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# Assessment of Management Scenarios for the Remediation of River Water Quality Based on Self-Purification (Case Study: Dez River)

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## Abstract

The most sustainable and cost-effective approach to enhance river water quality is by actively managing its self-purification. This study's aim is to explore potential management scenarios for enhancing the river's self-purification capacity. The QUAL2Kw model was used to simulate the water quality and self-purification capacity in Dez River in Iran. The model was calibrated and validated using recorded data of three monitoring stations along the river. Five parameters, namely DO, BOD, COD, NO<sub>3</sub>-N, and NH<sub>4</sub>-N were calculated and compared with field data. The Margin of Safety was presented and added to the value of each parameter for better water management and protection. Sensitivity analysis was conducted to identify the most influential parameters in water quality simulation for Dez River. The study presented and compared the self-purification capacity across six proposed scenarios for managing water quality. The results showed that the oxidation rate, nitrification rate, and denitrification rate were the most influential parameters in simulating water quality using QUAL2Kw. Among the scenarios considered, the fourth scenario, which included urban and industrial sewage point sources as diffuse sources, exhibited the highest level of self-purification, estimated at 2,246,170.01 kg/day. In all scenarios, the self-purification capacity for COD exceeded that of other parameters along the river, with the highest COD self-purification reaching approximately 167,034.9 kg/day.

**Keywords:** Margin of Safety, QUAL2KW Model, Self-Purification, Sensitivity Analysis, Water Quality.

## 1. Introduction

Rivers play a vital role in providing water for various purposes including industrial, urban, and agricultural uses. However, human activities such as urbanization and industrialization have a significant impact on the quality of river water (Singh et al., 2005). The entry of nutrients and biodegradable pollutants into rivers, including sanitary wastewater, agricultural and industrial residues can significantly affect the water quality and

disturb the Dissolved Oxygen<sup>1</sup> balance (Zhang et al., 2015).

The river reception capacity or the self-purification should remain within acceptable limits to have a proper water qualities management. Different management approaches or regulatory measures have been developed to sustain water quality, such as ambient water quality standards, total emission caps (Jolma et al., 1997).

<sup>1</sup> Dissolved Oxygen (DO)



Among all the approaches, river self-purification is the most cost-efficient approach for water quality control. However, with the increase in water usage and pollution, the river self-purification capacity could also be significantly affected. It is important to keep the water usage and pollution level within certain limits to sustain the river self-purification capacity ([Campolo et al., 2002](#)).

One of the most cost-effective ways to study water quality along rivers and their self-purification is to use simulation through numerical models, which have been widely used by researchers such as: ([Rehana and Mujumdar, 2011](#); [Zhang et al., 2012](#); [Zhang et al., 2015](#); [Indriani et al., 2016](#); [Cristea and Burges, 2010](#); [Babamiri et al., 2021](#); [Zare Farjoudi et al., 2021](#); [Pashmchi et al., 2022](#)).

Two classes of simple models and comprehensive models are used in water quality simulation studies. Simple models are easy to use but cannot describe complex fluid dynamic processes. In contrast, comprehensive models are difficult to calibrate but these models are able to describe complex fluid dynamics. However, complex models may not be the most useful tool in some studies with the lack of field data for calibration ([Lindenschmidt, 2006](#)). Some complex models have been developed for different systems, such as river systems (QUAL series), river-reservoir systems (WQRRS, WASP and CE-QUAL-W2). The QUAL2Kw model is the latest model of the QUAL series that is widely used in rivers and canals to evaluate the impacts of urban, industrial and agricultural wastewaters' pollutants ([Chapra and Pelletier, 2006](#)). This model has been used to determine the maximum daily load into rivers in the United States and many other countries ([Gikas, 2014](#)). Additionally, hydraulic properties of rivers can also be simulated using the QUAL2Kw model ([Bottino et al., 2010](#); [Gikas, 2014](#)).

The QUAL2Kw model is a highly accurate and comprehensive tool for simulating river water quality. It has the capability to simulate a wide range of quality parameters, making it a versatile and effective model ([Pelletier et al., 2006](#); [Chapra et al., 2008](#)). QUAL2Kw is a model that simulates the transport and fate of conventional (i.e., non-toxic) pollutants across the rivers.

The QUAL2Kw model has been used to simulate the level of BOD ([Fang et al., 2008](#), [Zare Farjoudi et al., 2021](#)), Nitrogen (N), Phosphorus (P) and COD ([Fan et al., 2009](#); [Grabic et al., 2011](#); [Babamiri et al., 2021](#)).

Some others used the QUAL2Kw for water quality management practice ([Gardner et al., 2007](#); [Azzellino et al., 2006](#); [Grabic et al., 2011](#); [Lin et al., 2010](#); [Saadatpour et al., 2019](#); [Pashmchi et al., 2022](#)).

Kannel et al. applied the QUAL2Kw model in Bagmati River in Nepal. It was found that the model was highly sensitive to water depth ([Kannel et al., 2007a](#)).

Oliveira et al. evaluated the model application for small basin rivers and a good agreement with field data was noted ([Oliveira et al., 2012](#)). The model was successfully applied in simulating the maximum and

minimum water temperatures in the United States ([Cristea and Bureges, 2010](#)).

QUAL2Kw provides a good simulation for DO in a river system comparing to other models. Many studies can be found using this model for analysis of river water quality purposes ([Pelletier et al., 2006](#); [Anh et al., 2006](#); [Fan et al., 2009](#); [Camargo et al., 2010](#); [Cho and Ha, 2010](#); [Gikas, 2014](#); [Sarda and Sadgir, 2015](#); [Mehrasbi and Farahmandkia, 2015](#); [Gupta et al., 2013](#)).

The model has been proved as a solid tool for water quality simulation with good validation ([Syafi'i and Masduqi, 2011](#)).

Heidarpour and Jamshidi, utilized the QUAL2Kw model to simulate the water quality of the Tajan River and determine location of the allocation of pollution ([Heidarpour and Jamshidi, 2019](#)).

Hoseini assessed the effectiveness of the QUAL2Kw model in examining the self-purification process of the Qarasu River. The study evaluated the model's performance in simulating pH, DO, BOD, NO<sub>3</sub>, and temperature during two different time periods. The findings of this research explored various levels of simulation capability of the model based on these parameters. The results demonstrated the model's satisfactory accuracy in simulating the mentioned parameters ([Hoseini, 2019](#)).

The QUAL2Kw model was used by ([Aryaee Nezhad et al., 2019](#)) to assess the water quality of the Shahrood River. The study found that the simulation accuracy of the model varied for each parameter, depending on its fluctuations along the river.

Maghsoudi et al. used the QUAL2Kw model to analyze the water quality of Beheshtabad river. The study focused on simulating various parameters including DO, BOD, T, EC, pH, and NO<sub>3</sub> ([Maghsoudi et al., 2021](#)).

The self-purification of AbbasAbad mountain river in Hamadan province was examined by ([Babamiri et al., 2021](#)). Their findings indicated that the oxidation rate has the most significant impact on the river's self-purification in mountainous rivers, and the power of self-purification is enhanced by the flow of headwater.

In the ([Farkhani, 2021](#)) study, the QUAL2kw model was used to assess the quality of Haraz River. The results revealed that the river's self-purification has been severely compromised as a result of the excessive release of sewage, particularly in relation to the BOD parameter.

Rafiee et al. investigated the self-purification of Baliqhli-Chai and Qare-sou rivers using the QUAL2Kw model in Ardabil province, their results showed that the most self-purification in the above rivers is related to the NO<sub>3</sub> parameter ([Rafiee et al., 2023](#)).

Also, studies have been conducted on the water quality simulation of the Dez River using the QUAL2Kw model, as demonstrated by ([Ghorbani et al., 2020](#); [Abdovis Sabdovis et al., 2020](#); [Jamalianzadeh et al., 2022](#)).

These studies have shown the accuracy of the model in simulating pollution parameters. However, it is



important to note that the focus of these studies was solely on simulating quality variables along the Dez River, and no management solution based on the river's self-purification was provided.

The Dez River has been severely polluted in recent years due to the discharge of urban and industrial sewage and agricultural effluents. On the other hand, one of the basic sources of water supply is the agricultural and industrial sector of Dez Plain. Hence, managing the water quality of the Dez River is essential, necessitating cost-effective solutions that include leveraging the river's self-purification capacity.

Therefore, the objective of this study is to model the water quality variables (DO, BOD, COD, NH<sub>4</sub>-N, and NO<sub>3</sub>-N) of the Dez River using QUAL2Kw and assess its self-purification capacity under current conditions as well as proposed scenarios. These scenarios include the removal of urban and industrial wastewater, treating urban and industrial sewage point sources as diffuse sources, and changes in upstream flow rates.

The study involves the following steps:

1. Simulating qualitative parameters (DO, BOD, COD, NH<sub>4</sub>-N and NO<sub>3</sub>-N) using the QUAL2Kw model.
2. Conducting sensitivity analysis to identify the parameters that have a significant impact on river water quality.
3. Determining the safety margin to improve the reliability of parameter simulation.
4. Calculating the self-purification capacity of the river under existing conditions, and proposed scenarios.

## 2. Materials and methods

### 2.1. Study area

Dez River, located in the southwest of Iran, plays a crucial role in the economic, social, and environmental well-being of southwest Iran. The river's water quality management is critical due to the various types of wastewaters (municipal, agricultural, and industrial) that pollute it, as it is the most significant source of water supply in the region. The Dez River basin has an area of about 21720 km<sup>2</sup>, divided into upstream and downstream by the Dez dam. It flows from north to south, with an average basin elevation of 1603 m. This study focuses on the downstream section, which is 173.78 km long, extending from Dez dam to Band-e Ghir (Fig. 1). The gross area of arable land around the Dez river from the Dez dam to Band-e Ghir is approximately 245,000 hectares. The study area has a semi-arid climate, an annual precipitation of 252.38 mm, an annual temperature of 25.1 °C, and a total evaporation of approximately 2035 mm. The Dez dam reservoir and river are the primary surface water sources in this area, while deep and semi-deep wells in the Dez plain serve as another source. Both surface and groundwater sources are utilized to meet the agricultural, drinking, and industrial needs of the region (Babamiri et al., 2021). Fig. 1 shows the study area's location, including plains, cities, rivers, and hydrometric stations.

### 2.2. Data and pollution sources

Many parameters are required for river water quality simulation, including hydraulic data in segments of river (headwater flow, river bed slope, river side slope, river width, and Manning's roughness coefficient), meteorological data (air temperature, wind speed, dew point temperature, solar radiation, and cloud cover fraction), and water quality of point sources and nonpoint sources (DO, BOD, COD, NO<sub>3</sub>-N, NH<sub>4</sub>-N, and surface water inflow).

Khuzestan Water and Power Authority (KWPA) and Khuzestan Department of Environment (KDOE) are the two main authorities of Dez River water quality monitoring and supervision (KWPA, 2001). Hydrometric and quality data at the stations, namely Dezful, Harmaleh, and Bamdezh were collected from KWPA and wastewater discharge data (point sources) were gathered from KDOE. Moreover, hydrodynamic data were obtained from the Dezab Engineering Company. Table 1 represents average values of quantitative and qualitative characteristics corresponding to the most important sources of pollutants in the study area. It can be seen that the concentration of BOD in urban and industrial pollutants is significantly higher than that of agricultural effluents, on the other hand, the amount of NO<sub>3</sub>-N in agricultural effluents is higher than urban and industrial wastewaters. It can also be seen that from 81.5km to the end of the river, the amount of NO<sub>3</sub>-N and COD increased significantly.

Fig. 2 shows the headwater discharge changes in fluctuation and its trend line in August at Dezful station from 1983 to 2021. As it can be seen, there is a decreasing trend in Dezful station discharge in August.

### 2.3. Quality simulation (QUAL2Kw)

QUAL2Kw model is used for qualitative simulation of Dez river (from the Dez dam to BandeGhir), which is bolded in Fig. 1. QUAL2Kw is the latest model of the QUAL model series which was approved by the United States Environmental Protection Agency (USEPA) and is widely used to simulate river water quality (Kannel et al., 2007a).

The framework represents the river as a one-dimensional channel with a non-uniform, steady flow, and simulates the impact of both point and non-point pollutant loadings. To determine the "concentration of qualitative parameters" in this model, the Finite difference method is used for the numerical solution of the Advection-Diffusion Equation (Chapra et al., 2008).

The QUAL2Kw model is capable of simulating over 15 qualitative parameters including DO, BOD, COD, temperature, NH<sub>4</sub>-N, NO<sub>3</sub>-N, pH, EC, etc., in the river.

The Dez River section was divided into a list of fragments (143 sections) based on the river's hydraulic conditions and pollutant discharge site as shown in Fig. 3. The general mass balance equation in the *i* section water column for all constituent concentrations can be written as (Equation 1):



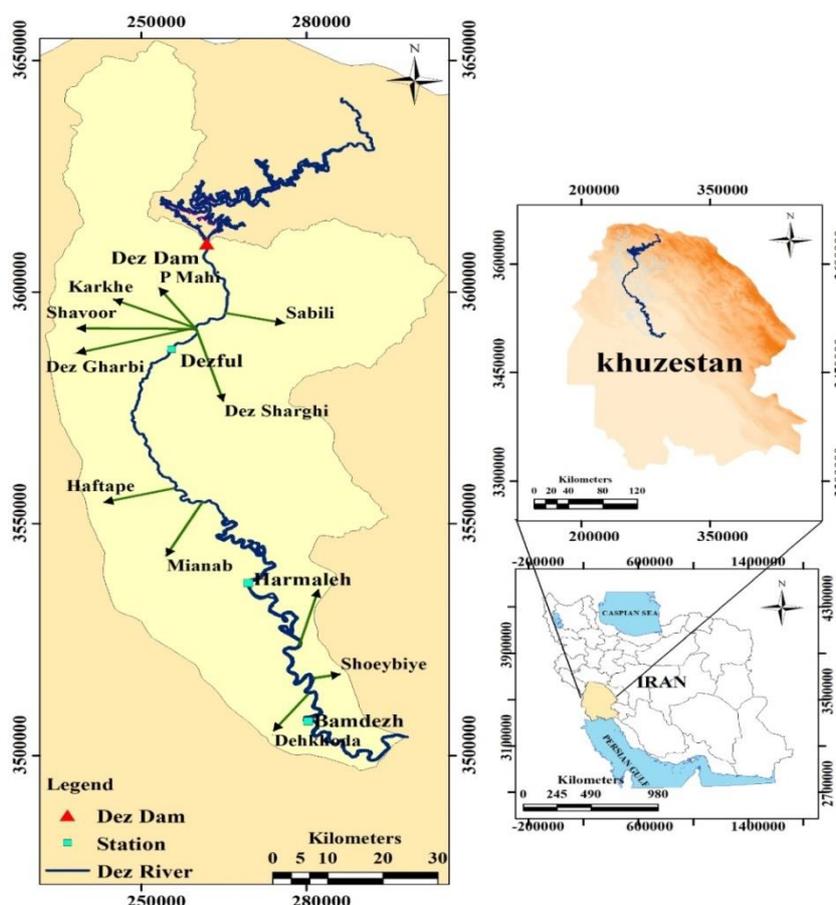


Fig. 1. Location of study area in Iran and Khuzestan province

Table 1. Average amount of river flows and monthly wastewater values of point sources pollutants

Sources	Name	Distance (Km)	Q (m <sup>3</sup> /s)	T (°C)	DO (mg/L)	BOD (mg/L)	COD (mg/L)	NH <sub>4</sub> -N (µg/L)	NO <sub>3</sub> -N (µg/L)
Urban wastewater (Pollutant sources)	Dezful	8.6	2.4	28	3.4	94.2	101.2	3500.4	2378.5
	Safiabad	26.6	0.4	24	4.7	20.8	50.7	2457.1	956.1
	Hor	37.5	0.5	24	5.2	23.8	47.6	1127.6	742.5
	Mianrood	40.3	0.6	24	4.8	25.6	51.4	2832.1	662.3
Industrial wastewater (Pollutant sources)	P Mahi	23.2	5.2	24	2.5	22.1	49.6	480.6	3688.5
	K Hafttapeh	38	1.8	26	4	110.6	66.3	421.8	2266.2
	Kagz Pars	69.2	0.6	28	2.2	150.3	53.2	1300.5	2026.3
Agricultural drainage (Pollutant sources)	Loor	4.7	1.3	16	6.2	3.8	26.3	856.3	1638.5
	Sabzab	23.5	3	24	8.1	4.2	27.8	945.4	2745.1
	Banehasan	31.4	1.3	26	7.6	3.2	32.1	1089.9	1683.2
	Sagari	33.2	4.2	23	8.7	3.7	21.5	1154.3	2596.4
	Haftapeh	43.3	1.3	25	7.6	2.4	29.7	784.1	2230.7
	Salimeh	55	2.8	24	6	3.3	32.4	952.4	2524.9
	Tapdarin	55.4	1.2	26	7.4	4.2	30.5	844.5	3884.3
	Atij	65.2	2.3	25	6.9	4.3	25.7	621.6	1920.5
	Mianab	107.5	3.5	29	3.1	2.8	33.4	951.7	2180.6
	Kharvar	134.7	2.2	31	3.5	5.5	44.3	723.6	2940.4
Hydrometric station	Shoaybiyeh	167.9	11.1	27	7.2	7.3	29.4	983.8	2655.4
	Dezful	0	174.9	18.2	8.6	3.6	4.1	302.8	813.37
	Harmaleh	81.5	123.4	28.6	5.5	3.5	12.6	382.1	1671.9
	Bamdezh	136.6	116.9	29.7	4.8	3.8	12.4	318.4	1717.1

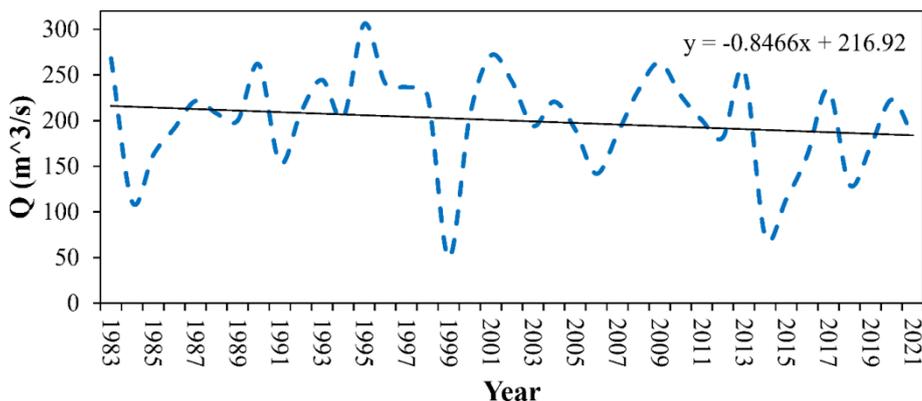


Fig. 2. The time series of August discharge in Dezful station, (1983-2018)

$$\frac{dc_i}{dt} \frac{Q_{i-1}}{V_i} c_{i-1} - \frac{Q_i}{V_i} c_i \frac{Q_{ab,i}}{V_i} c_i \frac{E_{i-1}}{V_i} (c_{i-1} c_i) \frac{E_i}{V_i} (c_{i+1} c_i) \frac{W_i}{V_i} + S_i + \frac{E_{hyp,i}}{V_i} (c_{2,i} - c_i) \tag{1}$$

Where

$c_i$ : is the concentration of a given water quality parameter in the reach  $i$  in terms of  $g/m^3$ ,  $V_i$ : is the volume of water passed from the elements of  $i$  in  $m^3/d$ ,  $t$ : is the time in terms of  $d$ ,  $E_i$ : is the emission factor between the reach  $i$  and  $i+1$ ,  $Q_i$ : is the flow rate in the  $i$ th reach in  $m^3/d$ ,  $W_i$ : is the external loading on quality parameter for the  $i$ th reach in terms of  $g/d$ ,  $S_i$ : is the production and consumption of quality parameter due to reactions and mass transfer mechanisms in the reach  $i$  in terms of  $g/m^3/d$ ,  $C_{2,i}$ : is the concentration of water quality reach in the hyperheic sedimentary zone and  $Q_{ab,i}$ : is the discharge of output pollutant of the  $i$ -th interval in  $m^3/d$ , which includes total point and non-point pollutants.

The QUAL2Kw model employs Manning's equation

to determine the flow velocity within each reach (Fig. 4), as depicted in equation 2 (Chapra et al., 2008)

$$Q = \frac{S_0^{1/2} A_c^{5/3}}{n P^{2/3}} \tag{2}$$

### 2.4. Sensitivity Analysis

The sensitivity analysis is conducted here to identify the input parameters that may have the maximum impact on DO, BOD, COD,  $NO_3-N$ , and  $NH_4-N$  values in output. Herein, the variations in oxidation rate, nitrification rate, and denitrification rate have been compared.

The normalized coefficient of sensitivity ( $S_{ij}$ ) is used here to determine the change rate in output variables for a certain percentage of change for each input variable (Palmieri and De Carvalho, 2006; Babamiri et al., 2021):

$$S_{j,i} = \frac{\partial y_j}{\partial x_i} \times \frac{y_j}{x_i} \tag{3}$$

Where

$S_{j,i}$  is Sensitivity analysis of the  $j$ th variable to the  $i$ th parameter,  $\partial y_j$  is the change rate in the variable  $j$ .  $y_j$  is initial value of the variable  $j$  (before change),  $\partial x_i$  is the

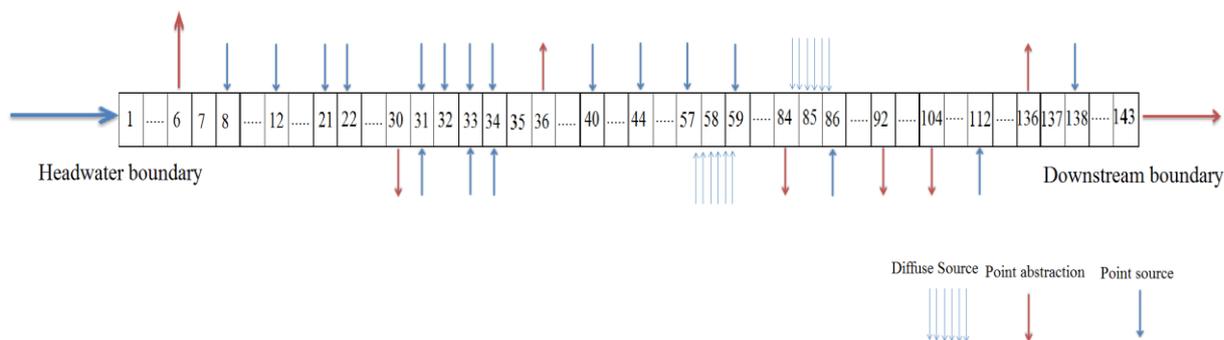


Fig. 3. Detachment pattern of the proposed simulation

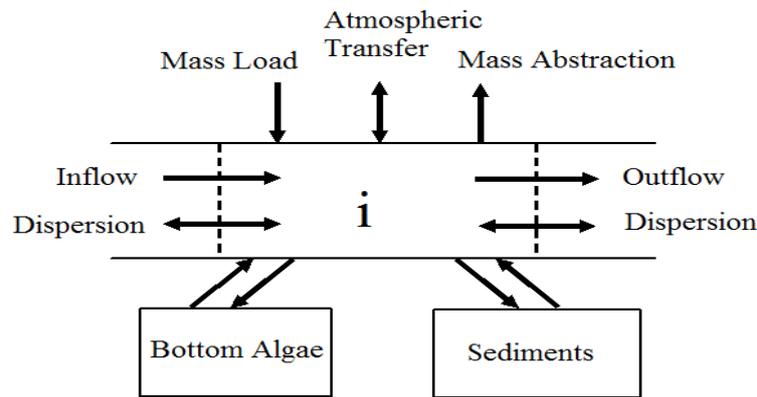


Fig. 4. Mass balance diagram in a distinct reach

change rate in the value of the input parameter  $i$ , and  $x_i$  is the initial value of the input parameter.

### 2.5. Model calibration and validation

The primary goal of Calibration is to reduce the disparity between the model output and the observed data. This objective is typically accomplished by accurately estimating the model parameters through optimization techniques. The QUAL2Kw model includes a sheet named Rates, where a set of parameters with specific ranges is defined. By adjusting each parameter within its range based on river conditions and comparing observed and simulated values, the model can be calibrated for the specific river. The key parameters considered in this study for pollution variables were the oxidation rate, nitrification rate, and denitrification rate. The model is automatically calibrated using a genetic optimization algorithm, aiming to minimize the variance between observations and simulations. The parameters defined in the Rates sheet serve as the decision variables for this process (Chapra et al., 2008). The model was calibrated by using the recorded data of three stations, namely Dezful, Harmaleh, and Bamdezh. The field data of dry season (August) from 2017 to 2020 were used to model calibration. Later, the data of August 2021 were used to model validation.

After the calibration and validation phases, the model error was determined by calculating the NSE (Nash and Sutcliffe Error), Standard Error (SE), and Mean Absolute Error (MAE) statistics as shown in equations 3, 4 and 5:

$$NSE = 1 - \frac{\sum_{i=1}^n (X_i^{obs} - X_i^{sim})^2}{\sum_{i=1}^n (X_i^{obs} - X_i^{mean})^2} \quad (4)$$

$$SE = \frac{RMSE}{X_{obs}^{mean}} = \sqrt{\frac{\frac{1}{n-1} \sum_{i=1}^n (X_i^{obs} - X_i^{sim})^2}{X_{obs}^{mean}}} \quad (5)$$

$$MAE = \frac{1}{n-1} \sum_{i=1}^n |X_i^{sim} - X_i^{obs}| \quad (6)$$

Where

$n$  is number of pairwise data,  $X_i^{obs}$  is the observed value,  $X_i^{sim}$  is the simulated value, and  $X_i^{mean}$  is

the mean of observed data for constituent being evaluated.

### 2.6. Self-purification

The self-purification of water systems is a complex process that often involves physical, chemical, and biological processes working simultaneously. In this study Ammonia ( $NH_4-N$ ), Nitrate ( $NO_3-N$ ), Chemical Oxygen Demand (COD), Biochemical Oxygen Demand (BOD) and DO parameters were selected for analysis. All of the four parameters are the main indicators of the river contamination. It is necessary to calculate the input load as well as the total outlet load from the beginning of the river to the control point to evaluate the ability of self-purification. The amount of self-purification is calculated here from the following equations (Indriani et al., 2016):

$$P_c = L_i - L_o \quad (7)$$

In which,  $P_c$  is the amount of self-purification,  $L_i$  and  $L_o$ , are the total input and output load, respectively.

The input load ( $L_i$ ) in the  $i$ th reach is calculated from the following equation:

$$L_i = (Q_h \times C_h) + (Q_p \times C_p) + (Q_{np} \times C_{np}) \quad (8)$$

Where

$Q$  and  $C$  are the discharge ( $m^3/s$ ) and concentration of the quality parameters, respectively. The indexes  $h$ ,  $np$ , and  $p$  refer to the headwater, non-point and point sources, respectively.

The output load ( $L_o$ ) in each branch is calculated using the following equation:

$$L_o = Q_{c.p} \times C_{c.p} \quad (9)$$

Where

$Q$  and  $C$  are the same as the previous definition, and the sub index  $c.p$  refers to the control point.

#### 2.6.1. Scenarios

Six hypothetical scenarios were proposed to improve the water quality of the river, considering the headwater

flow and providing cost-effective and applicable solutions as follows.

1. The self-purification with normal discharge of upstream flow;
2. The self-purification with upstream flow rate decreases by 20%;
3. The self-purification with removed urban and industrial sewage point sources;
4. The self-purification with considering urban and industrial sewage point sources as diffuse sources. Herein, each point source is evenly distributed within 5 kilometers of the river;
5. The self-purification with scenario 2 + scenario 3 (reduction of upstream flow by 20% plus removal of urban and industrial sewage point sources);
6. The self-purification with scenario 2 + scenario 4 (reduction of upstream flow by 20% plus considering point sources as diffuse sources).

According to (Krenkel and Novotny, 1980), the water quality of rivers can be categorized into the four distinct classes. Class 1 represents the best water quality and is suitable for most general purposes, and class 4 shows the worst water quality, which is inappropriate for most of the applications. Owing to the climatic and economic conditions of Iran, class 1B is selected for Dez River. According to (Krenkel and Novotny, 1980) standard, the allowed thresholds for DO, BOD, COD,  $\text{NH}_4\text{-N}$ ,  $\text{NO}_3\text{-N}$  parameters for class 1B are equal to 5 mg/L, 5 mg/L, 25 mg/L, 500  $\mu\text{g/L}$ , and 10,000  $\mu\text{g/L}$ , respectively.

### 3. Results and discussion

#### 3.1. Sensitivity analysis

The results of sensitivity analysis are presented in Table 2. Parameters of DO and BOD related to denitrification and nitrification rates had the lowest sensitivity coefficients (0.039, 0.006) while oxidation rate had the highest coefficient sensitivity (0.8, 0.217). A similar conclusion can be found in the works of (Sharma et al., 2015; Ahsan 2004; Paliwal et al., 2007; Parmar and Keshari, 2012).

The COD had the greatest sensitivity to the intake discharge. Meanwhile, it was neutral to oxidation rate, nitrification and denitrification. The finding is consistent with that of the (Kannel et al., 2007b).

Parameters of  $\text{NO}_3\text{-N}$  and  $\text{NH}_4\text{-N}$  had the greatest sensitivity to nitrification. The  $\text{NO}_3\text{-N}$  was less sensitive

to oxidation rate and  $\text{NH}_4\text{-N}$  is neutral to BOD oxidation and denitrification rate. The river had the highest effect from nitrification rate (82%) on  $\text{NO}_3\text{-N}$  and from BOD oxidation (80%) on dissolved oxygen, which can be supported by (Oliviera et al., 2012).

#### 3.2. Models' calibration and validation

The NSE, SE, and MAE calculations are presented to evaluate the simulation results, as shown in Table 3. A very good model performance based on NSE achieved in simulation process for all the parameters. The computed values of NSE for calibration and validation lies within the ranges of 0.779~0.961 and 0.916~0.995, respectively, which implies a satisfactory simulation when using the preset model. In calibration phase, the highest SE was equal to 11.95 % for COD, and the lowest SE value was about 5.74% for BOD. In validation process, the highest SE was 6.38% for BOD, and the lowest value was 2.34% obtained for  $\text{NH}_4\text{-N}$ . The range of SE calculated from the present simulation was an indicator of how good the validated model was. Also, the low MAE indicated a good simulation of the models.

#### 3.3. Margin of safety (MOS)

The MOS reflects the effects of uncertainty of stochastic parameters that are not considered in the modeling that may cause a difference between simulation and observation. The margin of safety was calculated by obtaining the probability distribution of simulation errors (the difference between simulated and observed data). The value representing the probability of not exceeding 50% was then derived from this distribution. This error value, equivalent to the probability of exceeding 50%, was added to the simulated model values as a safety margin in the simulation. Fig. 5 shows the cumulative of selected variables. It was found that, the parameters of DO, BOD, and COD followed the normal distribution. The parameters of  $\text{NH}_4\text{-N}$  followed the Pearson distribution; while  $\text{NO}_3\text{-N}$  followed the log-normal distribution. Overall, the normal distribution had the best fit with the data. The MOS values of DO, BOD, and COD were equal to 0.12, 0.02 and 0.22 mg/L, respectively. The MOS values of  $\text{NH}_4\text{-N}$ , and  $\text{NO}_3\text{-N}$ , were about 60.54, and 16.98  $\mu\text{g/L}$ , respectively. The above MOS values can be added to the simulated parameter to better protect water resources.

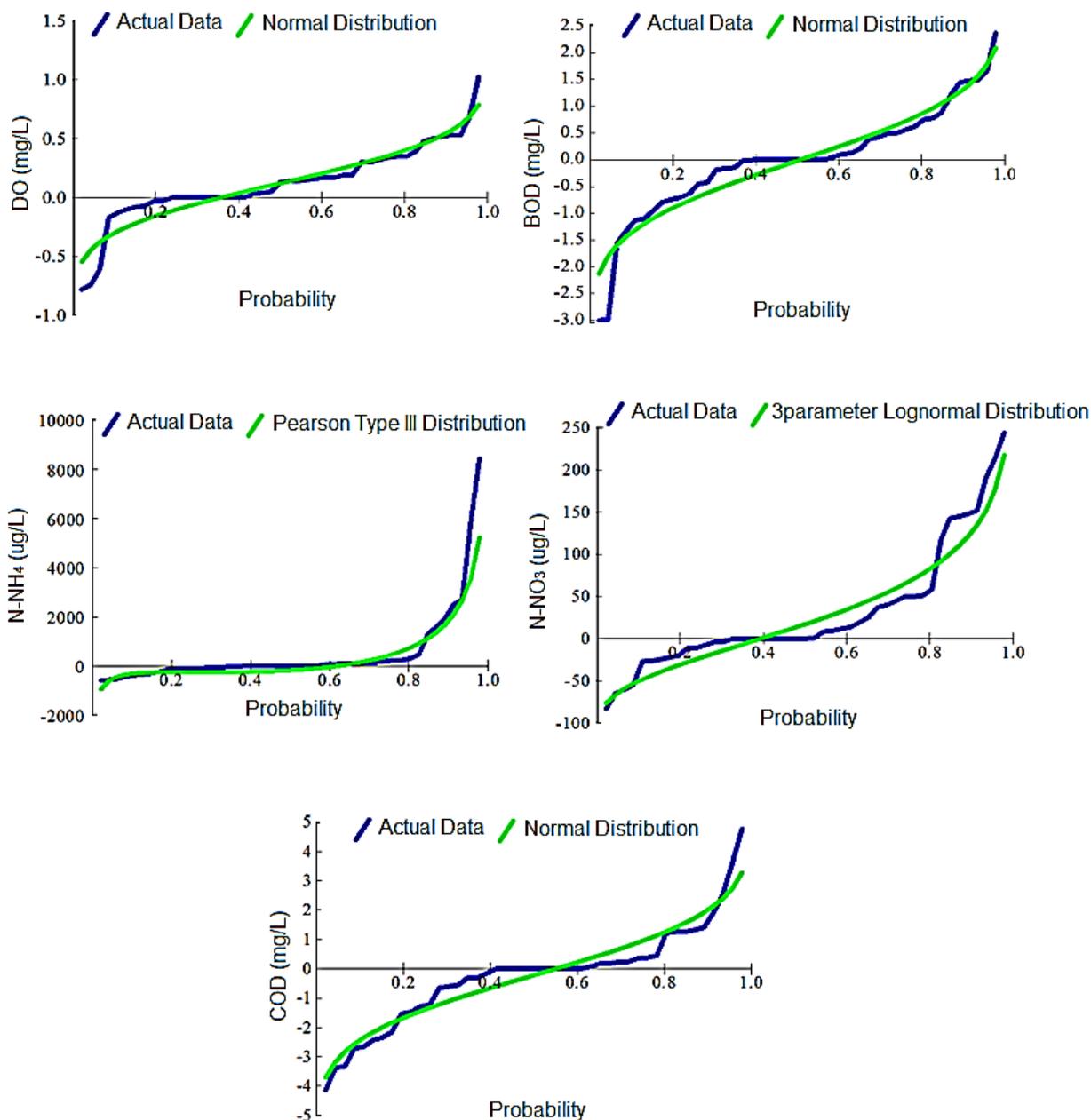
Table 2. Sensitivity analysis for the parameters

	Oxidation rate	Nitrification rate	Denitrification rate	Head water flow	Point source flow
DO	-0.8	-0.711	0.039	0.072	-0.119
BOD	-0.217	-0.006	-0.028	-0.143	0.026
COD	-0.02	0.019	0	-0.121	0.019
$\text{NH}_4\text{-N}$	0.03	-0.44	0	-0.173	0.347
$\text{NO}_3\text{-N}$	-0.014	0.821	-0.33	0.085	0.211



**Table 3.** The performance criteria of QUAL2KW in both calibration and validation of phases

Parameter	Calibration			Validation		
	NSE	SE%	MAE	NSE	SE%	MAE
DO (mg/L)	0.956	5.78	0.19	0.995	3.04	0.09
BOD (mg/L)	0.779	5.74	0.10	0.916	6.38	0.16
COD (mg/L)	0.845	11.95	0.21	0.921	4.53	0.17
NH <sub>4</sub> -N (µg/L)	0.815	9.58	19.50	0.988	2.34	4.90
NO <sub>3</sub> -N (µg/L)	0.961	8.65	83.18	0.971	5.11	51.96



**Fig. 5.** The cumulative probability of distribution of the selected parameters in the present study

### 3.4. Scenarios analysis

Fig. 6 shows the variation of parameters namely DO, BOD, COD,  $\text{NH}_4\text{-N}$ ,  $\text{NO}_3\text{-N}$  for the first and second scenarios compared with the existing conditions along the Dez River. According to the first scenario (upstream normal discharge), DO increased by 3.1% compared to the existing condition. But, the values of BOD, COD,  $\text{NH}_4\text{-N}$ , and  $\text{NO}_3\text{-N}$  decreased by 2.7%, 12%, 6.5%, and 6.6%, respectively. According to this scenario, the water quality of the river has improved. In the second scenario (20% reduction in upstream discharge), the DO value

decreased by 2.9, while the values of BOD, COD,  $\text{NH}_4\text{-N}$ , and  $\text{NO}_3\text{-N}$  increased by 4.4, 19.3, 10.9 and 10.7, respectively. The rate of BOD exceeded the allowable threshold of Class 1B from 6.5 km to 19.7 km and 39.6 km to 50.8 km of the river. Accordingly, the amount of contaminants entering the river in a reach from the upstream to 50.8 km should be reduced by 8461.4 kg/day.

The change trends of the studied parameters under these two scenarios were the same with the changing trends of the existing condition along the river.

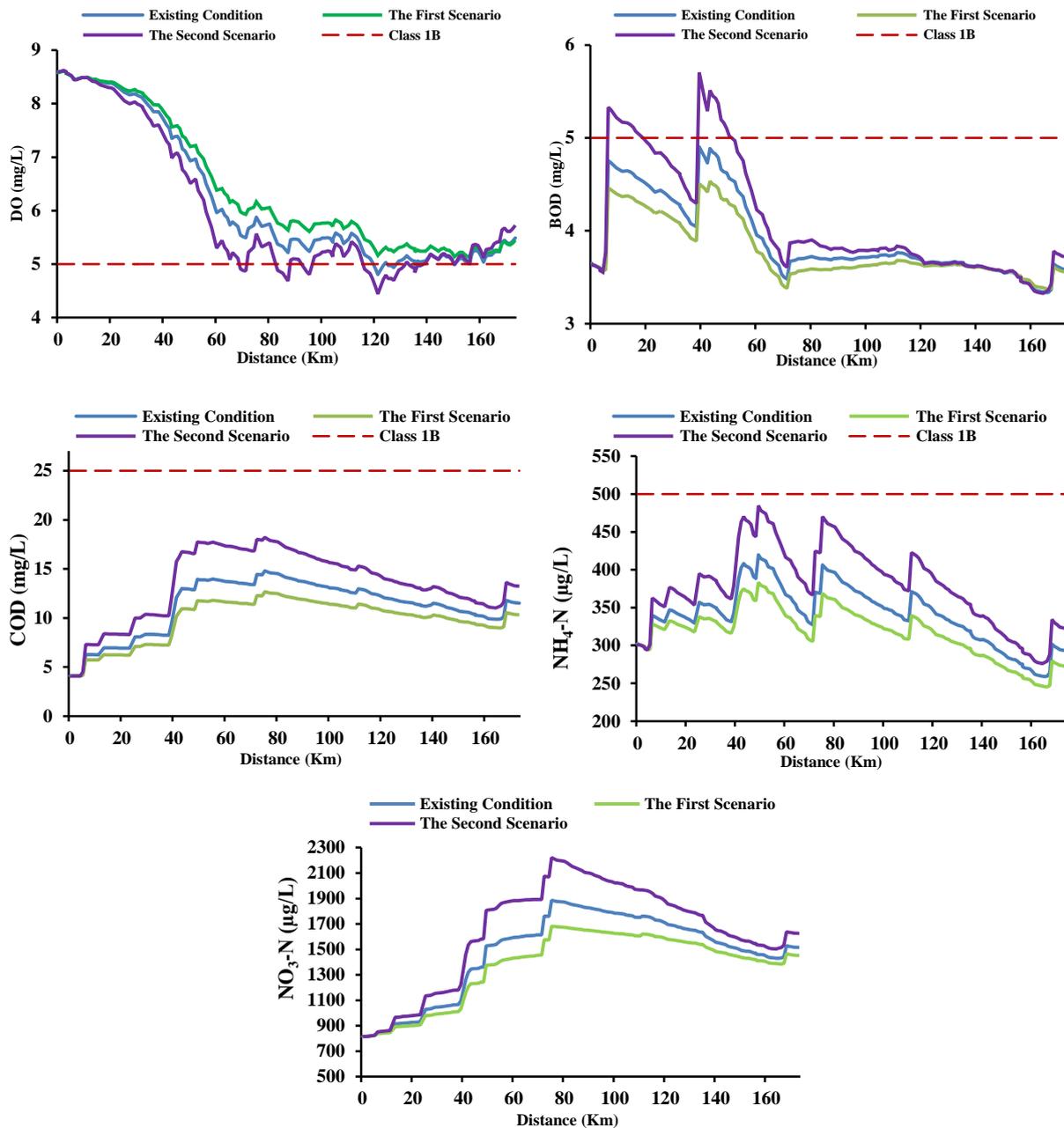


Fig. 6. Concentration of DO, BOD, COD,  $\text{NH}_4\text{-N}$ , and  $\text{NO}_3\text{-N}$ , parameters under the first and second scenarios compared to existing condition



Fig. 7 shows the variation in parameters of DO, BOD, COD, NH<sub>4</sub>-N, and NO<sub>3</sub>-N for the third and fourth scenarios compared to the existing conditions. Under the third scenario (removal of urban and industrial wastewater point sources entering the river), the DO value increased by 21% compared to the existing condition. Also, the amount of BOD, COD, NH<sub>4</sub>-N, and NO<sub>3</sub>-N parameters decreased by 28.1%, 71.4%, 52.6% and 40.3% along the river, respectively. According to this scenario, the change trend for DO was similar to the existing condition change trend, but the other parameters have a different trend than the existing situation.

The BOD value decreased from the beginning of the river to 72.9 km. It increased later from 72.9 km to the end of the river. The values of COD and NH<sub>4</sub>-N were decreased slightly through the river. The trends NO<sub>3</sub>-N was insignificant along the river. Under the fourth scenario (the distributed of urban and industrial point

sources pollution along the river) the DO value increased by 10.9% compared to the existing condition. The BOD value remained unchanged along the river but the amount of COD, NH<sub>4</sub>-N, and NO<sub>3</sub>-N decreased by 40.1%, 36.2%, and 31.5%, respectively along the river. The water quality of the river improved under this scenario, in other words, the self-purification of the river for the parameters of COD, NH<sub>4</sub>-N, and NO<sub>3</sub>-N increased by the distribution of urban and industrial wastewaters along the river.

The BOD values are lower than existing condition from 76.2 km to 129.1 km and are higher from 129.1 km to the end of the river. The change trends of COD, NH<sub>4</sub>-N, and NO<sub>3</sub>-N parameters from upstream to 39.3 km of the river were similar to the change trend in the existing condition; however, a descending trend observed from the 39.3 km to the end of the river.

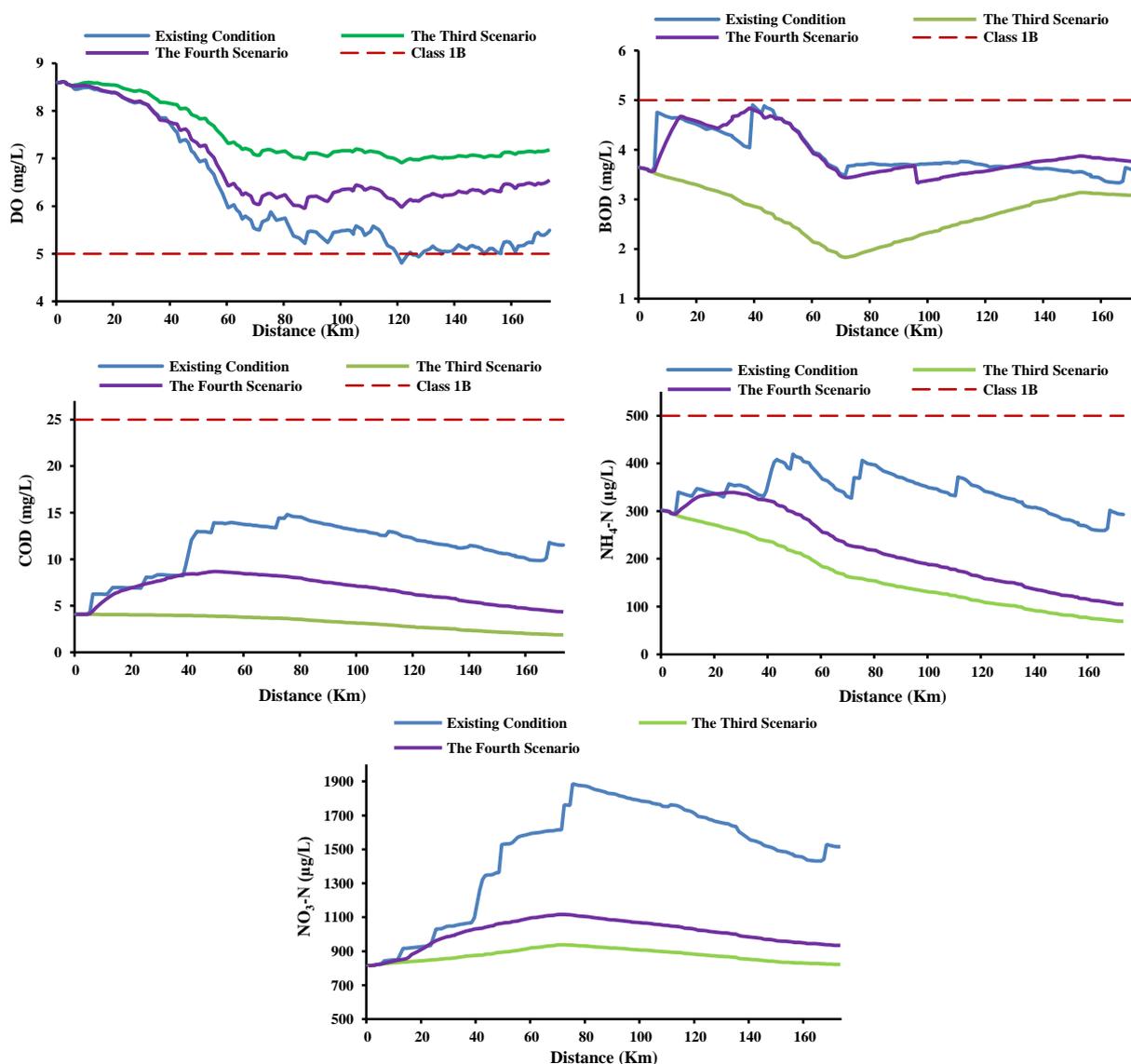
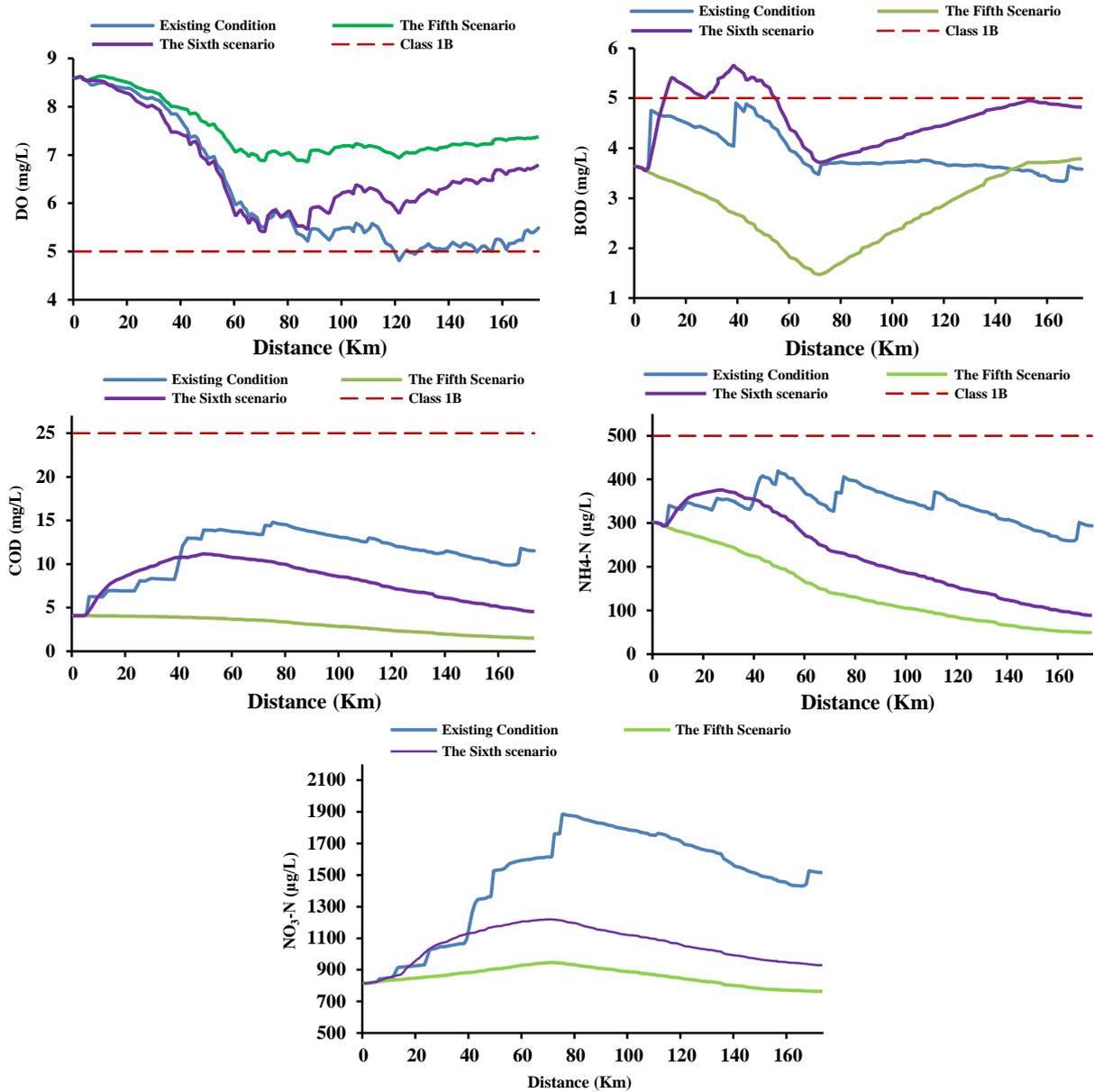


Fig. 7. Concentration of DO, BOD, COD, NH<sub>4</sub>-N, and NO<sub>3</sub>-N, parameters under the third and fourth scenarios compared to existing condition





**Fig. 8.** Concentration of DO, BOD, COD, NH<sub>4</sub>-N, and NO<sub>3</sub>-N, parameters under the fifth and sixth scenarios compared to existing condition

Fig. 8 shows the variations in the parameters of DO, BOD, COD, NH<sub>4</sub>-N, and NO<sub>3</sub>-N for the fifth and sixth scenarios compared to the existing condition along the river. Under the fifth scenario, the DO value increased along the river by 20.7%, but the amount of BOD, COD, NH<sub>4</sub>-N, and NO<sub>3</sub>-N decreased by 25.8%, 73.2%, 57.9%, and 41.7%, respectively. The change trends of the studied parameters in this scenario were similar to the third scenario. Under the sixth scenario, the amount of DO increase by 8.8%. Along the river, the BOD value increased by 5.7%, and the values of COD, NH<sub>4</sub>-N, and NO<sub>3</sub>-N decreased by 29.3%, 35.2%, and 28.4%, respectively. The BOD value exceeded the allowable

threshold of the Class 1B between the 13.3 km and 53.7 km of the river. Under these conditions, the amount of contaminants entering the river from the upstream to 53.7 km should be reduced by 10321 kg/day. The change trends of the studied parameters in this scenario were similar to that of the fourth scenario.

### 3.5. Self-purification capacity

Table 4 shows the results for the self-purification capacity of the Dez River based on the aforementioned scenarios. According to the Table 4, the highest rate of self-purification for the BOD was 42666.36 kg/day, obtained in the third scenario, which was 1970.33 kg/day



**Table 4.** The self-purification capacity (kg/day) based on the studied scenario of the studied parameters in the Dez River

Scenario	BOD	COD	NH <sub>4</sub> -N	NO <sub>3</sub> -N
Existing condition	40696.03	71296.04	4042.16	2407.95
The scenario 1	41143.91	71568.17	4449.89	3101.10
The scenario 2	37853.59	70852.13	3613.41	1495.05
The scenario 3	42666.36	161876.50	5876.29	10176.06
The scenario 4	40753.61	167034.91	6331.75	10496.74
The scenario 5	38452.57	158180.96	5370.01	10052.88
The scenario 6	39379.74	1620375.24	5802.91	10232.86

higher than the rate in the existing condition. In other words, the removal of urban and industrial point sources pollution from the river led to an increased self-purification for BOD, so that, it takes the highest value compared to the other scenarios. The highest values for COD, NH<sub>4</sub>-N, and NO<sub>3</sub>-N were 167034.91 kg/day, 6331.75 kg/day and 10496.74 kg/day, respectively, which were obtained in the fourth scenario. In other words, the distribution of urban and industrial point sources pollution into the river result in an increased self-purification for these parameters, so that, they take the highest value compared to the other scenarios.

In each scenario, the highest amount of self-purification was related to the COD parameter, and the highest amount of self-purification belonged to the COD was 167034.9 in whole river length. By comparing the first and second scenarios, it can be found that, the amount of self-purification capacity increased with an increase in the amount of upstream discharge. In other words, the capacity of self-purification along the river affected by the amount of upstream discharge. Similar conclusions can be found in the works of (Kannel et al., 2007b; Marzouni et al., 2014).

#### 4. Discussion

The studies conducted so far using the QUAL2Kw model show the acceptable accuracy of the the model in simulating water quality parameters in rivers such as BOD, DO, COD, NO<sub>3</sub>-N, P-PO<sub>4</sub>... (Moghimi Nejad et al., 2018; Babamiri et al., 2021; Rafiee et al., 2023; Farkhani, 2021).the study of the self-purification of the Dez River showed that with the increase in the discharge of the headwaters, the amount of self-purification of the river increases, which can be due to the increase in the amount of dissolved oxygen in the river as well as It has been found in studies by (Moghimi Nejad et al., 2018; Rafiee et al., 2023) that, they have shown that river self-purification increases during wet seasons.

In this research, the self-purification capacity of the Dez River was found to be greater for the COD parameter compared to other parameters. Conversely, the study by Rafiee et al., in 2023 on the Balighli-Chai River in Ardabil province revealed that the NO<sub>3</sub>-N parameter exhibited higher self-purification potential than the other parameters studied. The examined pollution parameters demonstrated a remarkable sensitivity to both Oxidation

Rate and Nitrification Rate, aligning with the findings of (Babamiri et al., 2021) study on the Abbas Abad Mountain River. This investigation also indicated that as point-source pollution spreads along the river, the river's self-purification capacity significantly increases. This phenomenon can be attributed to the expansion of pollution sources, resulting in a greater extent of self-purification opportunities for the river.

#### 5. Conclusion

Six theoretical management scenarios aimed at enhancing the self-purification of the river to improve water quality were suggested. To achieve this objective, the QUAL2Kw model was used to simulate the qualitative parameters within the Dez River in Iran. The results of the applied scenarios demonstrated that relocating and dispersing urban and industrial wastewater discharge points along the river resulted in a noteworthy enhancement of the river's self-purification capacity. The findings indicate that in all the suggested scenarios, the self-purification of COD in the Dez River surpasses that of other quality parameters. In simpler terms, the COD value decreases more significantly with the improvement of river self-purification compared to other parameters along the river. It can be concluded that the amount of river upstream discharge has a great effect on the amount of self-purification of quality parameters. The sensitivity analysis of the parameters revealed that the oxidation rate and nitrification rate have the most significant impact on the qualitative parameters examined in Dez River.

Rivers undergo numerous transformations throughout their extensive courses, and they possess a degree of inherent self-purification capability, enabling the removal of various pollutants. Consequently, it is imperative to take measures to preserve and enhance this self-purification capacity, a task achievable solely by safeguarding the integrity of this precious resource. This necessitates the prevention of pollution, especially from agricultural waste, domestic, and industrial wastewater.

Another proposed approach in the ongoing research aims to efficiently control river water quality by enhancing its self-purification ability through careful consideration of the timing and intensity of pollutant discharge. In other word, optimizing the timing and



intensity of pollution discharge using evolutionary optimization methods according to the objective function of the amount of self-purification.

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## 7. Conflicts of interest

The authors declare no conflict of interest.

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