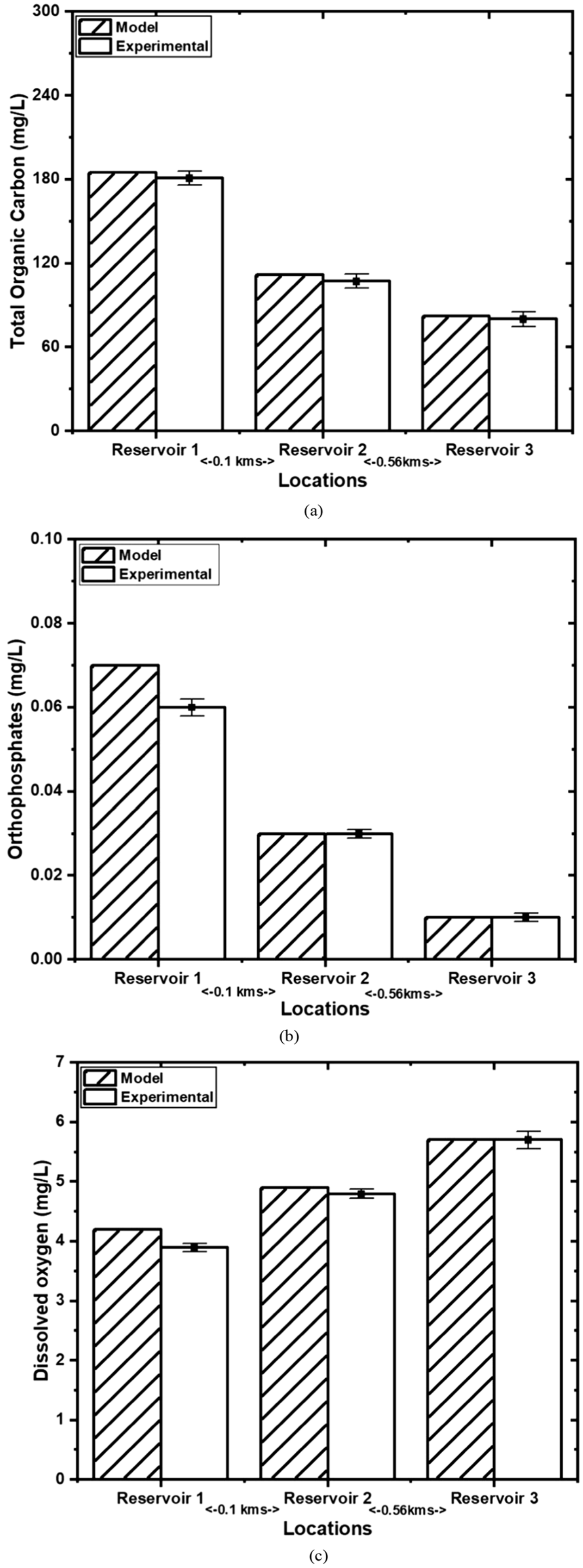


Fig. 3 Comparison of model vs. field observations (time averaged) of **a** TOC, **b** orthophosphate, and **c** DO at the outlet of the three reservoirs

components: soluble reactive phosphorus (SRP), particulate organic phosphorus (POP), and dissolved organic phosphorus (DOP). The SRP is a measure of orthophosphate and is bioavailable for phytoplankton uptake and is then converted into POP. The POP is then either captured by zooplankton or is solubilized into DOP (Li and Brett 2013). The DOP, in turn, is mineralized into SRP. The rates of SRP uptake depend on the rate of phytoplankton growth and the DO availability.

A minimum amount of DO is essential for the plankton to sustain. This is referred to as critical DO concentration, and it is the level at which oxygen supply is sufficient to support their respiration needs (Stumm and Morgan 1970). The critical DO concentration can vary depending on the specific species of plankton and environmental conditions, including temperature, light, and nutrient availability (Stumm and Morgan 1970). However, in general, most plankton species require a minimum DO concentration for growth. Several studies in the literature have consistently shown that DO concentrations below 2 mg/L, often referred to as hypoxia, are detrimental to the sustenance of plankton (Karpowicz et al. 2019, 2020; Miller et al. 2002; Tasnim et al. 2021; Tellier et al. 2022; Vanderploeg et al. 2009a, b; Weinstock et al. 2022).

In hypoxic reservoirs, the metabolic rates of plankton can decelerate (can reduce up to 0.09–0.14 $gO_2\ m^{-3}\ h^{-1}$ for net primary productivity and 0.15–0.20 $gO_2\ m^{-3}\ h^{-1}$ for gross primary productivity), and their capacity for growth can be significantly hindered (Tellier et al. 2022; Vanderploeg et al. 2009a). Furthermore, certain plankton species exhibit greater tolerance to low oxygen conditions than others. In reservoirs experiencing hypoxia, there may be an observable shift in the composition of plankton species. More resilient species that can thrive in hypoxic conditions may become dominant, while those sensitive to low oxygen levels may decline (Tellier et al. 2022; Vanderploeg et al. 2009a, b). Additionally, hypoxia can lead to the release of nutrients from the sediment, which, in turn, stimulates algal blooms and exacerbates nutrient pollution in the reservoir (Tellier et al. 2022; Vanderploeg et al. 2009a, b). In conclusion, a dissolved oxygen level exceeding 2 mg/L is essential for the survival of plankton. In the context of the three reservoirs under study, it is noteworthy that the dissolved oxygen concentrations exhibit a consistent range, typically falling between 3.5 and 5.5 mg/L (as seen in Fig. 3). Among these reservoirs, it is evident that reservoir 3 consistently exhibits the highest DO concentration levels. This observation provides valuable insights into the dynamics of oxygen levels within these aquatic ecosystems. The phenomenon of DO concentration in the reservoirs finds a basis in scientific literature. As elucidated by Mackay et al. (2020) in their research, DO concentrations within reservoirs are predominantly governed by two critical processes: photosynthetic oxygen generation and total plankton respiration. This research underscores the vital role of both natural processes in influencing the oxygen dynamics within aquatic environments.

Photosynthetic oxygen generation, as observed in the reservoirs, plays a pivotal role in elevating DO concentrations. It is an inherently biological process where aquatic plankton and algae utilize sunlight to convert carbon dioxide and water into organic compounds, releasing oxygen as a byproduct. This photosynthetic activity occurs during daylight hours and is particularly pronounced in shallow regions of the reservoirs where sunlight penetrates the bed of the reservoir.

It is essential to contextualize these findings within the broader ecological dynamics of these reservoirs. The observed increase in DO concentrations coincides with a noticeable depletion of nutrients, specifically nitrogen and phosphorus (Buckingham et al. 2022). This depletion can be attributed to the efficient uptake and utilization of these nutrients by the flourishing plankton communities. As plankton thrive and proliferate, they act as effective biological filters, sequestering nutrients from the water column. Consequently, this nutrient removal, driven by plankton growth, contributes to the observed increase in DO concentrations (Taipale et al. 2019). The research findings in this context establish a clear relationship between nutrient dynamics, plankton growth, and DO concentrations within the three studied reservoirs.

Table 6 shows the average reaction rate (day^{-1}) of parameters for all the three reservoirs as calculated from field observations, and Fig. 4 shows the comparison of model vs. field observed reaction rates of (a) NH_4-N, (b) NO_3-N,

Table 6 Average reaction rate (day^{-1}) of parameters for all the three reservoirs

Parameters	Average reaction rate (day^{-1}) of reservoirs			Reaction rate reported in the literature (day^{-1})
	Reservoir 1	Reservoir 2	Reservoir 3	
NH_4-N	0.05	0.03	0.05	0.022–1.175
NO_3-N	0.05	0.04	0.03	−0.096 to 2.402
TN	0.05	0.05	0.03	0.006–0.449
TOC	0.05	0.04	0.02	−0.02 to 0.09
Organic phosphorous	0.08	0.05	0.04	0.001–0.12

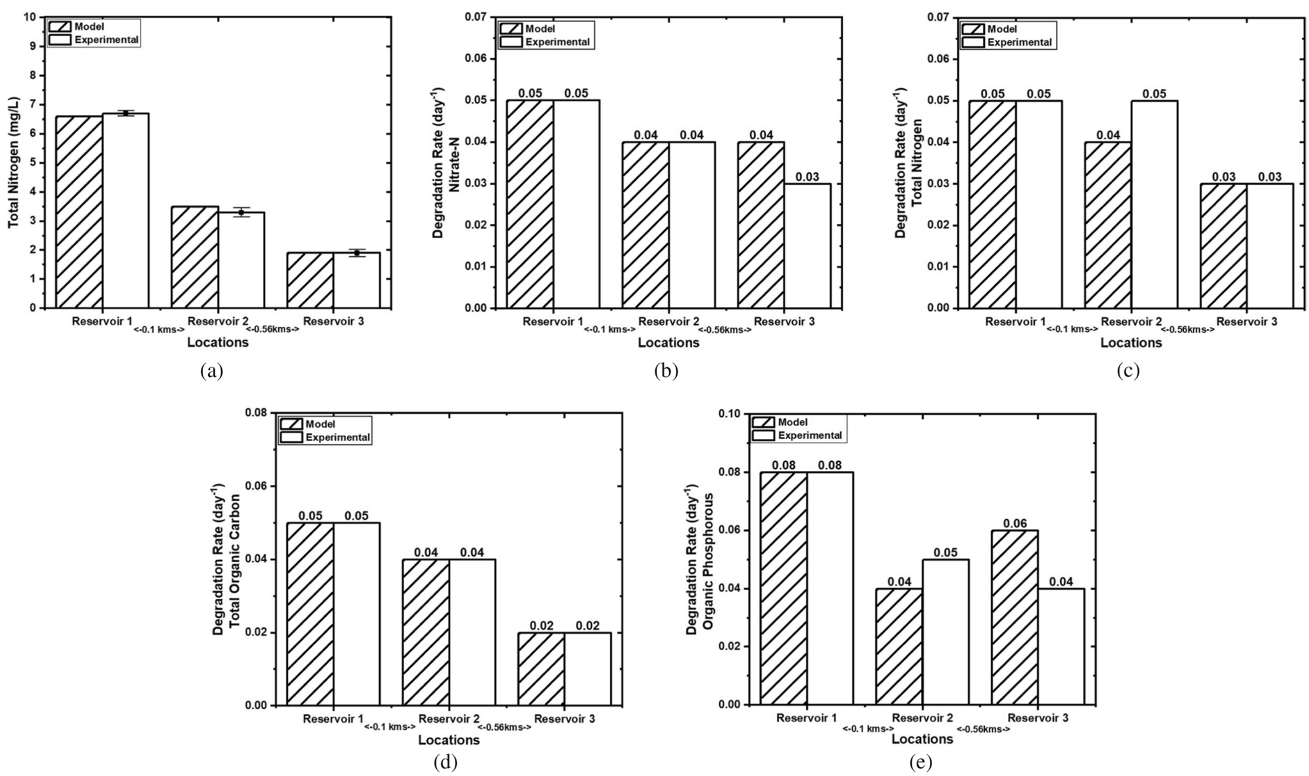


Fig. 4 Comparison of model vs. field observed reaction rates of **a** NH_4-N, **b** NO_3-N, **c** TN, **d** TOC, and **e** orthophosphate in the three reservoirs

(c) TN, (d) TOC, and (e) orthophosphate in the three reservoirs. The typical value of reaction rate constant for NH_4-N reported in literature varies between 0.022 and 1.175 day^{-1} (Guo et al. 2020). Similarly for NO_3-N and TN, the reaction rate constants were observed in between 0.096 and 2.402 day^{-1} and between 0.006 and 0.449 day^{-1}, respectively (Guo et al. 2020). It was observed that high water temperature promotes biochemical reactions and the reaction rate coefficient for all forms of nitrogen (Noori et al. 2022a, b; Zhao et al. 2013, 2015). Hence, the maximum reaction rates for nitrogen were observed in temperatures between 20 and 30 °C. In the present study, the reaction rates were within the literature observed range. Also, the simulated reaction rate constants (by back calculating the reaction rates from the simulated parameter concentrations) were matching well with the field observed value, thereby validating the model.

The literature studies on the reaction rate of TOC in warmer or tropical climate are less. However, it was observed that the reaction rate varies anywhere between – 0.02 to 0.09 day^{-1} in colder temperature ranging between – 6 to 27 °C (Magyan and Dempsey 2021). The reaction rate observed in the current study for TOC varied between 0.02 to 0.05 day^{-1} (at an average water temperature of 26 ± 4 °C). Long-term nutrient degradation experiments and models in literature have revealed that reaction rate constants for DOP to orthophosphates ranged from 0.001 to 0.12 day^{-1} with an average value of 0.01 day^{-1} (Thompson and Cotner 2018). These rates were geographically variable across a wide range of temperature and were as high as or higher than DOC reaction rate constants. Moreover, the total bioavailability of DOP ranged from 0 to 100% with an average of 78%, showing that DOP bioavailability was highly variable across temperature (Thompson and Cotner 2018). For the present study, the reaction rate of DOP varied between 0.04 and 0.08 day^{-1} and was higher than the DOC reaction rates.

Seasonal variation of parameters (period of 12 months) in the surface reservoirs

The simulated seasonal variations (for a period of 12 months) of (a) NO_3-N, (b) orthophosphate and phytoplankton, (c) DOC, and (d) average temperature for all the three reservoirs are given in Figs. 5, 6, and 7, respectively. It is observed that

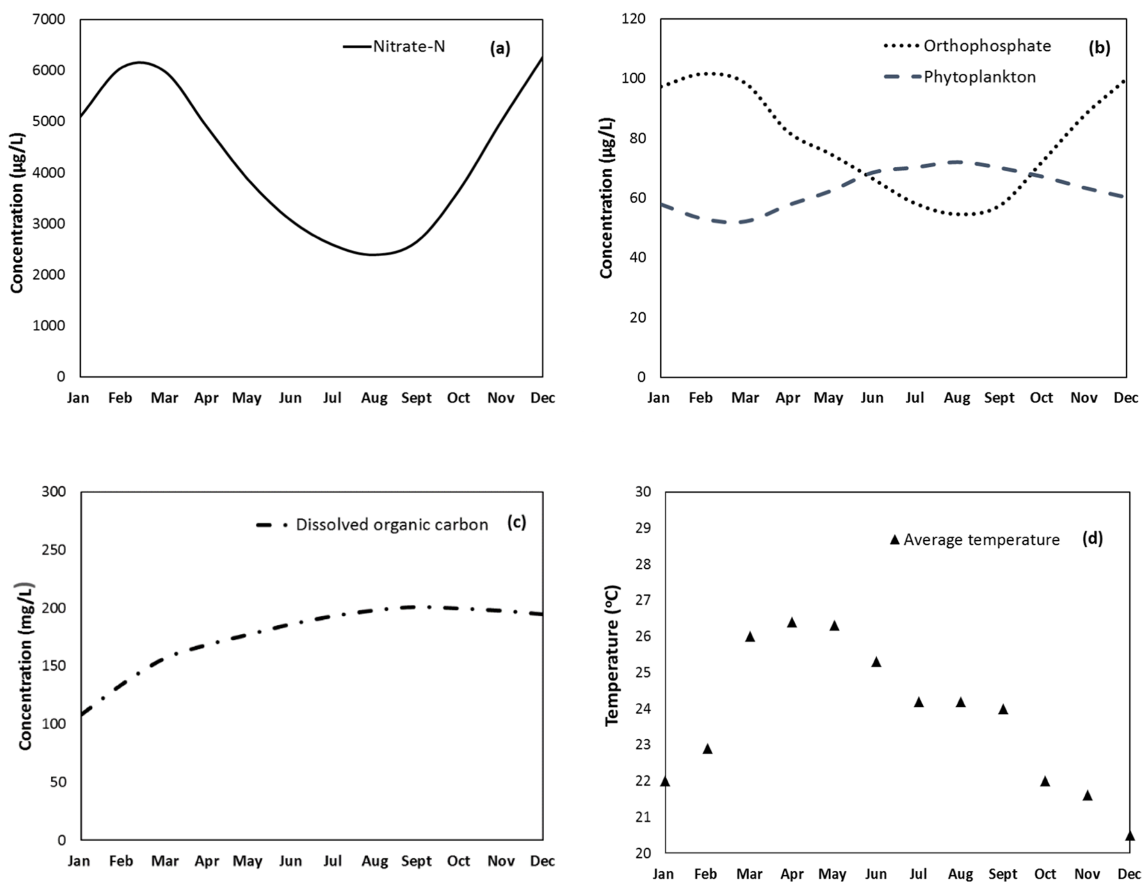


Fig. 5 Model simulation of seasonal variation (12 months) of **a** NO_3-N, **b** orthophosphate and phytoplankton, **c** DOC, and **d** average temperature at reservoir 1

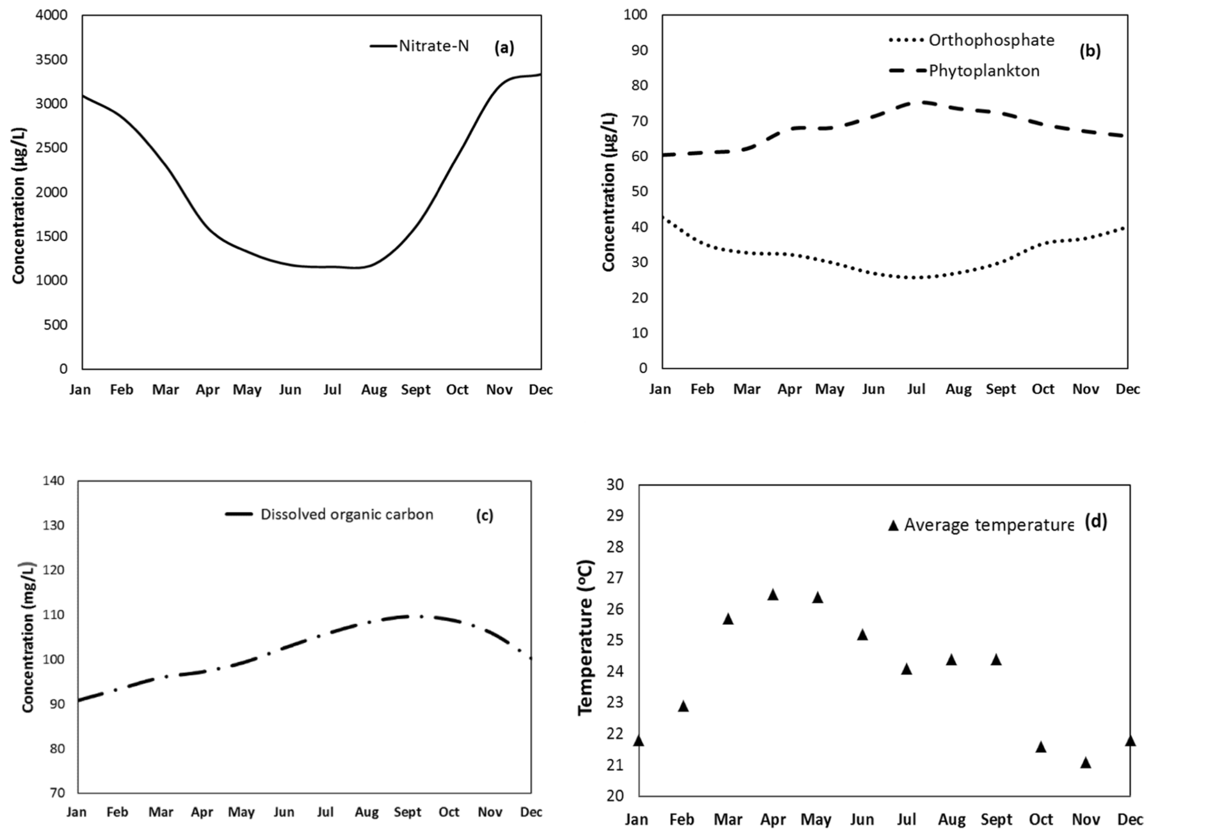


Fig. 6 Model simulation of seasonal variation (12 months) of **a** NO_3-N, **b** orthophosphate and phytoplankton, **c** DOC, and **d** average temperature at reservoir 2

the maximum growth rate of phytoplankton is in the months of July, August, and September for reservoirs 1, 2, and 3, respectively. Several studies have analyzed and concluded that the growth rate of phytoplankton increases under an optimum temperature range of 8.5–31.5 °C, with maximum growth rate attained at temperatures around 24 °C (Pulsifer and Laws 2021; Rasconi et al. 2015). Specifically for the study area (Kolar, India), for the period of July–August, the average temperatures were around 24 ± 5 °C, which was in the optimum range for plankton growth. The light availability was also favorable throughout the study period. The maximum phytoplankton concentration was observed as 76 µg/L for reservoir 3. The model predicts a gentle decline in phytoplankton biomass after the maximum growth period with the approach to turnover.

It was observed that warmer climates favored the growth of smaller autotrophic pico-phytoplankton (Rasconi et al. 2015). It was also observed that phytoplankton in warmer climate can have a different plankton structure, food web interactions, and higher community turnover as compared to their counterparts in colder climate, and that is an area of research that needs to be further explored.

The nutrient pool (nitrate–N and orthophosphates) was depleted during the maximum growth period of the plankton (Figs. 5, 6, and 7). The minimum concentrations of nitrate–N and orthophosphates were observed when the plankton concentrations in the reservoirs were at maximum. This juxtaposition of model results for phytoplankton and nutrients confirmed the applicability of the model to simulate the reservoir dynamics. The DOC concentrations were observed to increase gradually in the beginning, reaching a maximum, and then decreased at the end of the study period. As discussed before, the DOC was taken up by the planktons in the absence of a nitrogen source. Also, DOC was produced through extracellular release where organic substances were released from phytoplankton cells during the growth phase. Polysaccharides comprises of 80–90% of the total extracellular release (Myklestad 1995). The maximum DOC concentration was observed to coincide with the maximum phytoplankton concentration, proving that the possible increase in DOC is through extracellular release. During the death and lysis cycle of planktons, POC is produced as compared to DOC, which explains the decreasing DOC concentrations at the end of study period.

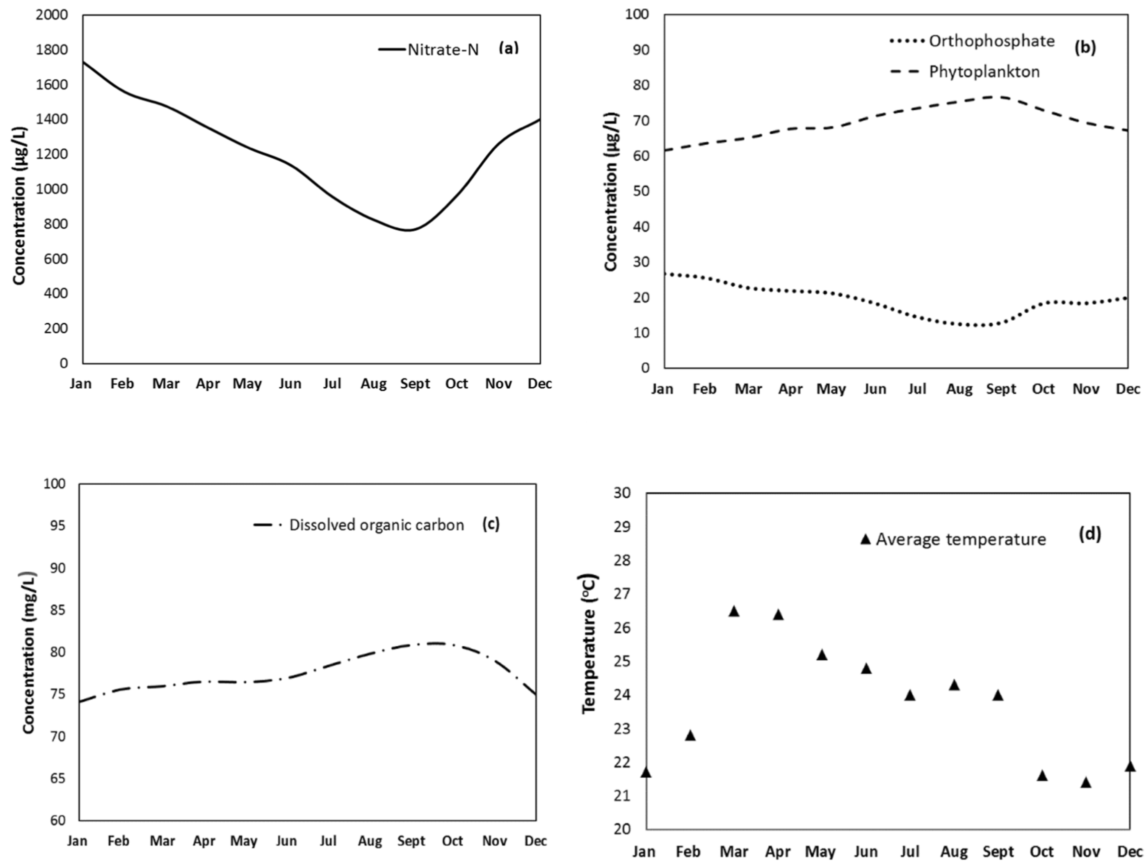


Fig. 7 Model simulation of seasonal variation (12 months) of **a** NO_3-N, **b** orthophosphate and phytoplankton, **c** DOC, and **d** average temperature at reservoir 3

Conclusion

This study proposes the use of the conceptual Lake2K model to evaluate the change in surface water quality as it passes through a series of reservoirs. The model was developed using reaction rate constants determined from field observations. The developed model was calibrated, validated, and used to investigate the seasonal fluctuations of water quality parameters. The major conclusions of the study were as follows:

- NH_4-N, NO_3-N, and the TN concentrations were significantly reduced as water moved in series through the three reservoirs due to the combined effect of nitrification, sedimentation, and nutrient uptake. The POC concentrations reduced, and DOC concentrations increased, and as a net, the TOC concentrations reduced at the outflow of all the reservoirs. The percentage reduction (from the inlet of reservoir 1 to the outlet of reservoir 3) of NH_4-N, NO_3-N, TN, TOC, and orthophosphates was observed as 90%, 78%, 79%, 67%, and 70%, respectively.
- The reaction rate constants of the water quality parameters including NH_4-N, NO_3-N, TN, TOC, and organic phosphorous were calculated as 0.043 day^{-1}, 0.04 day^{-1}, 0.043 day^{-1}, 0.055 day^{-1}, and 0.056 day^{-1}, respectively. And, these constants were on the higher end of the literature range, synonymous to the reaction rate constants observed in warmer climates.
- It was observed that the maximum growth rate of phytoplankton was in the months of July, August, and September (for reservoirs 1, 2, and 3), with the average temperature around 24 °C which is the optimum range for plankton growth.
- The minimum concentrations of nutrients (nitrate–N and orthophosphates) were observed during the maximum growth period of plankton. This juxtaposition of model results confirmed the applicability of the model to simulate the dynamics of reservoirs in series.

In summary, surface water quality monitoring is a fundamental tool for achieving SDG 6 by ensuring safe and clean water, protecting ecosystems, managing groundwater resources, promoting public health, and facilitating data-driven policies and targets.

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Author contribution K. V. (corresponding author): concept and study design, site selection, data collection, analysis, and drafting of the manuscript; R. M. T.: study design, analysis, modeling (Lake2K model), and drafting of the manuscript; M. M.: study design and review; S. J.: site selection, sample and data collection, analysis, and plotting graphs; S. R. M.: site selection, sample, and data collection; A. T. P.: site selection, sample, and data collection; L. R.: conception, designing of the study, and review of the article.

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Data availability The datasets used and analyzed during the current study are available from the corresponding author on reasonable request.

Declarations

Ethics approval and consent to participate Not applicable.

Consent for publication Not applicable.

Competing interests The authors declare no competing interests.

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