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Numerical Simulation of Water Quality and Self-Purification in a Mountainous River Using QUAL2KW

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ABSTRACT. Understanding the water quality in mountainous rivers is critical for sustainable water resources management. By using the rivers' self-purification to improve water quality is also the most economical and sustainable way to clean water. In the present study, the QUAL2KW model is applied to investigate the water quality and self-purification capacity in a mountainous river. The Abbasabad River in Iran is used as the study site. The river is divided into two intervals based on the main purpose of water usage: drinking and agriculture. The model is calibrated and validated using field data from five monitoring stations along the river. Six parameters, COD, BOD, DO, P-PO_4, N-NO_3, and N-NH_4 are calculated and compared with field data. The Margin of Safety (MOS) is presented and added to the value of each parameter for better water resources protection. The sensitivity analysis is conducted to identify the most influential parameters in water quality simulation for mountainous rivers. It is revealed that the parameters of oxidation rate, nitrification rate, and denitrification rate have the maximum influence on water quality simulation for mountainous rivers using QUAL2KW. Additionally, three scenarios are tested for water quality and self-purification. It is found that the river flow rate has a stronger impact for water self-purification in mountainous rivers and the location of point-source pollution has very limited impact.

Keywords: margin of safety (MOS), mountainous river, QUAL2KW, self-purification, TMDL, water quality

1. Introduction

Rivers are important water resources and main arteries of water supply for industry usage and urban consumption. Most of the major rivers have headwaters in highlands and more than half of humanity relies on the freshwater that accumulates in mountainous rivers (Karamouz et al., 2004). Mountainous rivers are also important sources of fresh water for both drinking and agricultural purposes. However, the water quality in mountainous rivers could be significantly impacted by human activities due to industrialization (Singh et al., 2005). Different management approaches have been developed to sustain water quality, such as, ambient water quality standards, total emission caps (Jolma et al., 1997). 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).

Numerical modeling is a cost-efficient tool to investigate river water quality and self-purification capacity, which has been widely used in the past to simulate the reaction of river systems to pollutants all over the world (Oliveira, 2012), such as India (Rehana and Mujumdar, 2011), China (Zhang et al., 2012, 2015). There are simple models and comprehensive models in the water quality simulation. Simple models are easy to apply, which cannot describe complex fluid dynamic processes. In contrast, comprehensive models are difficult to calibrate considering complex fluid dynamics. Complex models may not be the most useful tool in some studies with the lack of field data for calibration (Lindenschmidt, 2006). Complex models have been developed for different water systems, such as river systems (WASP), river-reservoir systems (WQRRS and CE-QUAL-W2). QUAL model is widely used in rivers and canals to evaluate the impacts of agricultural pollutants (nitrogen and phosphorus) (Chapra and Pelletier, 2003). 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 can also be simulated in this model (Bottino et al., 2010). The QUAL2KW model is the latest model of the QUAL series and one of the most comprehensive models is water quality simulation. QUAL2KW is a modernized framework for the simulation of water quality in streams and rivers, which can track the transport of conventional (non-

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toxic) pollutants. The framework represents the river as a one-dimensional channel with non-uniform, steady flow, and simulates the impact of both point and non-point pollutant loadings. QUAL2KW can be used to simulate a wide range of parameters, including temperature, dissolved oxygen, electrical conductivity, pH, BOD, suspended solids, ammonium nitrogen, organic phosphorus (Pelletier and Chapra, 2008; Chapra et al., 2008), BOD (Fang et al., 2008), Nitrogen (N), Phosphorus (P) and COD (Fan et al., 2009). The model can also be used for water quality management practice (Lin et al., 2010).

The model has been well used by many researchers around the world. Gardner et al. (2007) used the model to investigate the water quality issues in a watershed in Mexico. The pollutant sources in European freshwater resources were examined and integrated for sustainable water management (Azzellino et al., 2006). Kannel et al. (2007) applied the QUAL2KW model in Bagmati River of Nepal. It is found that the model can be highly sensitive to water depth. The model was successfully applied in simulating the maximum and minimum water temperature in the United States (Cristea and Bureges, 2010). Additionally, QUAL2KW provides a good simulation for dissolved oxygen comparing to other models. Further studies can be found in Gupta et al. (2013), Pelletier et al. (2006), Sarda and Sadgir (2015).

The model has been proved as a solid tool for water quality simulation. However, to date, very limited research can be found to apply this model in mountainous rivers. To fill in this gap, the present study is conducted. The self-purification capacity in a mountainous river in Iran is tested using TMDL (Total Maximum Daily Load) method under three scenarios. Six water quality parameters (DO, BOD, COD, N-NH_4, N-NO_3 and P-PO_4) are simulated and compared with field data. The Margin of Safety (MOS) is added to self-purification for better water protection.

2. Methodology

2.1. Study Area

The Abbasabad River basin is located in the province of Hamedan, Iran, which is a mountainous region with the elevation varies from 3,312 m to 1,951 m (Figure 1). The total length of the Abbasabad River is 18 km long, which flows from South to North. The field data of May, June and August between 2011 and 2012 were used for model calibration, which were collected by the Environmental Protection Agency of Hamadan from five monitoring stations. The data in May, June and August 2015 were used for model validation. The – following parameters were collected during the proposed month: COD, $CBOD_f$, DO, PO_4-P, NO_3-N, and NH_4-N. The simulation was carried out in two seasons, wet season (May and June) and dry season (August). The Manning's coefficients (0.028 ~ 0.035) were used based on field measurement.

Many parameters are required for river water quality simulation, including hydraulic data in each fragment (headwater flow, river bottom slope, river side slope, river bottom width, and manning's coefficient), meteorological data (temperature, wind speed, dew point temperature, solar radiation, and cloud cover percentage), and water quality of point sources and non-point sources (COD, $CBOD_f$, DO, PO_4- P, NO_3-N, NH_4-N, and surface water inflow). The detailed requirement can be found in Chapra and Pelletier (2008).

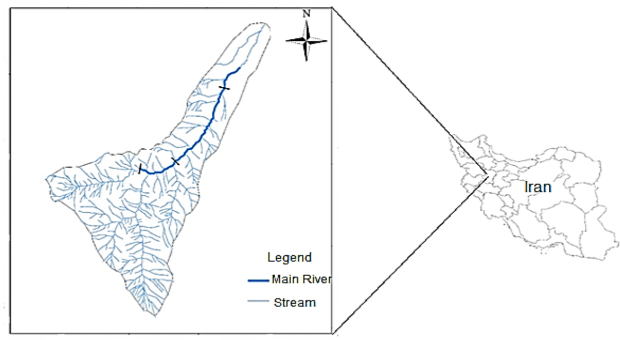

Figure 1. The site location of the Abbasabad River, Iran.

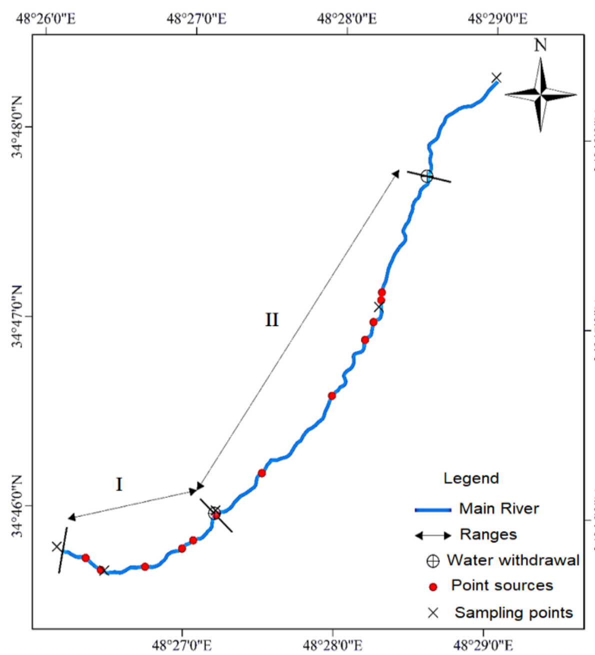

Figure 2. Location of the Interval I (drinking) and Interval II (agricultural) with point sources of pollutants, water withdrawal, and sampling points.

The upstream 7 km of the Abbasabad River is used for the present study, which is divided into two sections according to the main purpose of water usage, drinking (Interval I) and agriculture (Interval II), as indicated in Figure 2.

2.2. Governing Equations

The river section is divided into a list of fragments as shown in Figure 3. The general mass balance equation in the *i* water column (as shown in Figure 4) for all constituent concentrations can be written as:

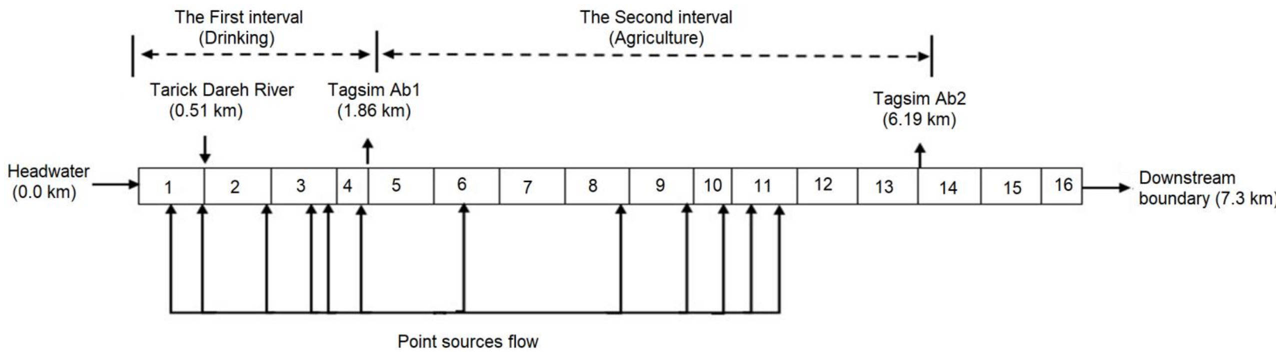

Figure 3. Detachment pattern of the proposed simulation.

$$\frac{dc_i}{dt} = \frac{Q_{i-1}}{V_i}c_{i-1} - \frac{Q_i}{V_i}c_i - \frac{Q_{ab,i}}{V_i}c_i + \frac{E'_{i-1}}{V_i}(c_{i-1} - c_i) + \frac{W_i}{V_i} + S_i + \frac{E'_{hyp,i}}{V_i}(c_{2,i} - c_i) \quad (1)$$

where C_i is the concentration of the specific parameter in the element i in terms of, g/m^3, V_i is the volume of the element i in m^3/d, t: is the time according to d, Ei' is the emission factor between the element i and $i + 1$, Q_i is the flow of element i in m^3/d, W_i is external loading on quality parameter for element i in terms of g/d, S_i is production and consumption of quality parameter due to reactions and mass transfer mechanisms in element i in terms of g/m^3/d, $C_{2,i}$ is concentration of the quality element 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.

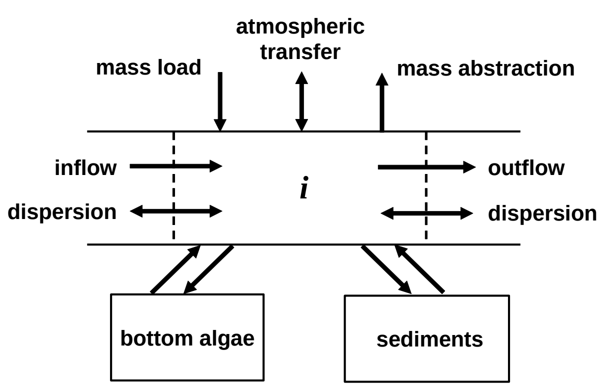

Figure 4. Mass balance for one fragment (cited from Chapra and Pelletier, 2008).

The river was divided into 16 sections and the Manning Equation is used to determine the depth and flow velocity in each section:

$$Q = \frac{S_0}{n}\frac{A_c^{5/3}}{P^{2/3}} \quad (2)$$

where Q represents flow (m^3/s); S_0 represents bottom slope (m/m); n represents Manning roughness coefficient; A represents cross sectional area (m^2); and P represents wetted perimeter (m).

2.3. Total Maximum Daily Load (TMDL)

The following equation is used as the framework for the TMDL analysis. The TMDL is the maximum amount of contaminant that can be accepted in the river system:

$$TMDL = (WLA + LA + MOS) \quad (3)$$

Waste Load Allocation (WLA) is the percentage of the total maximum daily load that assigned to a current or future point source of pollution. Load Allocation (LA) is percentage of the total maximum daily load that is considered as a present or future non-point contaminant source. The total sum of WLA for point sources and LA for non-point sources in addition to Margin of Safety (MOS) is equal to the TMDL. Thus, the maximum waste volume in the river can be determined.

To assess self-purification capacity and maximum loading capacity, it is necessary to calculate the total load. The capacity of self-purification of the river in the intervals of drinking (Interval I) and agricultural (Interval II) is considered. The maximum input load (L_i) is then calculated from the following equation:

$$L_i = (Q_h \times C_h) + (Q_p \times C_p) + (Q_{np} \times C_{np}) \quad (4)$$

where, Q and C are discharge (m^3/s) and concentration of quality parameters (mg/L), respectively. h, np, and p refers to headwater, non-point and point resources, respectively. In the present study, the TMDL method was used to calculate the self-purification capacity.

3. Results and Discussions

3.1. Sensitivity Analysis

The sensitivity analysis is conducted to identify the input parameters that may have the strongest impact on the output simulation of COD, $CBOD_f$, DO, PO_4-P, NO_3-N, and NH_4-N. Herein, the variations in oxidation rate, nitrification rate, and

Table 1. 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
N-NH4	0	-0.44	0	-0.173	0.347
N-NO3	-0.014	0.821	-0.33	0.085	0.211
P-PO4	0	0	0	-0.174	0.073
COD	0	0	0	-0.121	0.019

Table 2. The Self-Purification Capacity (kg/day) In Scenario I

Interval I	BOD	COD	N-NH$_4$	N-NO$_3$	P-PO$_4$
Loading current	52.86	134.36	2.55	16.26	3.80
Surplus capacity	49.05	37.58	23.75	165.53	0
Self-purification capacity	101.92	171.95	26.30	181.78	3.80
Interval II	BOD	COD	N-NH$_4$	N-NO$_3$	P-PO$_4$
Loading current	27.08	58.89	2.55	0.55	0.81
Surplus capacity	960.79	1672.90	65.82	25.66	32.67
Self-purification capacity	987.87	1731.79	68.36	26.21	33.49
Total river	BOD	COD	N-NH$_4$	N-NO$_3$	P-PO$_4$
Loading current	79.94	193.25	5.10	16.81	4.62
Surplus capacity	1009.85	1710.48	89.56	191.19	32.67
Self-purification capacity	1089.79	1903.73	94.66	208	37.29

denitrification rate have been compared. The following coefficient is used to determine the change rate in output variables for a certain percentage of change for each input variables (Palmieri and Carvalho, 2006):

$$S_{ij} = \frac{\Delta y_j / y_j}{\Delta x_j / x_j} \tag{5}$$

where S_{ij} is the normalized coefficient of sensitivity, Δy_j is the change rate in variable *j*. y_j is original value of variable *j*, Δx_i is the change rate of input variable *i*, and x_i is the original value of variable *i*.

The results of sensitivity analysis for the dry season can be found in Table 1. Parameters of DO and BOD on denitrification and nitrification rates have the least sensitivity (0.039, 0.006) while oxidation rate has the largest sensitivity (0.8, 0.217). Parameters of P-PO$_4$ and COD have the greatest sensitivity to the river discharge and they are neutral to oxidation rate, nitrification and denitrification. Parameters of N-NO$_3$ and N-NH$_4$ have the greatest sensitivity to nitrification. N-NO$_3$ has the least sensitivity to oxidation rate and N-NH$_4$ is neutral to rate of BOD oxidation and denitrification. For N-NO$_3$, the impact from nitrification rate is around 82% and for DO, the impact from oxidetion is around 80%.

3.2. Margin of Safety (MOS)

The MOS reflects the impacts of parameters that are not considered in the modeling that may cause a difference between simulation and measurement. Firstly, the difference between measured and simulated data was calculated to determine the safety coefficient following calibration and validation of the model. The SMADA software was used to determine the distribution. The probability of 50% was used and mine the distribution. The probability of 50% was used and added to the standard value of each parameter. Based on the specific usage of water in the research area, the standards of drinking water and agriculture water from Iran (Environmental Protection Agency of Iran, 2011) is used for self-purification analysis. The safety margin can be determined following the selection of standards. The distribution curve based on chi-square test for each parameter can be seen in Figure 5. It is found that, the parameters of DO, BOD, and COD follow the normal distribution. The parameters of N-NH$_4$ and P-PO$_4$ follow Pearson distribution. While N-NO$_3$ follows the three-parameter log normal distribution. Overall, the normal distribution has the best fit with the data. The MOS of DO, BOD, and COD is 0.12, 0.02 and 0.22 mg/L, respectively. The MOS of N-NH$_4$, N-NO$_3$, and P-PO$_4$ is 175.54, 16.98 and 6.63 µg/L. The above MOS can be added to standard level of each parameter to better protect water resources.

3.3. Scenario Analysis

To further understand the water quality and self-purification of the mountainous river, three hypothetical scenarios are presented in the following.

- The self-purification with 35 years average flow rate in the river;
- The self-purification with reduced flow rate of 10%, 20% and 30%, respectively;
- The self-purification with point-source pollution relocation.

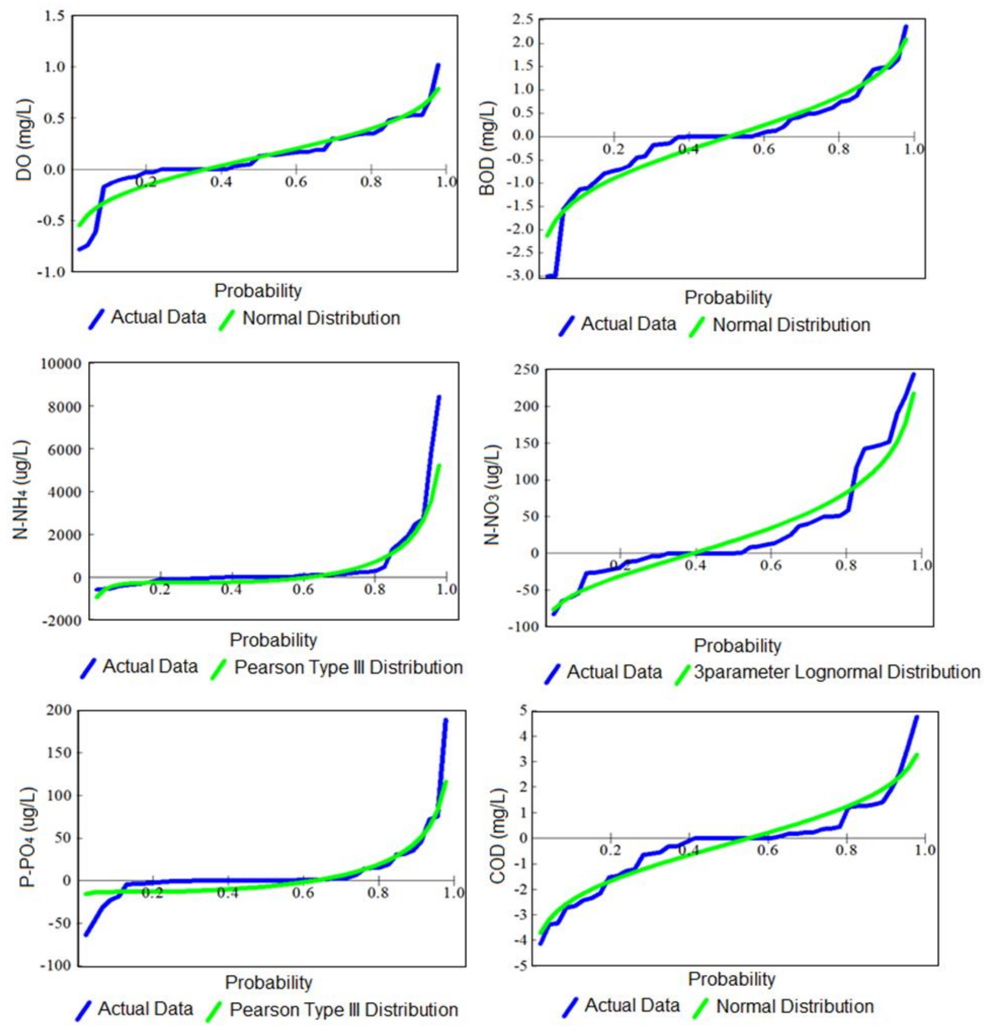

Figure 5. Distribution diagrams for the parameters studied.

3.3.1. Scenario One

Figure 6 shows the changes of water quality and pollution level in the river along the two intervals between the 35 years average discharge and the 2015 flow rate. In this scenario, the DO level does not change from 0 to 1 km but decrease by 1.5% from 1 to 4.1 km. From 4.1 km to the end of the river, the DO level has a 5% increase. The average decrease of BOD and COD is 45%. The level of N-NO_3 is increased with a decrease in N-NH_4 due to the nitrification process along the river. In Interval I, the reason for the increasing BOD and COD is the increase in flow rate. While in Interval II, the decrease in BOD and COD dues to the self-purification process.

Self-purification capacity. The self-purification simulation is given in Table 2. Under this scenario, at Interval I, the drinking water standards can still be satisfied even with increased concentrations of BOD, COD, N-NH_4 and N-NO_3 are up to 49.05, 37.08, 23.75 and 165.53 kg/day, respectively. It should be noted that the phosphate concentration in this interval is always higher than that in the drinking water standard. There fore, it should be reduced to 2.43 kg/day. While for agricultural usage (Interval II), even with BOD, COD, N-NH_4, N-NO_3 and P-PO_4 concentrations up to 960.79, 1672.9, 65.82, 25.66, and 32.67 kg/day, the agricultural water standard can still be satisfied. The self-purification is consistent with simulations from Zhang et al. (2012).

From the analysis, the self-purification can be maintained in the river with a 1903.73 kg/day for COD and 37.29 kg/day for PO_4-P. In this scenario, the maximum self-purification capacity is 3333.47 kg/day. The allowed thresholds for the parameters are plotted in two intervals in Figure 7. The maximum load for BOD, COD, N-NH_4, N-NO_3, and P-PO_4 are 49.98 mg/L, 99.78 mg/L, 4824.46 μg/L, 9983.02 μg/L, and 1993.37 μg/L respectively following agricultural water standard. The maximum load for BOD, COD, N-NH_4, N-NO_3, and P-PO_4 are 4.98 mg/L, 9.78 mg/L, 1324.46 μg/L, 9983.02 μg/L, and 193.37 μg/L, respectively, following drinking water standard.

3.3.2. Scenario Two

Figure 8 shows the changes of parameters along the river

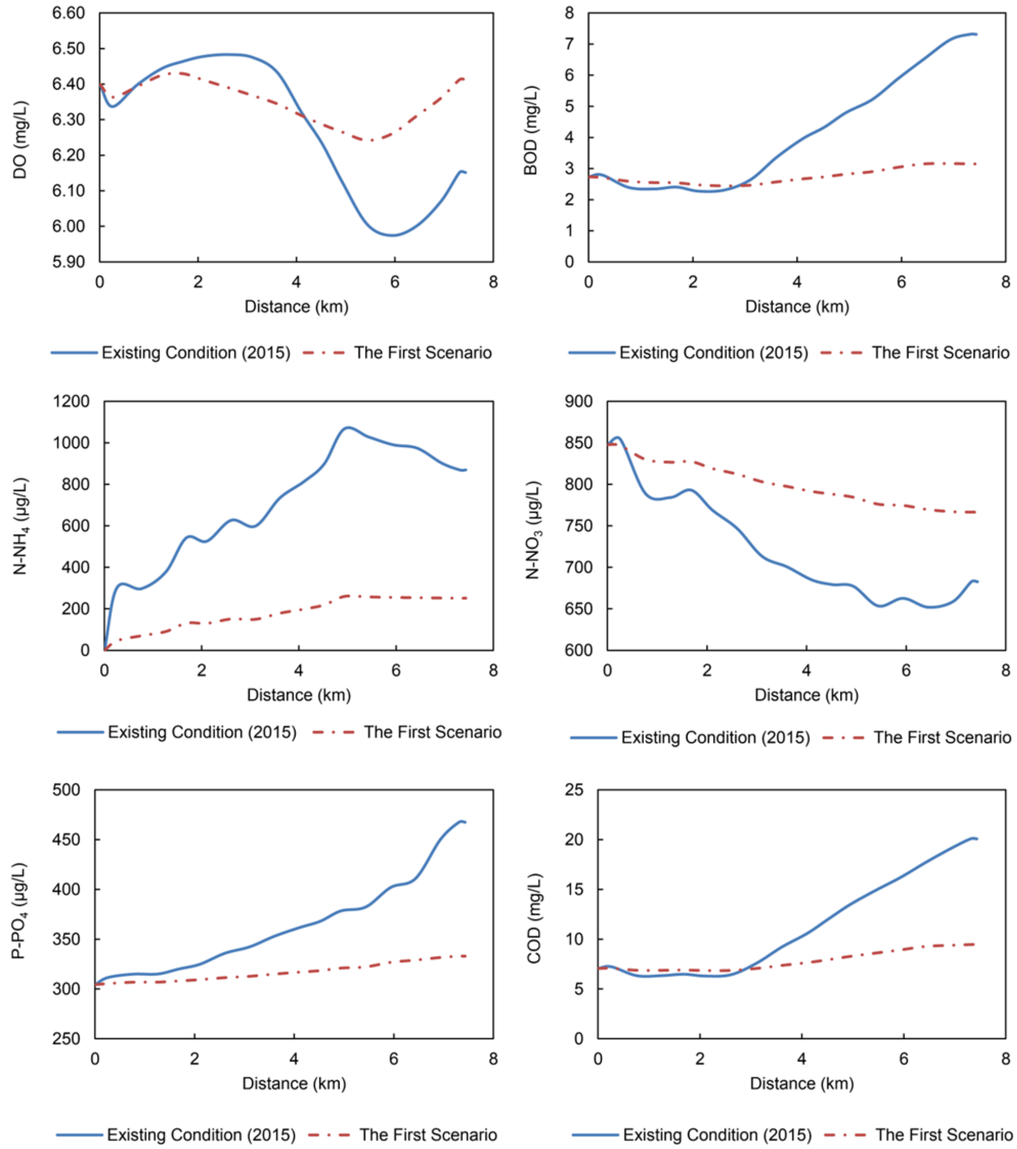

Figure 6. BOD, DO, N-NO_3, N-NH_4, COD, and P-PO_4 diagrams under scenario one compared to existing condition (2015 flow rate).

comparing to the original conditions. The DO level has no change from 0 to 4.5 km. From 4.5 km to the end of the river, the DO value is decreased due to the reduction in discharge. The average reduction is less than 2%. The flow rate is the main cause of changes in CBOD and DO concentration in a river system (Alhassan et al., 2007). The COD, BOD, and P-PO_4 values are not changed significantly from 0 to 3.1 km. However, from 3.1 km to end of the river, the concentration of these parameters are increased significantly due to a 30% re-duction in flow rate from 6.44 km to the downstream. The NH_4 level is increased due to the decrease in flow rate from 0 to 6.44 km. However, the NH_4 level is decreased from 6.44 km to the downstream, which may due to the decreased water depth and increased oxygenation (Chapra et al., 2008). The process is known as the nitrification process, which converts NH_4 to NO_3.

Self-purification capacity. The result of self-purification analysis is provided in Table 3. In this scenario, with a 10% flow reduction, the self-purification capacity of BOD, COD, N-NH_4 and N-NO_3 are 24.69, 42.43, 5.83, 35.88, and 0.88, respectively, in Interval I (drinking purpose). Similarly, the concentration of BOD, COD, N-NH_4, N-NO_3 and P-PO_4 can be increased up to 129.44, 311.78, 13.52, 18.66, and 6.43 kg/day in Interval II (agricultural purpose). Agricultural water standards can still be satisfied. It should be noted that the level of phosphate is always higher than that in the drinking water standard. Therefore, the concentration of phosphate should be reduced to 0.54, 0.52, and 0.5 kg/day, with a decreased 10%, 20%, and 30% flow rate, respectively. BOD and COD have a higher self-purification capacity than the other parameters from the analysis. The lowest amount of self-purification in the

Intervals I and II was 7.06 kg/day for P-PO_4 along the river. The self-purification capacity along the river is most significantly affected by flow rate.

3.3.3. Scenario Three

Figure 9 shows the parameters changes along the river compared to the original condition. In this scenario, it is assumed that the sewage point sources in Interval I is collected and transferred to the beginning of Interval II (after Tagsim Ab1). Therefore, the contaminant level is decreased in the upstream from 0 to 1.86 km (Interval I) and increased from 1.86 km to downstream (Interval II). There is a slight decrease in river water quality parameters, except DO and NH_4. Overall, the water quality in this scenario has very limited change comparing to other scenarios.

Table 3. The Self-Purification Capacity (kg/day) Based on the Second Scenario

	BOD			COD			N-NH_4	
Interval I								
Discharge reduction	10%	20%	30%	10%	20%	30%	10%	20%
Loading current	11.92	11.22	10.53	28.60	26.80	25	2.55	2.55
Surplus capacity	12.76	12.76	11.11	13.82	13.82	13.23	3.28	2.88
Self-purification capacity	24.69	23.99	21.63	42.43	40.63	38.23	5.83	5.43
Interval II								
Discharge reduction	10%	20%	30%	10%	20%	30%	10%	20%
Loading current	27.08	27.08	27.08	58.89	58.89	58.89	2.55	2.55
Surplus capacity	129.44	116.95	108.48	311.78	291.02	265.49	13.52	12.53
Self-purification capacity	156.52	144.03	135.56	370.67	349.91	324.39	16.07	15.08
Total river								
Discharge reduction	10%	20%	30%	10%	20%	30%	10%	20%
Loading current	39	38.30	37.61	87.49	85.69	83.89	5.10	5.10
Surplus capacity	142.21	129.72	119.59	325.61	304.85	278.72	16.81	15.41
Self-purification capacity	181.21	168.02	157.20	413.10	390.54	362.62	21.90	20.51
	N-NH_4	N-NO_3			P-PO_4			
Interval I								
Discharge reduction	30%	10%	20%	30%	10%	20%	30%	
Loading current	2.55	3.55	3.33	3.12	0.88	0.84	0.80	
Surplus capacity	2.50	32.33	32.19	29.89	0	0	0	
Self-purification capacity	5.05	35.88	35.52	33.01	0.88	0.84	0.80	
Interval II								
Discharge reduction	30%	10%	20%	30%	10%	20%	30%	
Loading current	2.55	0.55	0.55	0.55	0.81	0.81	0.81	
Surplus capacity	11.20	18.66	17.26	16.16	6.43	5.96	5.44	
Self-purification capacity	13.75	19.21	17.82	16.72	7.25	6.77	6.26	
Total river								
Discharge reduction	30%	10%	20%	30%	10%	20%	30%	
Loading current	5.10	4.10	3.89	3.67	1.69	1.65	1.61	
Surplus capacity	13.70	50.99	49.45	46.05	6.43	5.96	5.44	
Self-purification capacity	18.80	55.09	53.34	49.72	8.13	7.61	7.06	

Table 4. Determine Self-purification Capacity (kg/day) in the Third Scenario

Interval I	BOD	COD	N-NH_4	N-NO_3	P-PO_4
Loading current	10.37	26.94	0	3.44	0.85
Surplus capacity	0	0	0	0	0
Self-purification capacity	10.37	26.94	0	3.44	0.85
Interval II	BOD	COD	N-NH_4	N-NO_3	P-PO_4
Loading current	30.54	64.07	5.57	0.94	0.97
Surplus capacity	174.50	345.48	12.57	43.62	6.88
Self-purification capacity	205.04	409.55	18.14	44.56	7.85
Total river	BOD	COD	N-NH_4	N-NO_3	P-PO_4
Loading current	40.91	91.02	5.57	4.38	1.82
Surplus capacity	174.50	345.48	12.57	43.62	6.88
Self-purification capacity	215.41	436.50	18.14	47.99	8.70

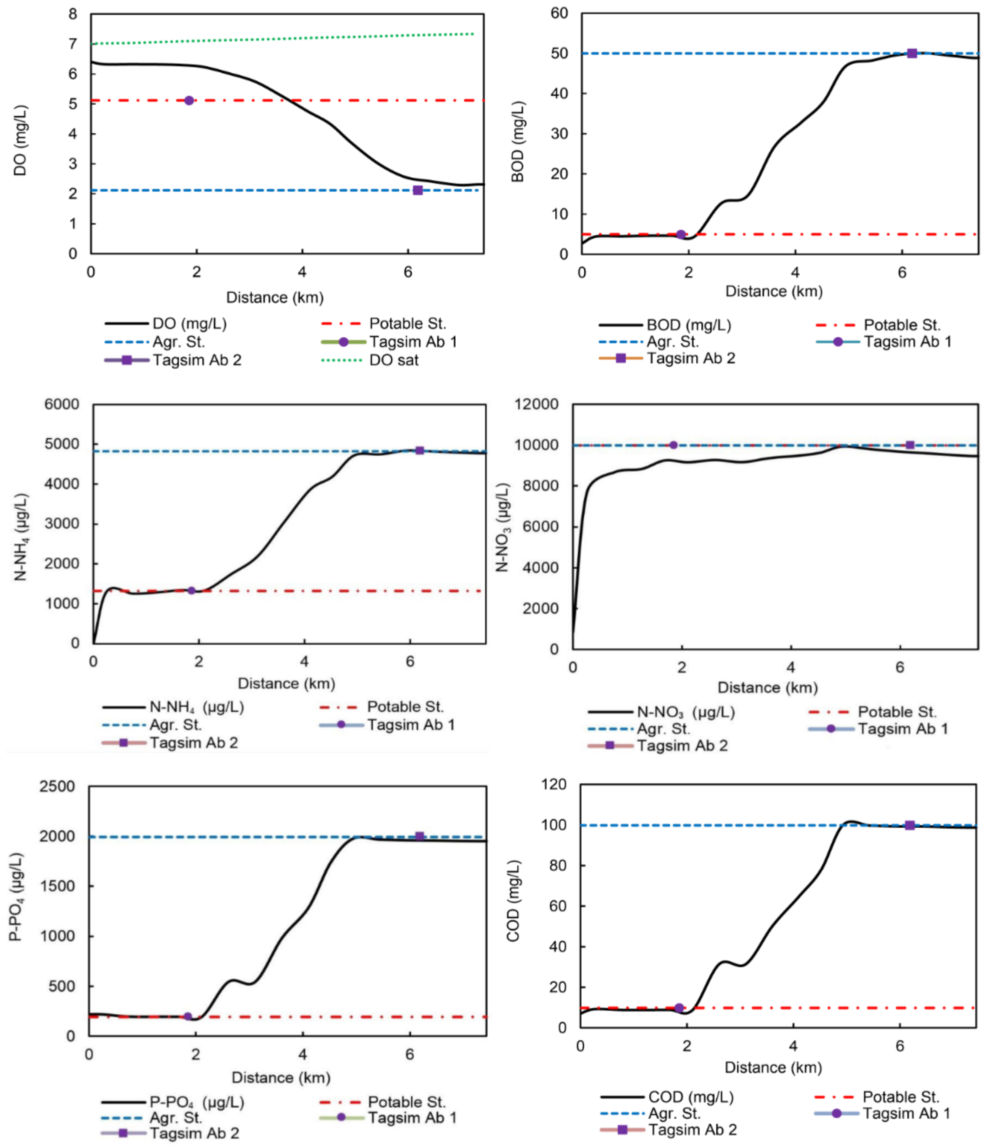

Figure 7. Allowed threshold for the parameters measured along the river based on first scenario.

Self-purification capacity. The results of self-purification capacity are presented in Table 4. In this scenario, the river cannot accept extra BOD, COD, $N\text{-}NH_4$ and $N\text{-}NO_3$ at Interval I for drinking purpose. The amount of phosphate is higher than the standard for drinking purposes and it must be reduced to 0.48 kg/day. At the agricultural interval, with the concentration of BOD, COD, $N\text{-}NH_4$, $N\text{-}NO_3$ and $P\text{-}PO_4$ increased up to 174.50, 345.48, 12.57, 43.62, and 6.88 kg/day, the standards can still be satisfied. The COD have a higher self-purification capacity than the other parameters from the analysis. In this scenario, the maximum self-purification capacity along the river was 726.74 kg/day for the studied parameters.

4. Conclusions

By simulating the water quality parameters in the Abbasabad River in Iran, the self-purification capacity in mountainous rivers was presented. The QUAL2KW model was applied with two intervals in the river. The model was calibrated and validated using field data from five monitoring stations along the river. Six parameters, COD, BOD, DO, $P\text{-}PO_4$, $N\text{-}NO_3$, and $N\text{-}NH_4$ were calculated and compared with field data. It is found that, the self-purification capacity of the COD is higher than the other parameters along the river (in all three scenarios). The river flow rate has a strong impact on self-purification capacity for mountainous rivers. Additionally, the relocation of sewage point sources has very limited impact on self-purification capacity. A sensitivity analysis is conducted to identify the most influential parameters for simulation. For mountainous rivers, the oxidation rate and nitrification rate have the largest influence on water quality output.

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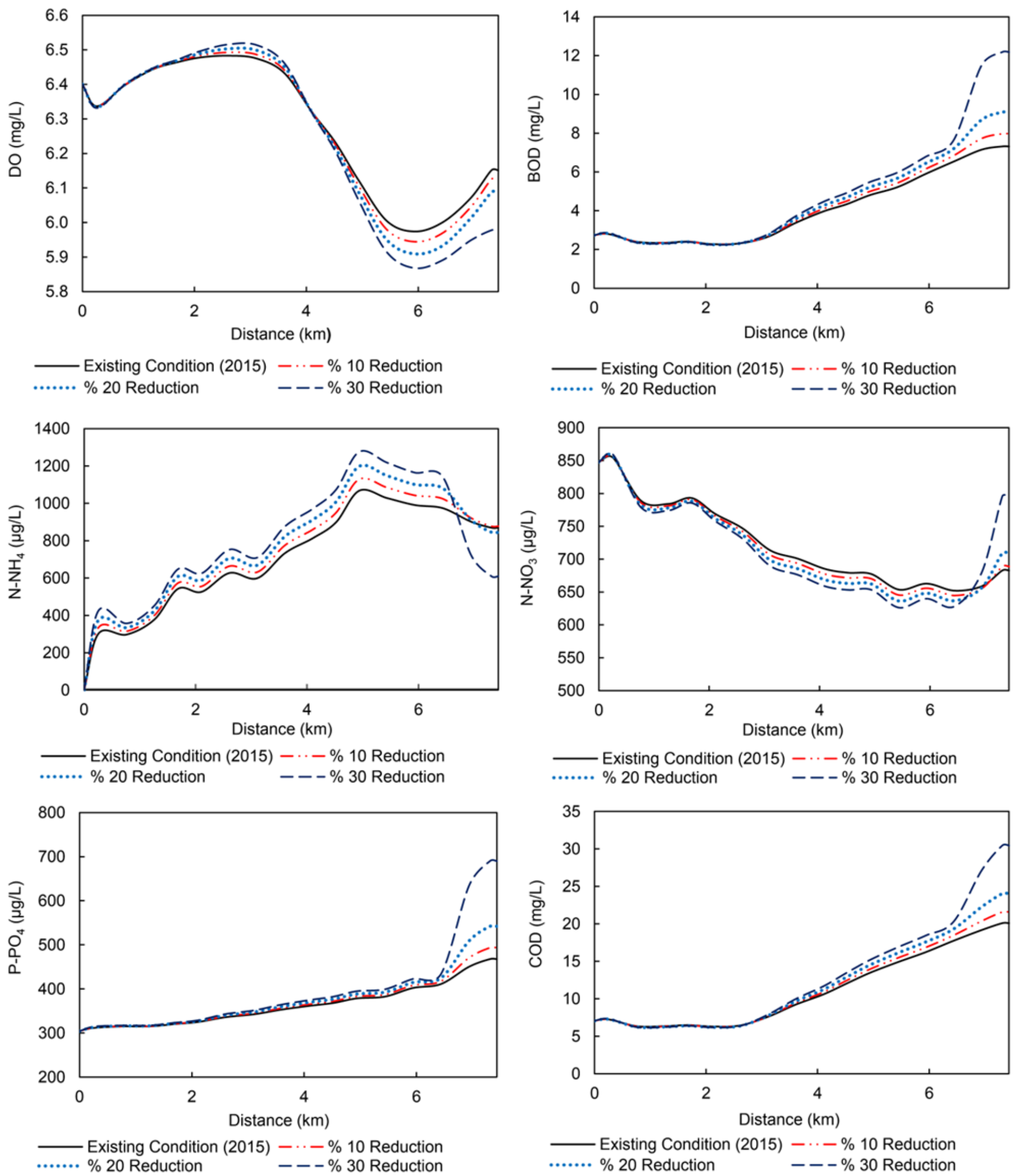

Figure 8. BOD, DO, N-NO_3, N-NH_4, COD, and P-PO_4 diagrams in Scenario two.

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