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Application of QUAL2K Model for Simulating Water Quality in Hilla River, Iraq

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ABSTRACT

The quality of the water in Iraq's Hilla River has been severely degraded as a result of human activities and industrial development. The QUAL2K model, a widely used one-dimensional water quality model, was used to simulate the river's water quality parameter of CBODu and DO utilizing river and point-source flows rate as well as quality of water metrics observed along the river. Despite a severe lack of data in the research region, the QUAL2K model was determined to be an adequate instrument for the evaluation of quality of water. Simulated results of DO, BOD_5, and temperature for the period (October 2022) showed the robustness of the model. Results showed that the two parameters (CBOD and DO) ranged between (9.5 and 10.65) mg/L and between (1.425 and 3.075) mg/L, respectively. Based on statistics, good agreement was found between the model predictions and field data. Thus, using QUAL2K model is an effective tool to manage the river water quality.

Keywords: water quality; QUAL2K; management modeling; Hilla River; BOD; DO.

INTRODUCTION

Due to the necessity of water for life to exist, it is the most fundamental component of all living thing. Food is what keeps living things alive, plants create this food, and water is necessary for plant growth. No animal on earth can exist without water, which threatens billions of lives [1, 2]. Environmental contamination is thought to be a very serious threat to humanity. Rapid population growth, industrialization, urbanization, and land development next to streams put more strain on the river's pollutants. River water quality has lately been the subject of a lot of researches due to its importance as one of the major and crucial supplies for many human activities such as industries, agricultural, and water supply. A variety of anthropogenic influences, including industrialization and urbanization, have contributed to an increase in pollutant concentrations in rivers [3]. It has become increasingly clear over time that the water we drink is less safe and more hazardous, and it is extremely clear from the observation of medical statistics that many people experience water-borne illnesses on a daily basis. Low quality of water also has the unfortunate side effect of destroying aquatic life and vegetation [1, 4].

The chemical, physical, and biological properties of water determine its quality. Prior to using it for a variety of intended purposes, such as drinking water, agriculture, recreation, or industrial water usage, it is crucial to evaluate its quality in both industrialized and a number of emerging nations, the prevention of water contamination has become crucially important. It's important to understand the complex relationship between wastes load from different source and the quality of water that results in the incoming waterways. Mathematical models are the best tools for describing these interactions. Quality of water models come in a variety of varieties, and each one calls for a certain level of assurance in the model's predictions. The common popular mathematical models that may be applied for a conventional contamination effect evaluation is QUAL2E. This model was created by the "United States Environmental Protection Agency (US EPA)". One of

QUAL2E's drawbacks is that it cannot convert algal death to (CBOD). USEPA has developed a new model called QUAL2K to serve as a more contemporary rendition of the QUAL2E model. A one-dimensional, steady-flow stream quality of water model is the QUAL2K model. It involves the modeling of novel interactions affecting water quality in rivers, including the conversion of algal deaths to BOD, the nitrogen removal mechanism, and the changes in DO caused by fixed plant. The drawbacks of QUAL2E can be overcome by these new parts. In circumstances when there is a lack of data, this beneficial program is free [5].

This model was applied to the lower part of the Diyala River's dissolved oxygen (DO) and biochemical oxygen demand (BOD_5) using hydraulic and quality of water data from the water resources ministry [5]. The model predictions covered a 16.90 km extent (January-April 2014). Four bridges, each less than 1 km long, were constructed by further segmenting the Tigris and Diyala Rivers (resulting in 26 segments). In order to control the quality of water at a crucial time, QUAL2K was used to simulate different scenarios (Changes in the pollutant load, increased flow, and localized oxygenation), using the input hydro-geometric data (low flow). The findings showed that the simulated and observed readings agreed well, and that the levels of DO and CBOD, which varied between (2.51–4.80 mg/L) and (18.75–25.10 mg/L), correspondingly, did not fall within the permissible limits. In addition, the local oxygenation and pollution load modification scenarios were successful in raising DO levels. For the Gargar River in Iran, the levels of DO, pH, CBOD, NH_4-N, NO_3-N, and phosphorous were simulated using a one-dimensional QUAL2K model [6]. Data was collected at different locations and from a variety of sewage discharge devices during the rainy and dry season. Using the simulation results, it was clear that the model had caught the quality of water profiles 20 km upstream accurately. Because the local data that was used to calibrate the equipment was not good enough, the levels of dissolved oxygen and nitrite in the river slowly went down. The general condition of Klang River water quality was assessed using a quality of water index (WQI), which consisted of the following six factors: biochemical oxygen demand (BOD), dissolved oxygen (DO), chemical oxygen demand (COD), ammoniacal nitrogen (AN), suspended solids (SS), and pH. Together with water quality models and the geographic information system (GIS), a management strategy for the available water resources was chosen [7]. The main stems of the Klang River's water quality conditions were forecasted and assessed using the QUAL2K simulation model. The modeling results for the current scenario showed that BOD differs between class II and III, while DO differ between class I and II upstream of the main stem of the Klang River. The Sewerage Treatments Plant (STPs) are the principal contributors of DO and BOD pollutants in the rivers system, based on the simulated results of the 3 options. Increased DO amounts (from 0% to 40.5%) were caused by the lack of Sewerage Treatments Plant (STPs) that met standards A and B. With the assessment of the physical-chemical characteristics and the application of the gathered data, a one-dimensional model of the QUAL2K was created to replicate the water quality in the Tigris River [3]. The Tigris River's 22 kilometers was examined. The model was used to mimic the river's DO, CBOD5, conductivity, temperature, alkalinity, and pH profiles during both low-flows (January 2019) and high-flows periods (April 2019). For model calibration and verification, four sampling sites from this river as well as several places among Jadiriyah and the confluence of the Tigris and Diyala River were chosen. Al-Jadriyah Bridge (S1), Al Dura energy plant (S2), Leather Factory (S3), and the confluence are some of these stations. The main finding demonstrated that DO was accurate at the minimum DO criteria of 4 mg/L, signifying adequate health for Tigris River in the research region. However, the CBODu and the dissolved oxygen have occasionally revealed some variations between the simulated and actual datasets. The CBODu simulation values were less than 5 mg/L in January and below 2.7 mg/L in April. In addition, the amounts of DO, BOD, and alkalinity constantly increased as the distance from the headwater increased as a result of activities along the riverbank. Station 4 has the highest concentration of BOD since it is closest to the confluence of the Tigris and Diyala River. In this paper, the DO and CBODu were simulated along Hillah River using the QUAL2K model, showing the longitudinal distribution and interaction of these parameters and the impact on the river water quality.

METHODOLOGY

Study area and sampling stations

Hilla River is the main water resources in Hilla City, Iraq (Figure 1). In the city center where the study was conducted, the river passes from the Bata Bridge upstream the river to its downstream at the Al-Farsi District. The distance from Bata Bridge to Al-Farise District is around 6.8 km, which is located between the latitudes of 32°27'54.35" and 32°30'56.39" and between the longitudes of 44°26'02.09" and 44°26'27.08". The approximate bed width of the river is 40 to 60 m with an average of 50 m. Its depth ranges from 7 to 15 m, and its flow velocity ranges from 0.3 to 0.5 m/sec. The flow rates were around 90, 100, 110, 130, 140, and 150 m^3/s in a number of locations along the river. In recent years, the river has been ignored and polluted by waste, prompting studies related to water quality. The river is used for farming, drinking water, tourists visiting [8].

The air temperature reaches to more than 40 degrees Celsius during Summer. From November through April, there is few and intermittent chance of precipitation. This has been impacting the river water quality recently. Hence, river management is very important. The Hilla River and water quality sampling locations are shown in Figure 1.

Nine sampling sites on the Hilla River were chosen at the research region for the model validation and calibration for the time frame (October, 2022), (Fig. 1). From the Bata Bridge to the AL Farise region, the study reach was covered by the sampling procedure based on the water resources ministry of Iraq. The samples were taken from the sampling station in water bottles. In order to prevent unexpected property change, water sample was obtained, analysis during 24 hours to be examined while being stored at +4 °C. The samples were analyzed at the U Science Scientific Lab. Temperature, BOD_5, and DO were measured for each sample. Fields sampling and lab testing are the first primary components of this study technique. Then, running the river water quality model based on the field data is the next step in this study.

Model description

The QUAL2K is an updated generation of the QUAL2E and measures the quality of water of rivers and streams. QUAL2K is distinguished by the traits listed below [9]: (i) One-dimensional (the stream is well-mixed vertically and laterally); (ii) Steady-state Hydraulic actuators (non-uniform, steady stream is simulated); (iii) Diurnal Heat Budget (the heat budget and temperature are

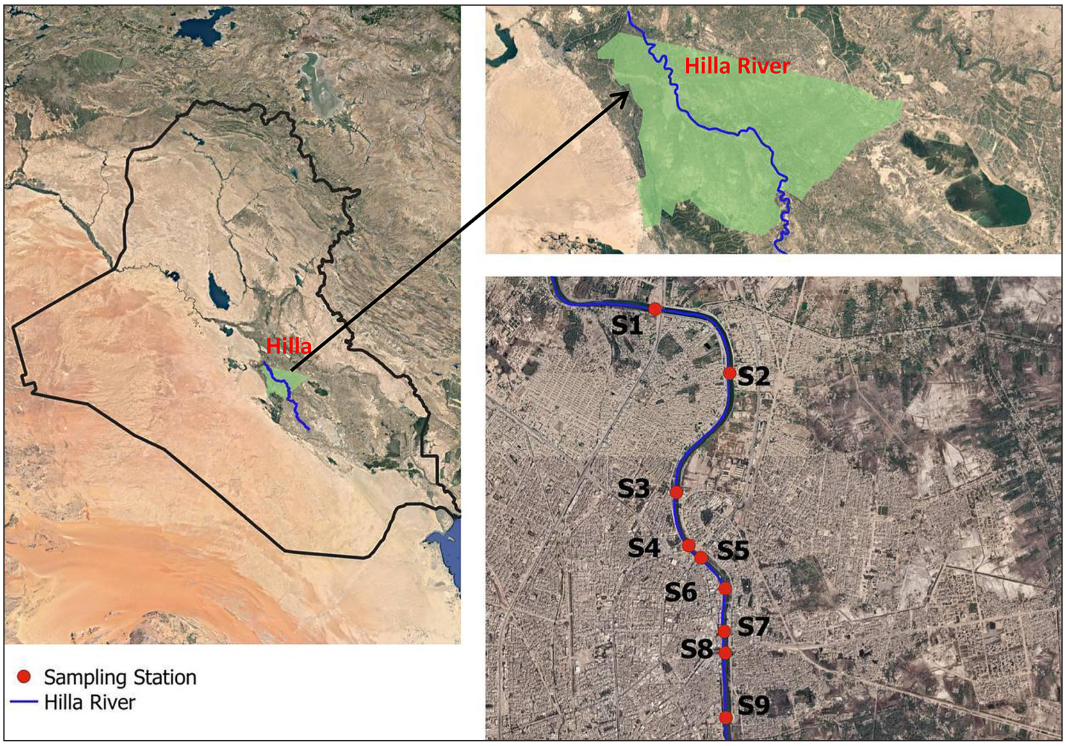

Figure 1. Map showing the study area along Hilla River

simulated as a function of meteorology on a diurnal time scale); (iv) Diurnal Water-Quality Kinetics (all water-quality variables are simulated on a (point and non-point loads and abstractions are simulated)”. The river is split into multiple reached in the QUAL2K model, then each reach is further subdivided into parts. A steady-state flows balancing is used for every modeling run:

$$Qi = Qi - 1 + Qin, i - Qab, I \quad (1)$$

where: Qi-1 – the inflows from the upstream reaches i-1 (m^3/d);
Qi – the outflows from reaching I into reaches i+1 (m^3/d);
Qab,i – the entire outflows from the reaches as a result of points and non-point abstraction;
Qin,i – the complete inflows in to reaches from points and non-point sources (both are expressed in m^3/d).

Weirs, ratings curves, and Manning formulas may all be used to determine the depth and velocities for each reach after the outflow has been determined for each one. Every river reach is treated in this study as a trapezoidal canal. The Manning equations can be employed to represent the connection among flows and depths with constant supply as follows:

$$Q = \frac{S^{\circ\frac{1}{2}}}{n} \frac{Ac^{\frac{5}{3}}}{P^{\frac{2}{3}}} \quad (2)$$

where: Q – the flow rate (m^3/sec);
$S°$ – the bottom longitudinally slope (m/m);
n – the Manning abrasion factor;
Ac – the cross-sectional area (m^2);
P – the wetted perimeter (m) [9, 10, 11].

The fundamental equation of QUAL2K is the one-dimensional advection-dispersion equations:

$$V\frac{\partial C}{\partial t} = \frac{\partial\left(AcE\frac{\partial C}{\partial x}\right)}{\partial x}dx - \\ -\frac{\partial(AcUc)}{\partial x}dx + V\frac{dc}{dt} + s \quad (3)$$

where: U (LT-1) – denotes averaged velocity;
Ac – denotes cross-sectional region (L2);
E – denotes longitudinally dispersion (L2T-1);
c – denotes concentrations (ML-3);
V – denotes volume (L3);
x – denotes distance (L);
s – denotes source and sink, which denote further inflows of water or component mass. This regulating equation is solved by QUAL2K under steady-state conditions for a component concentrations ci in the water column of a stream reach i (excluding hyporheic exchange) (Figure 2).

This results in a generic mass material balance (the loads and transportation factors for the modelling of bottom algae are excluded), which can be written as follows [12, 13]:

$$\frac{dci}{dt} = \frac{Qi-1}{Vi}ci - 1 - \frac{Qi}{Vi}ci - \\ -\frac{Qab,i}{Vi}ci + \frac{Ei-1}{Vi}(ci+1-ci) + \\ +\frac{Ei}{Vi}(ci+1-ci) + \frac{Wi}{Vi} + Si \quad (4)$$

where: Qi – stands for stream at achieve i (L/d);
Qab,i – for abstraction stream at achieve i (L/d);

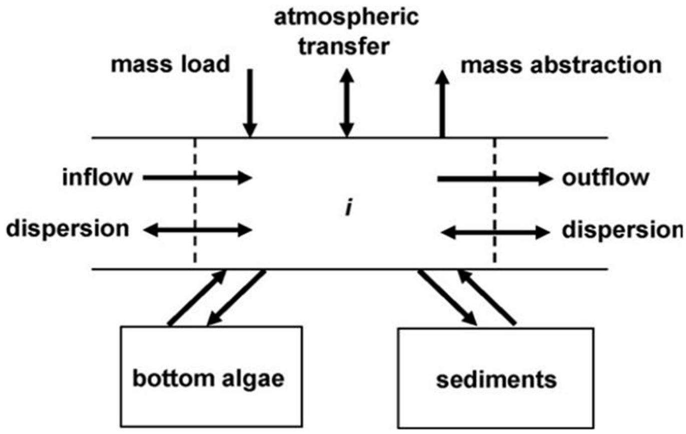

Figure 2. Mass balance in a reach segment I (from Chapra et al., 2006)

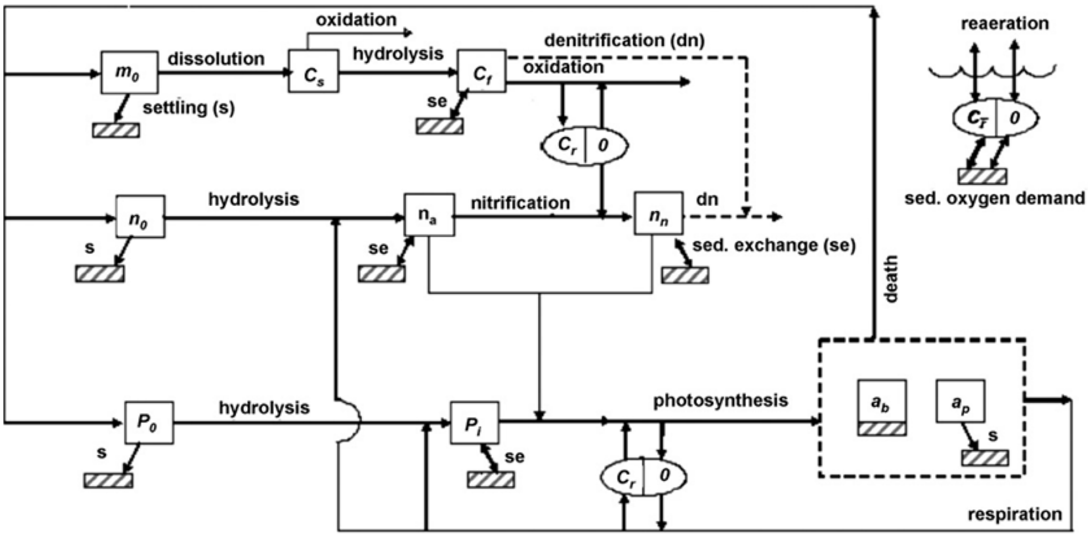

Figure 3. Schematic diagram of interacting water quality state variables (from Chapra et al. 2006)

Vi – for reach i's volume (L);
Wi–fortheconstituent'simpactload(mg/d);
Si – for the constituent's sources and sinks because of reaction and fluid flow techniques (mg/L/d);
Ei – for the bulk diffusion coefficient among extends (L/d);
Ei1 and *Ei+1* – for the bulk.

The model's interdependent quality of water system parameters, that are viewed as sources and sinks, are schematically shown in Figure 3 (Equation 4). In [14], which contains constituent-specific governing equation, the full description of mechanisms and mathematical representation of the interdependent status parameters are provided.

Model implementation

The Hilla River (6.8 km research area) has been split into six levels, along with the sites of the detected point source of water (Figure 4). The QUAL2K modelling program is built on this fragmentation. The model assumes 1.5 times the measured $CBOD_5$ [14] because it simulates ultimate CBOD. The model's input variables also contained data of river flows, temperatures, DO, and BOD_5, in addition to the following:

Geographical traits (height, longitudes, and latitudinal), meteorological traits ("temperature, wind direction, dew step, shade, cloud cover"), hydrodynamic traits ("morphological components, Manning abrasion co-efficient, stream curve"), and biological, chemical, and physical traits of rivers and local sources are all examples of geographic traits. In this study, the reach section length and geographic latitude and longitude were calculated using Google Earth. The fragmentation, placement, and length of every segments of the input model are displayed in Table 1.

The QUAL2K model was calibrated using the observed data from October 2022 (Table 2). In order to calibrate the model, several parameter of the model, such as the oxidation rates were changed until a good agreement between the values of the simulated and observed values. Equation 5, 6, and 7 show (RMSE), (MAE), and (RE) used to compare the predicted results and actual data for quality of water. Model calibration and

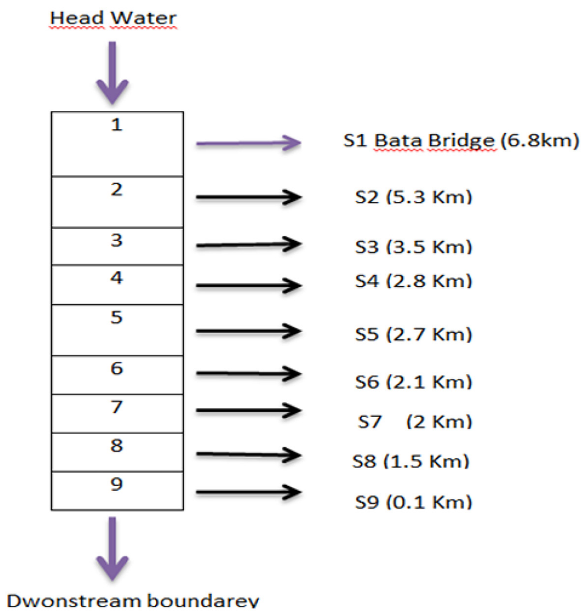

Figure 4. System segmentations with locations of pollution sources along Hilla River

Table 1. Model segmentation, location and length of each reach

Reach	Downstream	Elevation		Downstream					
	Location	Upstream	Downstream	Latitude			Longitude		
	(km)			Degree	Minute	Second	Degree	Minute	Second
S1	1.5	31	31	32	30	56.39	44	26	02.09
S2	2.4	31	31	32	30	34.53	44	26	14.81
S3	0.9	31	30	32	29	16	44	26	02.64
S4	0.5	30	30	32	29	43.1	44	26	23.21
S5	1.5	30	29	32	28	49.37	44	26	22.67

model validation frequently employ these statistical error characteristics [15, 16, 17, 18, 19].

$$\mathrm{MAS} = \frac{1}{N}\sum_{n=1}^{N}|O^n - p^n| \quad (5)$$

$$\mathrm{RMS} = \sqrt{\frac{1}{N}\sum_{n=1}^{N}(O^n - p^n)^2} \quad (6)$$

$$RE = \frac{\mathrm{MAS}}{\mathrm{Observed\ Mean}} * 100 = \frac{\frac{1}{N}\sum_{n=1}^{N}|O^n - p^n|}{\bar{O}} \quad (7)$$

where: N – number of observation–prediction pairs;
O^n – the value of observed data;
p^n – the value of the predicted data;
O – observed mean of the state variable (i.e., DO, CBOD, etc.).

RESULTS AND DISCUSSION

Observed data from field was used to calibrate the QUAL2K model. Many built-in input parameters were used to process the calibration. Data from October 2022 was used to calibrate the model. In order to boost the model's stability, the computation step has been set to 0.03 h. The model was run until the system's parameters were properly adjusted, and there was a good match between the model's predictions and field measurements. Two quality of water parameters (CBOD and DO) were included in the study. These parameters are the main stream indiction for the river health. The output of the model provides the observed and simulated concentrations of several quality of water parameters throughout the chosen river reach length. The simulation of CBODu in the specified extension is shown in Figure 5. The simulated CBOD values follow well the field data, revealing good agreement for the model robustness. The simulated results showed that the observed data for all stations listed below are very similar to the field data, with an increase in CBOD values at the selected stations (3, 4, 5) that is not seen at the other stations. This is due to the effect of the source of river pollution by organic matter.

The simulated DO values displayed in the Figure 6. Good agreement to the field conditions exist clearly, where the values are nearly constant at all stations with the exception of a discrepancy at certain locations where the water is still and not flowing. The generated curves start from the first station point and do not exhibit the tiniest changes and stay virtually constant towards the lower areas, which is the same direction as the simulated data presented by the model. The simulated values vary from 9 to 10 mg/L.

Based on Table 3, it can be concluded that all expected quality of water standards at all river stations are within the permissible limit of drinking water standard and are safe for use as a source of drinking water or for other purposes.

Based on the calibration findings, the model's effectiveness was assessed using statistical

Table 2. The measured data from the Hilla River station

Parameter	Stations of sampling								
	S 1	S 2	S 3	S 4	S 5	S 6	S 7	S 8	S 9
BODu (mg/l)	0.975	1.425	1.425	2.1	2.7	3.075	2.85	2.1	2.325
DO (mg/l)	10.4	10.65	10.4	10.5	9.65	10.45	9.85	10.5	9.5
Temperature C°	23.4	23.65	23.4	23.3	23.35	23	23	23	23

metrics (MAE, RMS, and RE). Table 4 displays the MAE, RMS, and RE for three stations during calibration period between predicted and actual value for quality of water indicators.

Thus, the observed and anticipated DO and BOD values match together well. These values of MAE, RMS, and RE show very small differences between the simulated and predicted values. The acceptable error values demonstrate that the QUAL2K models is a useful tool for predicting the quality of water of rivers and can be utilized to support management of quality of water and decision-making, particularly in developing countries where the sources of finance for repeated observation advertisements and higher accuracy analysis [20]. As listed in Table 4, there is an inverse link between temperature and dissolved oxygen. In addition, there are temperature drop and dissolved oxygen concentration rises. As a result, it is clearly that the temperature almost constant. Dissolved oxygen, on the other hand, showed a rise from 9.5 to 10. Additionally, there

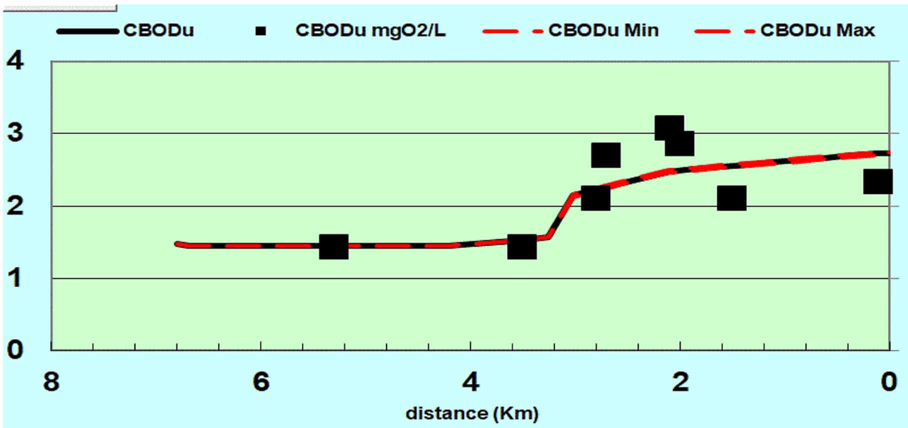

Figure 5. Simulated CBODu profile along the study area

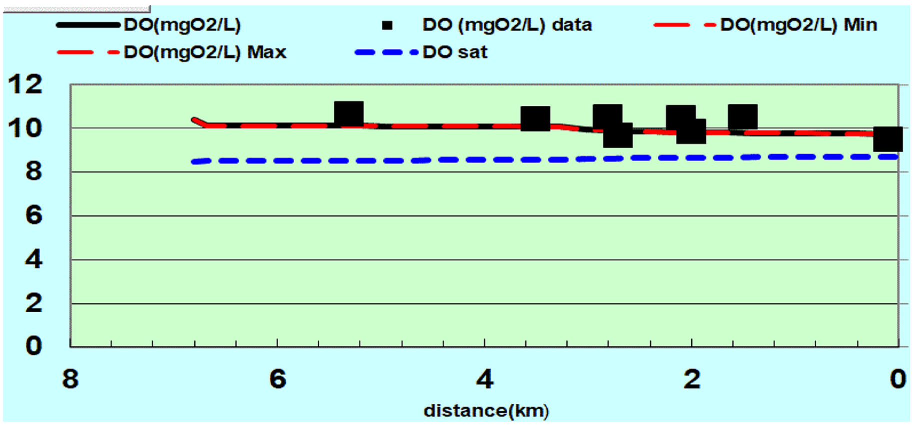

Figure 6 Simulated DO profile along the study area

Table 3. The concentration of parameters predicted at the Hilla River study area

Parameter	Name of station								
	S 1	S 2	S 3	S 4	S 5	S 6	S 7	S 8	S 9
CBODu (mg/l)	1.47	1.45	1.53	2.23	2.31	2.40	2.48	2.54	2.73
DO (mg/l)	10.4	10.11	10.08	9.91	9.88	9.85	9.82	9.80	9.75

Table 4. Statistical errors for the predicted and measured quality of water parameters

Parameters	Mean absolute error (MAE)	Root mean square error (RMS)	Relative error (RE)%
CBODu (mg/l)	0.337	0.386	0.15
DO (mg/l)	0.362	0.436	0.787

is an inverse link between the BODs value and dissolved oxygen. Nevertheless, several limitations that may be encountered when modeling the river, including the prediction of extraction efficiency from non-point source including livestock and discharge from agricultural operations. Thus, the model was able to forecast the quality of the water in various scenarios [21]. The model's outputs have demonstrated that the study area's dissolved oxygen levels are above 4 mg/L minimum standards level [22–25].

CONCLUSIONS

QUAL2K river water quality model was used to simulate Hilla River water quality at the Hilla City for management purposes. The study focused on the parameters: CBOD and DO due to their impact on the river health. The main findings showed that the indicators (CBOD and DO) ranged between 9.5 and 10.65 mg/L and between 1.425 and 3.075 mg/L, respectively, along the river. It is obvious that QUAL2K simulated the river's water quality efficiently due to the very low statistical errors and can be used as a useful tool for directing managements strategies for the Hilla River. Thus, more researches are required regarding optimization strategies and accuracy assessment under different conditions based on the use of QUAL2K.

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