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Surface Water Resources Assessment and Planning with the QUAL2KW Model: A Case Study of the Maroon and Jarahi Basin (Iran)

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Abstract: Mathematical models are useful for predicting the reactions of watercourses such as rivers due to the entry of contaminants. Some of these models are able to simulate the effects of present and future loadings as well as aid managers and officials in making decisions even if the data are sparse. In other words, river water quality preservation requires more investment in wastewater treatment and/or the installation of collection and control systems; it may also limit activity expansion in the river basin. The conservation of watersheds such as the Maroon and Jarahi basin, which provide water for drinking and for industrial and agricultural use, is socio-economically vital. Therefore, the first stage of managing the conservation of water resources is understanding their qualitative changes. For this purpose, the QUAL2KW mathematical model was utilized to simulate the river water quality in this example region. According to the reported values of water quality parameters and pollutants at monitoring stations, it was established that the river is at a critical condition in terms of biochemical oxygen demand (BOD) pollution due to the discharge of urban and industrial wastewater, as well as high electrical conductivity (EC) due to the drainage of agricultural lands. Based on the statistics calculated during the validation step, the authors concluded that the QUAL2KW water quality model is reliable in the simulation of qualitative parameters and the pollution data of the study area; namely the Maroon and Jarahi river basin located in the south-west of Iran. This will help stakeholders to better manage watersheds with sparse data. This region has been suffering from climate change which has led to droughts and the construction of several dams to retain water. For the second and third stations, the NASH (named after the mathematician John Forbes Nash) values were 0.96 and 0.92, respectively, indicating a relatively high model accuracy. The evaluation using the root mean square errors (RMSE) and NASH showed that the quality of water at the second station was better than the other two stations based on the coefficient of determination R^2. Since there were three drains at station number 3, the wastewater entering the Maroon River had a higher level of contamination.

Keywords: QUAL2KW; quality monitoring station; Maroon and Jarahi basin; water quality

1. Introduction

Water pollution has posed a serious threat to human and natural ecosystems in recent decades. So, the detection of changes in water quality is one of the important challenges for the optimal use of water resources. Various types of agricultural, industrial and municipal pollutants are discharged into rivers, which are the main sources of water for drinking, industrial and agricultural purposes. This has led to an environmental crisis. Pollution and surface water contamination is one of most important challenges in the built environment. Therefore, achieving good quality surface water is a common societal goal [1–15]. The quality of the surface water depends on many complicated physical and biochemical processes [16]. The water quality cannot simply defined be as good or bad, but it is appropriate to assess how sufficient or insufficient the water quality is for urban or agricultural consumption using water quality standards [2]. River geomorphology and urbanization have an impact on the water quality that is characterized by physical, biological and chemical water quality parameters [12].

Operational management and measurements aim to improve and maintain water quality. Toxic substances are assessed for their impact upon the human body. In fact, these substances are present in surface water and feature in many water quality standards. The various components in water depend on physical, chemical and biological properties such as temperature, ions and microbes [10]. Wastewater has harmful and long-term effects on some physical and chemical parameters such as dissolved oxygen (DO), BOD, phosphorus, temperature and pH and biological parameters such as bacteria, algae and organisms. Sewage can have a detrimental effect on water in the environment [3–9].

Mathematical models allow stakeholders to make suggestions with the aim to prevent damage to the conditions of water resources [8]. One-dimensional models are commonly used for rivers. They simulate processes with only one direction in space and they show flow through the mean velocity in the cross section and eliminate the vertical and horizontal dimensions [14]. These models typically include simulations of DO, BOD, nitrate, EC, toxins and heavy metals. Promising water quality models include QUAL2E, MIKEll, HSPF, WASP6, EXAMS, CE-QUAL-W2, CE-QUAL-ICM, HEC5Q and SALMON-Q [4]. Furthermore, researchers investigated six water quality models to simulate DO [5,6]. These models were SIMCAT (simulation), TOMCAT (general model for reservoirs), QUAL2KW, QUAL2EU (advanced water quality model), WASP7 (water quality's analysis and simulation) and QUASAR (simulation of water quality along rivers). These models showed differences between input data, hypotheses and modeling processes [4].

The SIMCAT and TOMCAT models are simple and are most useful for rapid analysis. The QUAL2EU model is widely used for qualitative analysis and assessments. On the other hand, QUAL2KW is the most mathematically heavy model for simulation purposes. This model is based on an automatic calibration system with new equations. Researchers validated the data of four hydrometric stations with the QUAL2KW model. Water quality data included BOD, EC, temperature and DO [17]. The results showed that at a flow rate of 190 m^3/s, BOD was very important for the Dez River.

A high EC has often been identified as a serious threat to the environment. River water quality was simulated by the QUAL2KW model for the Shahroud River. The results showed that the minimum and maximum EC values were 0.19 and 163.89 ds/cm, respectively. The DO ranged between 6.94 and 9.99 mg/L [13].

Researchers analyzed DO using the QUAL2K model. They showed that the most important concern in their case study was BOD within the QUAL2K water quality model. However, low photosynthetic algae also had a significant effect on DO [18]. Furthermore, BOD and DO were examined at 12 stations at Zayandehrood. The results showed that the flow rate sharply decreased at the last station due to agricultural water abstraction. In addition, the concentration of DO was very low due to industrial sewage and human wastewater inputs [19]. Some experiments on the water quality of the Kinevers River were carried out. Their simulation results showed that the QUAL2KW model was a practical tool for crisis management [20]. The QUAL2KW model was applied to simulate DO and BOD in the Karun River [21]. They studied the diversity of the seasonal treatment of Karun River water by applying three scenarios: a 30% decrease in sewage flow, a 30% increase in monthly river flow and a 30% decrease in sumps. Their results showed that nitrate depletion in January and February and a total BOD decrease throughout the month, except for 30% in October, had the greatest impact on river water quality. Moreover, a 30%

reduction in effluent flow containing pathogens had the greatest impact on river water quality [22]. These researchers used the QUAL2KW model to simulate DO concentration as a function of river water temperature, organic pollutants, algae respiration and to identify river self-purification. They concluded that if the city of 'Lamia' located in the north of India had a secondary effluent treatment plant with a minimum efficiency of 76%, the dissolved oxygen concentration of the river should not be less than 5 mg/L [23]. Mutiga et al. [24] examined the coordination between the water supply and the demand for water resources using the Qual model during a study in the Ovasoniro Basin in Kenya to minimize the conflicts related to overuse of the water in the basin. They concluded that the highest demand and, therefore, the cause of the conflict was in the agricultural sector. Mutiga et al. suggested that rain-fed cultivation should be developed in the region to solve this challenge.

This team used the Fischer equations to estimate the longitudinal dispersion coefficients in the Qual2k equations [25]. Their simulations showed that this parameter is important in tracking contamination densities [26]. They simulated the water quality of the Karun River in the range of Bandaghir to Ahvaz using the QUAL2K model. For this purpose, they used qualitative data from 2012 to 2014. The results of their research showed that the amount of ammonium and nitrate increased downstream of the river and the QUAL2K model had a good simulation accuracy [27]. The management of water resources is a complex activity that requires structural tools to assist in decision making. There are many applications with graphical interfaces and models that provide the most convenient way to make decisions.

To qualitatively optimize the Dez River system, the environmental flow had to be determined and the quality of the river needed to be simulated by the QUAL2K model [28]. Researchers evaluated the water quality by calibrating the QUAL2K model and subsequently examining five qualitative variables including water temperature, dissolved oxygen, pH, electrical conductivity and turbidity. The results showed that some factors such as rainfall, land use and land slope affected the amount of dissolved oxygen in water in particular [29]. They simulated the water quality by using the QUAL2K model. The results showed that the total nitrogen and total phosphorus should be reduced to 15% and 19%, respectively, to achieve the desired water quality goal in the river [25]. In this research, by considering the quality parameters and using the QUAL2K model and also considering the defined water quality and land use standards, the self-purification potential of this river was evaluated. The BOD, DO, nitrate and total coliform parameters were selected as indicator parameters to evaluate the self-purification capacity of the river [30].

The agricultural lands downstream of the river met their needs only from the river water compared to the lands upstream of the plain, which were simultaneously harvesting surface and groundwater. The lower areas faced water shortages between September and December. Environmental needs were not fully met for the Maroon and Jarahi Rivers in contrast to the Allah River. The water needs of agriculture during the dry periods were never met. However, the needs of the drinking water and other industries were fully met. Therefore, the aim of this research was to test a broader quantitative and qualitative water quality simulation model for planning purposes in the Maroon and Jarahi basins linked to scarce data availability. The authors applied the QUAL2KW modeling principles to properly manage the reduction in surface water pollution. This paper highlights the application of a simple model to support decision makers with the effective assessment of water resources within regions located in developing countries characterized by sparse data.

2. Materials and Methods

2.1. Example Study Area

The study area is located in the southwest of Iran covering the provinces of Khuzestan, Kohgiluyeh and Boyer-Ahmad on the slopes of the Zagros. The area of this basin is nearly 3824 km^2. The Maroon River rises from the Zagros Mountains and flows into the Maroon Dam Reservoir Lake. Thereafter, it joins the Allah River in the continuation of its path. This river is called Jarahi. The Maroon and Jarahi basin has a cold climate in the mountainous areas. These areas are composed of resistant limestone, which often has steep slopes. The formation of this basin includes alluvial rocks. The locations of these rivers in the study area are shown in Figure 1. This study investigated the quantity and quality of water in the rivers of the Maroon and Jarahi catchment area, as well as the conditions for the development and identification of bottlenecks and challenges resulting from increasingly excessive water exploitation actions.

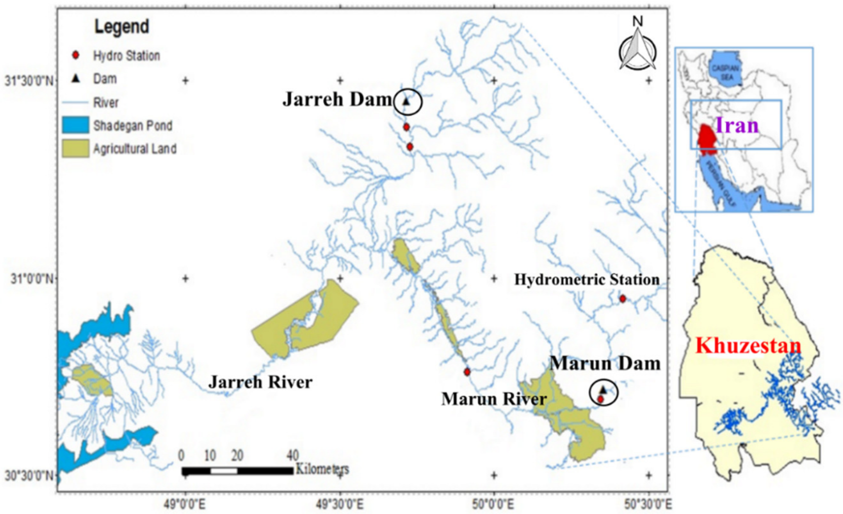


Figure 1. Location of the studied rivers in the Maroon and Jarahi basin.

The authors established a simple water balance model for the catchment (3801 km^2) around the Maroon Dam. Rainfall data for the main basin (Idnak) and the catchment area of the Maroon Dam were used to estimate the inflow to the dam. The findings indicated that the dam overflowed during the calibration period. Therefore, several other methods were used to estimate the inflow to the dam more accurately. However, all the alternative methods did not match the model well. For a 60-year simulation period, a regression analysis was finally used to optimize the model's predictions.

2.2. Description of the Basic Equations used in the QUAL2KW Model

2.2.1. The QUAL2KW Model

The QUAL2KW model was developed in 2006 by Pelletier and Chapra, but it is actually a modernized version of the Qual2e model [22]. This updated model is the latest in the series of QUAL models which have been recommended by the United States Environmental Protection Agency (USEPA) and have been extensively used to simulate river water quality [5]. A typical QUAL2KW working model simulates a river in one dimension with a steady and non-uniform flow. The flow simulation can consider pollution as either a point or non-point source. In order to calculate the density of the qualitative limitations to this model, a finite difference method is used to solve the advection-diffusion equation [31]. The QUAL2KW model can simulate more than 15 water quality parameters such as DO, BOD, temperature, ammonia–nitrogen and nitrate–nitrogen in rivers.

2.2.2. The Flow Balance Relationship in the QUAL2KW Model

The relationships utilized in the QUAL2KW model are flow, temperature and mass balance. Along the river, assuming complete mixing, relationships such as Equation (1) are used to perform a steady flow for each element [32].

$$Q_i = Q_{i-1} + Q_{in,i} - Q_{ab,i} \tag{1}$$

where Q_i is the output flow from each i, Q_{i-1} is the output flow from each $I-1$, $Q_{in,i}$ is the input flow from the point and non-point sources for each i and $Q_{ab,i}$ is the output flow from all non-point and point sources of each *i*. Figure 2 shows a schematic overview of the flow balance.

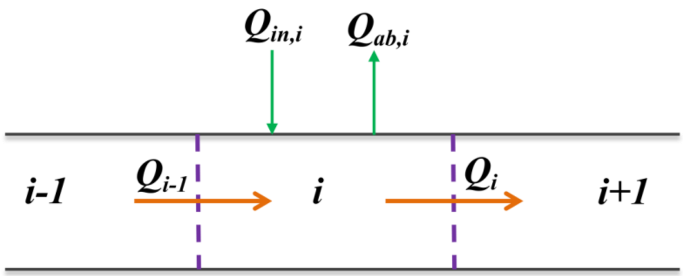


Figure 2. Flow balance for the first period of rivers.

2.2.3. Temperature Balance Relationship in the QUAL2KW Model

One of the most important parameters in the simulation is the mean temperature of each spot along a river. A changeable temperature has effects on the river water quality in terms of DO and BOD. Some effective factors in determining temperature are as follows: the initial temperature of the river water, bed surface temperature and the temperature of the point or non-point river inlet sources. The temperature can be balanced for each *i* as shown in Figure 3 [32].

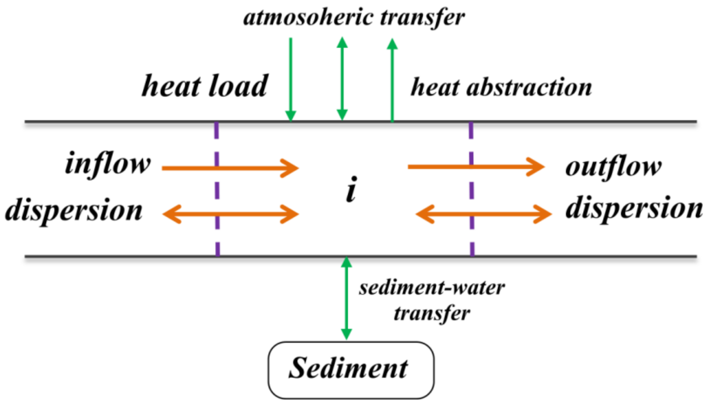


Figure 3. Temperature balance for the *i*-th period of rivers.

The heat balance in each river is calculated according to Equation (2):

$$\frac{dT_i}{dt} = \frac{Q_{i-1}}{V_i}T_{i-1} - \frac{Q_i}{V_i}T_i - \frac{Q_{ab,i}}{V_i}T_i + \frac{E'_{i-1}}{V_i}(T_{i-1} - T_i) + \frac{E'_i}{V_i}(T_{i+1} - T_i) + \frac{W_{h,i}}{\rho_w C_{\rho w} V_i}\left(\frac{m^3}{10^6 cm^3}\right) + \frac{J_{h,i}}{\rho_w C_{\rho w} H_i}\left(\frac{m}{100cm}\right) + \frac{J_{s,i}}{\rho_w C_{\rho w} H_i}\left(\frac{m}{100cm}\right) \quad (2)$$

where Q represents flow (m^3/day), T is the water temperature (°C), t is time (day), V_i represents the water volume (m^3), E' denotes the volumetric diffusion coefficient between reach i and $i + 1$ (m^3/day)), $W_{h,i}$ represents the amount of received pure heat from point and non-point sources in the i-th reach (cal/day), ρw represents the water density (gr/cm^3), C_{pw} is the specific heat of water (J/g), $J_{h,i}$ is the heat flux between the i-th reach and air (cal/(cm^2 day)), $J_{s,i}$ is the heat flux between water and sediment (cal/(cm^2 day)) and H_i represents the mean water depth in each i-th of the river (m).

2.2.4. Mass Balance Relationships in the QUAL2KW Model

One of the basic principles in the formulation of water quality models is the conservation of mass. The authors used the default Fischer equation of the Qual2k model. The main equation that the QUAL2KW model solves is the one-dimensional advection-dispersion equation, which was calculated for all parameters except for marine algae according to Equation (3).

$$\frac{dc_i}{dt} = \frac{Q_{i-1}}{V_i}c_{i-1} - \frac{Q_i}{V_i}c_i - \frac{Q_{ab,i}}{V_i}c_i + \frac{E'_{i-1}}{V_i}(c_{i-1} - c_i) + \frac{E'_i}{V_i}(c_{i+1} - c_i) + \frac{W_i}{V_i} + S_i + \frac{E'_{hyp,i}}{V_i}(c_{2,i} - c_i) \quad (3)$$

where W_i is the load of pollutants in each river branch (g/day), S_i represents the sources of pollutant input and output (g/(m^3/day)), C_i is the concentration index in the river water reach at i and c_2 is the concentration index in the sediment. Surface water quality models estimate many aspects of water quality at steady and unsteady conditions. Figure 4 shows the mass balance equation for the first section of the river in the QUAL2KW model.

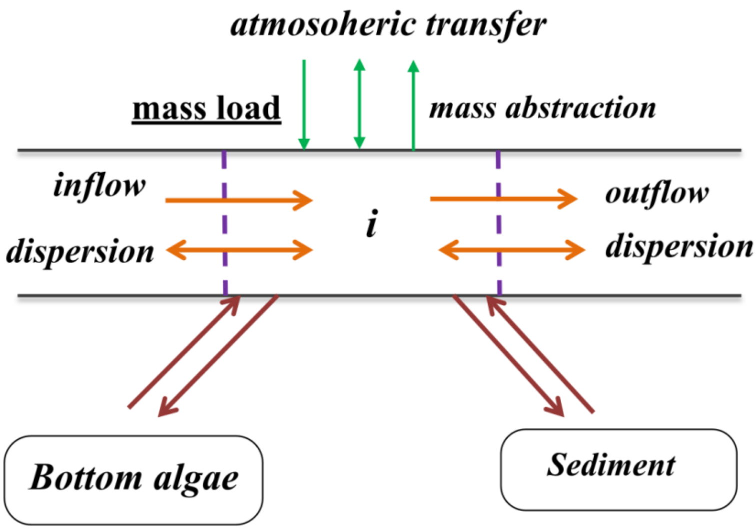


Figure 4. Temperature balance for the first river section.

2.3. Qualitative Simulation of the Maroon and Jarahi Rivers with the QUAL2KW Model

After collecting the data, all the necessary parameters for the qualitative simulation were entered into the QUAL2KW software. The data included interpolations and some characteristics of river hydraulics, meteorological information and water quality data, which relate to rivers and sources of contamination. The entry and exit of contaminants were considered based on the time steps of the monthly simulation and the metric computing unit. The commencement month of the simulation in the model was defined as January, but in the model settings, the number of days of the contracted Gregorian months was entered in the order equal to the number of days of the corresponding solar month in order not to disturb the calculations.

At the validation stage, the authors used another series of measured data after running the QUAL2KW model to determine errors. The model calculated for each simulated parameter the correlation coefficient (normalized mean square error), the root mean square error and the NASH equilibrium parameter linked to the NASH Equilibrium used in game theory. The NASH equilibrium builds on the notion that every player finds his or her best response to each of his or her rivals' strategy in a game.

For all simulated parameters, the correlation coefficient r and *NASH* were close to 1. The *NRMSE* was always about 0. It follows that all data were associated with a high level of accuracy. Table 1 shows the evaporation during the sampling period as one of the validation parameters.

Table 1. Potential evaporation during the sampling period (mm).

River	Parameter	Sep	Jul	Jun	May	Apr	Mar	Feb	Jan	Dec	Nov	Oct	Aug
Maroon	Evaporation	173.6	218.7	237	221.8	152.8	88.1	54.7	32.4	20.9	26.7	59.1	115.9
	Vaporization	173.6	218.7	237	221.8	149.8	65.1	20	20	10	10	23.5	106.4
Jarahi	Evaporation	190.4	218.9	219.7	196.3	134.6	81.3	48.8	36.8	34.5	44.7	85.7	135.9
	Vaporization	189.8	218.7	219.4	1963.3	123.6	33	20	20	10	10	46.8	133.6

2.3.1. Hydraulic Data and River Partitioning

The flow simulation in the QUAL2KW model is based on hydraulic river partitioning. Therefore, partitioning was performed based on the hydraulic conditions of rivers and locations of pollutant input. Figure 5 shows the locations of different sources of input sewage and pollution control stations located on the Maroon and Jarahi Rivers.

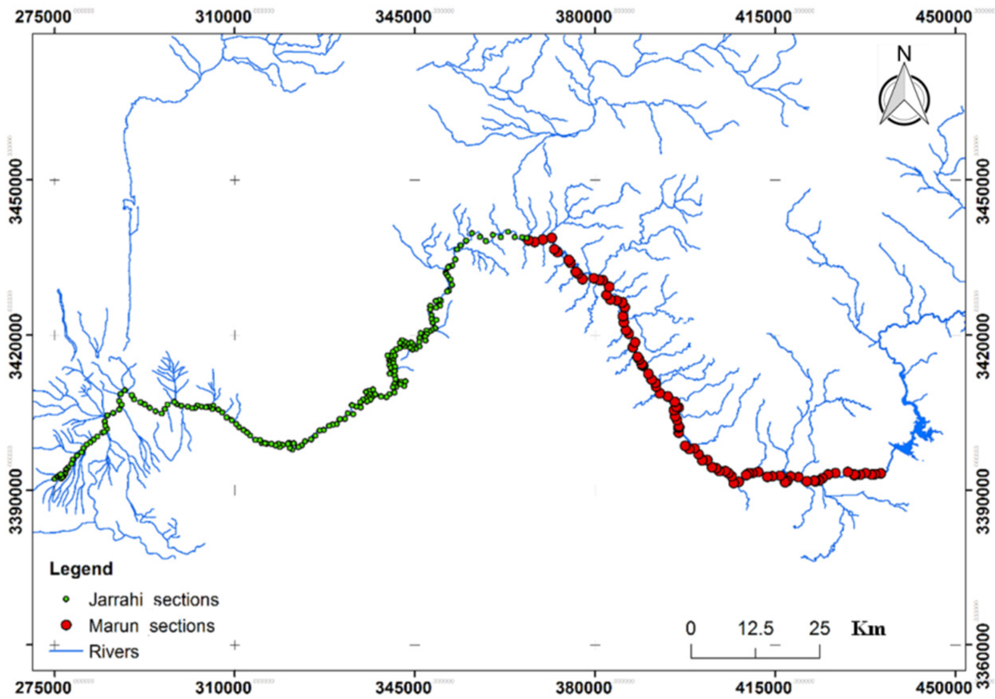


Figure 5. Location of 281 river sections in the Maroon and Jarahi study area.

Agricultural areas, urban sewage discharge, watercourses and other features of interest along the river were identified. The distance between Behbahan station and the end of the Jarahi River was divided into 281 partitions with different lengths. The locations of input water and associated pollutants as well as output water were defined based on mileage to the end of each river in the QUAL2KW model. Figure 5 shows the point sources of pollutants in this area.

In each zone, geometric characteristics such as canal longitudinal slope (0.13), wall slope (0.04), river longitudinal slope (0.1), canal height (0.6 cm) and sediment bed width (0.72 cm) were calculated with Auto-CAD software and then entered into the model. The QUAL2KW model calculated the depth and velocity of the flow based on the Manning's equation and the assumption that river partitions are trapezoidal [32]. After partitioning, some other essential information such as the Manning's coefficient were chosen from the reference material and after visits to all fields around the river sections. As a result, the authors determined the coefficient to be approximately 0.038. In addition, the input and output sources of the Maroon and Jarahi Rivers were also introduced to this model. Maroon Jarahi is a complete basin in terms of access to all hydrometric stations and water reservoirs;

therefore, this model was calibrated for the process of simulating input data based on the water cycle algorithm.

The authors entered all sources based on physical observations and made preliminary estimations of unknown parameters. Then the model was executed and its output was compared with the observed values. This method was continued until two outputs matched best together. This approach in the QUAL2KW model is performed by setting various parameters in the rates worksheet. After manual changes, the parameters and coefficients of the model were determined by trial and error by repeating the execution of the model.

Finally, after the calculation parameters were close to the observational parameters, the final values of the calibrated parameters were accepted as the best values in the calibration stage. The QUAL2KW model minimizes the distance between the observed results and the computational results using the RMSE technique to optimise the fitting processes. Non-point source inputs and outputs were linearly simulated in this model.

2.3.2. Meteorological Data

The meteorological parameters include solar radiation, wind speed, dew point temperature, air temperature, the percentage of cloud cover and shadow. Table 2 shows the monthly average values of several meteorological parameters at Behbahan synoptic station for the researched region. Table 3 shows information about the initial parameter conditions. Figure 6 indicates the model configuration for the boundary conditions. The model parameters comprise general information such as year, the month of the simulation start, the length of the planning period, time step and the model settings. In order to model the studied basin using Qual2KW software, the supply and consumption components according to the size of the basin and the variety of resources and uses were determined.

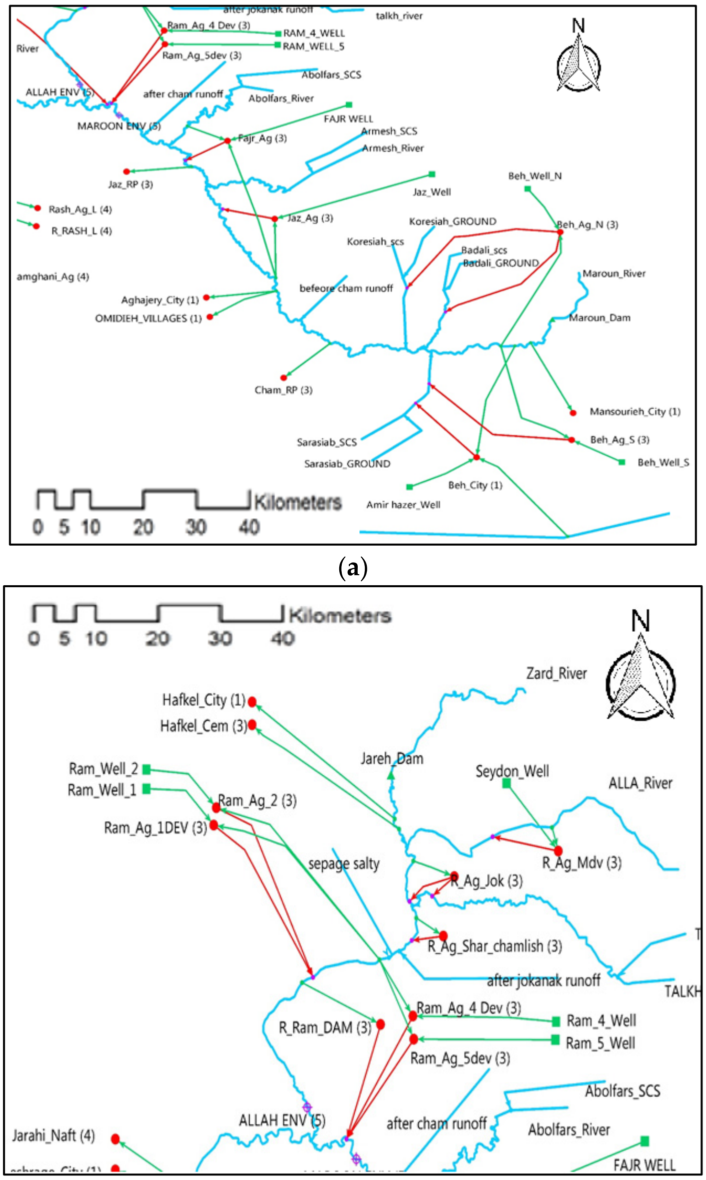
Table 2. Monthly average meteorological parameters at Behbahan synoptic station (2010–2011).

Parameter	September	October	November	December	January	February	March	April	May	June	July	August
Air temperature (°C)	28.2	24.12	14.4	11.8	13.2	16.8	21.4	28.2	33.9	36.1	36.6	34.6
Dew point (°C)	9.7	8.8	6.5	6.2	6.6	8.1	10.1	9.4	8.9	12.1	13	10.4
Sun hours (h)	270	198	194	194	176	181	221	200	281	267	34	232
Wind speed (m/s)	1.1	0.9	0.9	0.9	1.2	1.4	1.6	2	1.9	1.6	1.5	1.3
Potential Evaporation (mm)	54	32	26	20	69	88	173	237	221	152	115	99
Rainfall (mm)	12	18	26	18	12	12	5	5	5	5	5	5

Table 3. Initial and upper and lower parameter values in the QUAL2KW model.

Parameter	Symbol	Initial Value	Low Limit	Upper Limit
Fast CBOD * (oxidation rate)	k_{dc}	0.706	0	5
T (°C)-atmospheric transmission coefficient	a_{tc}	0.83	0.7	0.91
Oxygen for CBOD * (oxidation)	r_{ac}	2.69	2.4	2.8
Temperature correction		1.006	1	1.07

* Carbonaceous biological oxygen demand.



(**a**)

(**b**)

Figure 6. Model configuration for the boundary conditions: (**a**) Maroon; and (**b**) Jarahi.

3. Background Information about the Data and Study Area

3.1. General Sources of Pollution in the Maroon and Jarahi Rivers

Surface watercourses such as rivers can naturally treat modest pollutant loads that enter them. Raw urban sewage, heavy industrial pollution and polluted agricultural wastewaters with different quality characteristics are the most important contamination sources that pose a serious environmental hazard. Surface waters cannot completely purify such pollution. The main sources of pollution are described in the following sub-sections.

3.1.1. Pollutions from Municipal Wastewater

Municipal wastewater in the case study area contained high levels of BOD and chemical oxygen demand, nutrients and pathogenic microorganisms, which are influenced by factors such as cultural features, eating habits and climate change. Pollution originates from domestic sewage linked to public places, baths, hospitals and offices, as well as surface runoff due to heavy rainfall, which directly enters rivers without any purification in the study areas. One of the primary causes of urban pollution in the research region included sewage from Behbahan, Meshrageh and Chamran cities, which are located within the Maroon and Jarahi basins.

3.1.2. Agricultural Wastewater

Agricultural expansion due to an increase in the population growth rate requires irrigation. Therefore, large amounts of surface water and groundwater have been used up by irrigation installations.

Agricultural drainage is affected by water quality, the type and efficiency rate of irrigation, the type of drainage system, the consumption of agricultural inputs, the type and characteristics of soil as well as the climate conditions in each location. The main characteristics of agricultural drainage are the high level of EC, phosphorus, nitrogen and pesticides. The main sources of this pollution are six major drains in the study area.

3.2. Quality Monitoring Station Findings

It is necessary to compare the simulated parameters linked to the model with observational data to evaluate the model's accuracy. Therefore, the main information gathered for this exercise comprised all hydrometric station data including Behbahan, Cham-Nezam and Meshrageh. Furthermore, water quality and pollution data linked to the six main agricultural drains discharged into the Maroon and Jarahi were provided by the Khuzestan water organization. The third data set comprised the annual field measurement data collected by the authors. Due to the lack of information on wastewater pollution, the authors took care of three water quality measurement stations (Behbahan, Cham-Nezam and Meshrageh) located along the Maroon and Jarahi Rivers as indicated in Table 4.

Table 4. Specifications of river water quality monitoring stations.

Name	Station′	Longitude	Latitude	Distance to the End of River (km)
Behbahan	S1	23°20′50″	29°40′30″	50
Cham-Nezam	S2	04°55′49″	53°44′30″	60
Meshrageh	S3	24°26′49″	22°00′31″	110

Table 5 shows all the sources of pollution at each measurement location. The Maroon and Jarahi hydrometric stations were used to calibrate the QUAL2KW model. These stations are shown in Figure 7. Although there are eight hydrometric stations in this basin, due to station relocations, inaccurate station information and inappropriate locations, only information from three hydrometric stations was used.

Table 5. Sources of inlet and point-source pollutants for the Maroon and Jarahi Rivers.

Incoming Pollutants	Contaminant Reagent	Source of Pollution	Distance to the End of River (km)
Agricultural Drainage	A1	p1	306
	A2	p2	305
	A3	p3	302
	A4	p4	109
	A5	p5	237
	A6	p6	221
Lateral River	R1	p7	195
Municipal Sewage	U1	Behbahan	306
	U2	Cham-Nezam	142
	U3	Meshrageh	64

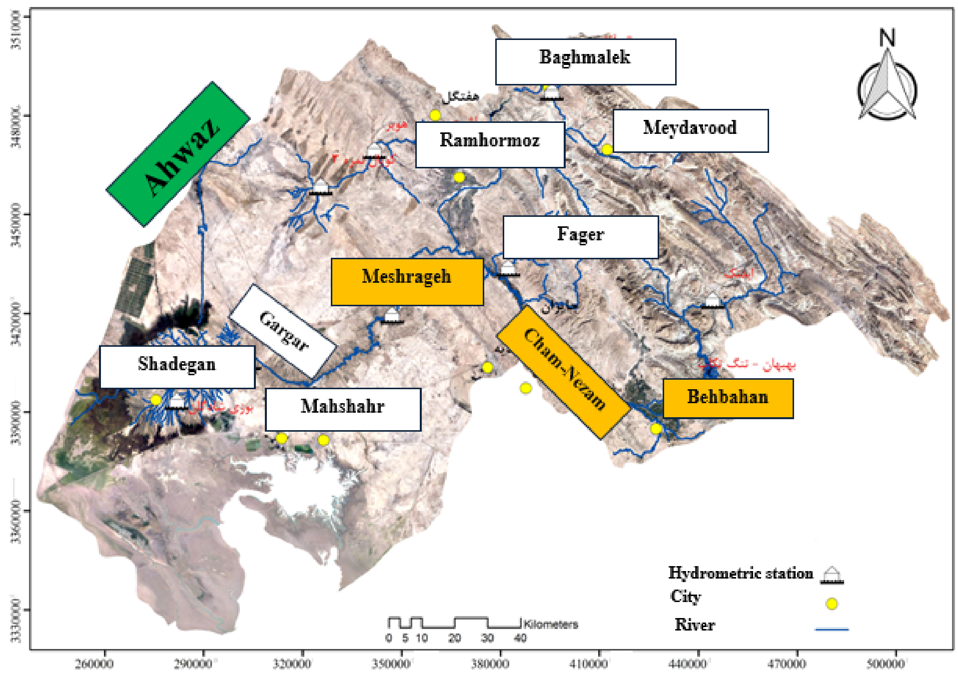


Figure 7. Location of hydrometric stations in the Maroon and Jarahi basin.

As the river has complex varying hydraulic conditions and variable pollutant input loads, it was necessary to simplify the input and output data. The authors considered that all hydraulic and quality parameters were constant in the model. Therefore, the model did not account for changing discharges [33].

Table 6 shows different river water quality characteristics grouped in four different categories. In this categorization, group one (1A, 1B) indicates the appropriate water quality for general consumption in contrast to the fourth group indicating the worst water quality, which is inappropriate for most consumption types. This table recommends the second group of water quality characteristics for Iran's rivers that support the economy [16]. Examples of the water quality parameters monitored at the Maroon and Jarahi river water quality monitoring stations are shown in Figure 8.

Table 6. Different river water quality standards (after [17]).

Parameter	Unit of Measurement	Different Water Quality Groups					National Standard of Iran	Selected Standard
		1A	1B	2	3	4		
Temperature	°C	≤20	20–22	22–25	25–30	>30	<21	1B
pH	-	6.5–8.5	6.5–8.5	6.5–8.5	5.5–9.5	>9.5 or <5.5	7.5	1B
Electric conductivity	mhos/cm	≤400	400–750	750–1500	1500–3000	3000<	<500	National Standard of Iran
Dissolved oxygen	mg/L	>7	5–7	3–5	-	<3	>7	1A
Five-day biochemical oxygen demand	mg/L	≤3	3–5	5–10	10–25	>25	<10	2
Nitrate	mg/L	-	≤44	-	44–100	100<	<44	National Standard of Iran
Ammonium	mg/L	≤0.1	0.1–0.5	0.5–2	2–8	>8	<0.5	1B

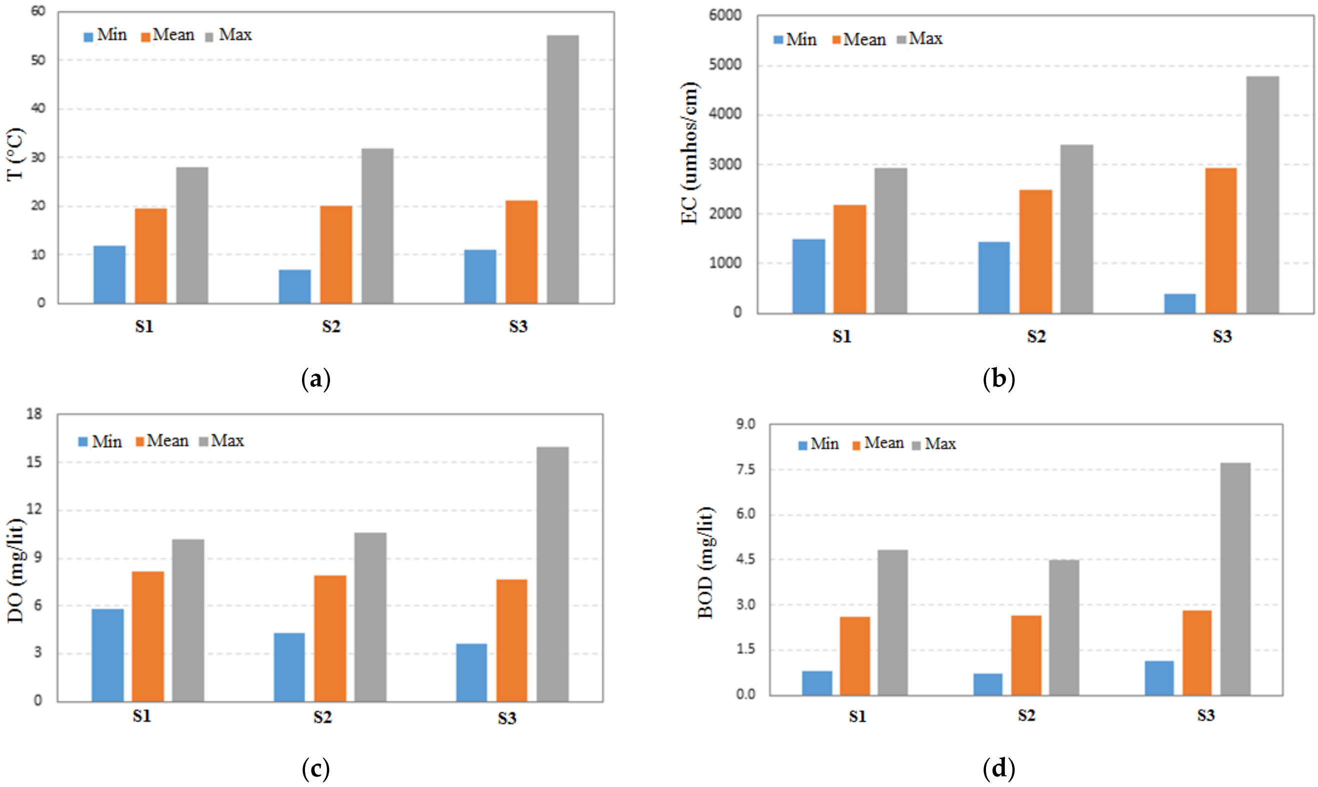


Figure 8. Example water quality parameters: (**a**) temperature (T); (**b**) electric conductivity (EC); (**c**) dissolved oxygen (DO); and (**d**) five-day biochemical oxygen demand monitored at the Maroon and Jarahi river water quality monitoring stations.

3.3. Qualitative Model Calibration Results

During the calibration stage, groups of hydraulic, meteorological and water quality data (obtained from the Water and Electricity Organization, Khuzestan Government,) were processed for the periods between May and September for the years 2019 and 2020. Then computational data were compared to the observational data. The main goal during calibration was to reduce the difference between the model output and observational data via optimization methods. Nevertheless, the final model should reflect as many realities as possible. Typically, there are two general calibration methods used in practice: (a) the trial and error (manual) method and (b) the automatic model (systemic) method. In the first method, the user enters all parameters based on physical observations and then makes suggestions as part of a set of preliminary tests. This method can be performed by the QUAL2K model. In the second method, the QUAL2KW model decreases the dichotomy (partition of a whole into two parts) between the computational results and the observational ones by a finite difference method. For this purpose, square deviation using the root mean square error as a selection criterion is the most practical manual regression method [11]. The average of simulated parameters using the QUAL2KW model is shown in Table 6. Regression analysis applying a genetic algorithm for automatic calibration was used. The application of genetic algorithms is suitable for evolutionary processes [34].

3.4. Validation of the Qualitative Model

By injecting various contaminants into the river, their transfer downstream was undertaken by the process of mixing with the flow and subsequent longitudinal, transverse and deep distribution. Contaminants are emitted longitudinally, transversely and deeply under the influence of the transfer and mixing processes. The capability and strength of river flows and other surface flows in the distribution of materials added to it are expressed in longitudinal, transverse and vertical directions. In the present study, based on the information collected in hydraulic stations and monitoring using SPSS software and optimal correlation applying the NRMSE equation, longitudinal mixing coefficients were obtained.

4. Results and Discussion

Modelling Findings

The results of the model calibration for the qualitative parameters are shown in Figures 9 and 10. There was little difference between the simulated and observational data for all stations. The water temperature increased from nearly 22 to 26 °C at the end of the Maroon River because of the input of polluted water with a higher temperature. Subsequently, the temperature decreased again to 21 °C due to water input from other branches of the river network. Furthermore, there was a considerable decrease in EC to nearly 1500 mmhos/cm along the river, especially after joining the Jarahi River. No interactions between the groundwater and surface water intake were considered in this paper when estimating EC levels. The agricultural industry downstream of the river meets their irrigation needs only from the river water. In contrast, agricultural activities upstream of the plain simultaneously harvest surface water and groundwater. The agricultural industry has faced water shortages in some months of the year (September to December). Furthermore, the environmental needs of the watercourses are not fully met (except for the Maroon River on some occasions) during most months of the year in the Maroon and Jarahi watershed. Finally, the needs of the potable water industry are met all the time.

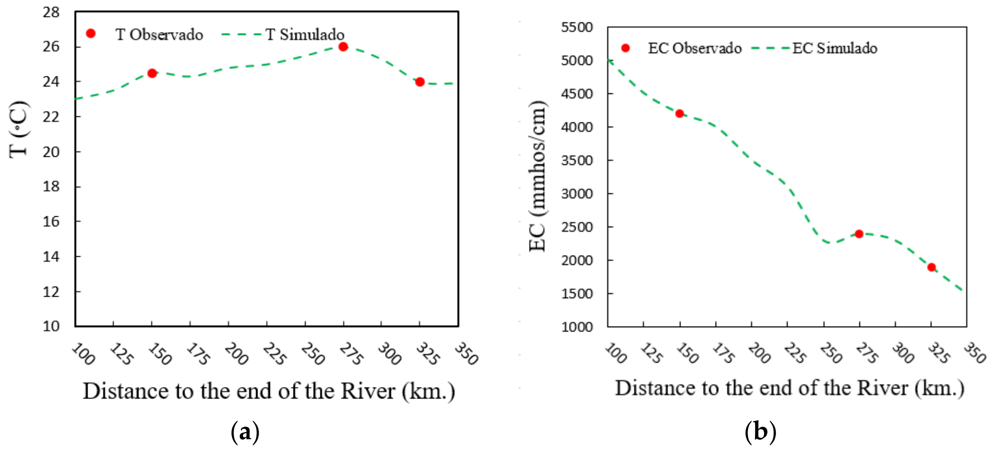
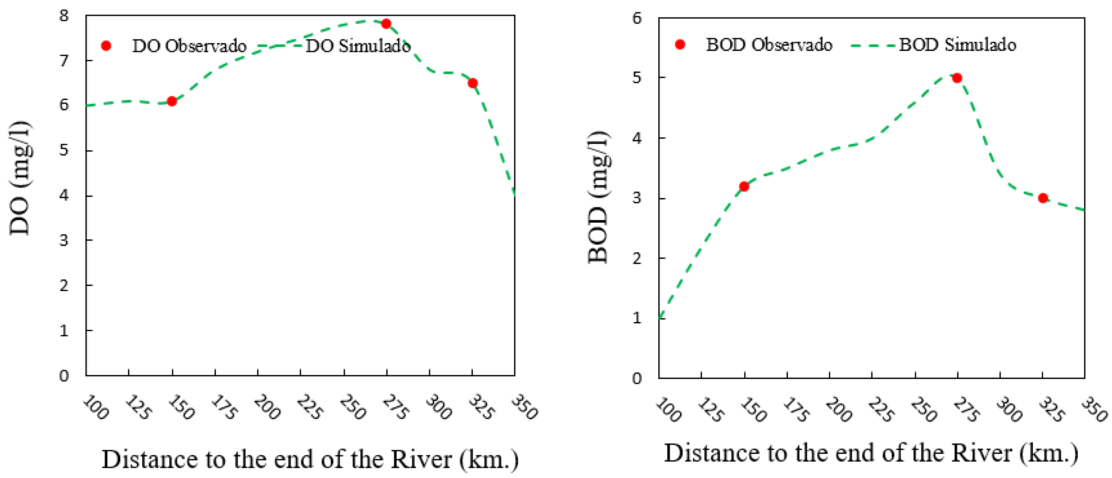


Figure 9. (**a**) Temperature; and (**b**) EC simulations along the Maroon and Jarahi Rivers.

Other water quality simulation findings are shown in Figure 10. The DO concentration increased slowly by 2 mg/L and then decreased rapidly by 4 mg/L. In comparison, the BOD parameter significantly increased from 1 to 5 mg/L because of discharged wastewater and urban sewage along the first half of the Maroon River. Thereafter, the BOD dropped by 3 mg/L due to other water discharges and self-purification especially around the Meshrageh station.

Tables 7 and 8 show all the results of the model calibration. Based on the mentioned assessed example parameters, the QUAL2KW model showed a high accuracy in simulating water quality parameters for the Maroon and Jarahi Rivers. The model used two forms of carbonaceous BOD to represent organic carbon. These forms were a slowly oxidizing form (slow CBOD) and a rapidly oxidizing form (fast CBOD; Table 9).

The lack of hydrometric stations in the Maroon–Jarahi basin was a great challenge to the modelling effort. For this reason, it was not possible to accurately calibrate the sections close to the end of the Maroon River. However, this area accommodates the vast majority of the irrigation and drainage networks. Therefore, it would be appropriate if at least one station could be located at the end of the Maroon River before crossing the Allah River.



(**a**) (**b**)

Figure 10. (**a**) Simulation of dissolved oxygen (DO); and (**b**) biochemical oxygen demand (BOD) along the Maroon and Jarahi Rivers.

Table 7. Test statistics in the validation stage.

Parameter	Temperature	Electric Conductivity	Dissolved Oxygen	Rapidly Oxidizing Carbonaceous Biochemical Oxygen Demand	Harati et al. (2015)
Correlation coefficient	0.97	0.97	0.98	0.97	0.87
Normalized mean square error	0.911	0.13	0.09	0.04	0.75
NASH parameter	0.94	0.91	0.96	0.93	0.95

Table 8. Indicators for the NASH parameter, root mean square error (RMSE) and the coefficient of determination (R^2) for observational and simulated data.

Name	Station	NASH	RMSE	R^2
Behbahan	S1	0.82	20.05	0.78
Cham-Nezam	S2	0.96	3.89	0.98

Table 9. Simulated sources of point-source pollution parameters for the Maroon and Jarahi Rivers using the QUAL2KW model.

Incoming Pollutant	Spot of Point-Source Pollution	Source of Pollution	*T* (°C)	*Q* (m^3/s)	*EC* (Umhos)	*DO* (mg/L)	*FastBOD* (mgO_2/L)
Agricultural Drainage	Maroon	p1	16	1.3	697	8.5	3.9
	Maroon	p2	24	3	787	8.1	4.2
	Maroon	p3	26	1.3	778	8.7	3.2
	Jarahi	p4	23	5.5	708	7.6	3.7
	Maroon	p5	26	1.3	1281	7.6	2.8
	Rood-Zard	p6	25	1.5	1545	7.6	1.7
Lateral River	Allah	p7	28	4.2	747	6.1	2.7
Municipal Sewage	Maroon	Behbahan	24	0.99	1750	6	113.5
	Maroon	Cham-Nezam	24	0.04	1750	5	20.8
	Jarahi	Meshrageh	25	0.04	1750	5	23.8

The highest amount of BOD along the Maroon River was related to the stretch located after the Behbahan Irrigation and Drainage Network due to the discharge of agricultural and urban effluents. The highest amount of BOD along the Maroon River was related to stations 1 and 2 due to the discharge of municipal and agricultural effluents from Behbahan city and other drains such as P2, P3 and P4 (Table 7) located near these two points.

The Qual2K software was used to simulate the water quality in the Maroon and Jarahi basin and genetic algorithms were applied to optimize variables of relevance for decision makers. The model had a good capacity to provide optimal answers concerning point-source pollutant load allocations. Calibrated parameters in the QUAL2KW model are shown in Table 10.

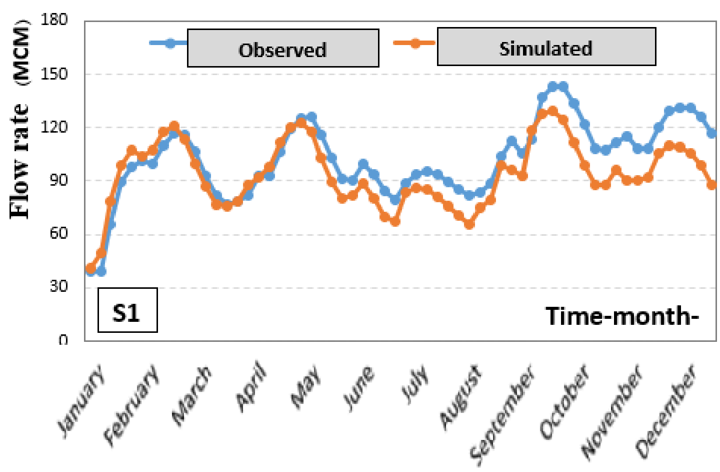
Table 10. Values of calibrated parameters in the QUAL2KW model using the genetic algorithm based on boundary conditions for this parameter.

ID	Parameter (M/Day)	Min	Max	Calibrated Value with GA
1	Biochemical oxygen demand	0	2	1.5
2	Dissolved oxygen	0	5	2.69
3	Nitrate	0	5	3.78
4	Ammonia	0	2	1.52
5	Phosphate	0	3	1.06
6	Organic nitrogen	0	2	0.25
7	Inorganic phosphorus	0	2	0.014

The model calibration parameters are shown in Table 11. Figure 11 indicates that the observed and simulated discharge values at each hydrometric station had similar trends and that differences were only observed for S2. The reasons for this are as follows: (a) highest need for water in summer; (b) (subsequent) release of large volumes of water by the dam; (c) challenges in measuring high discharges at station S1; and (d) absence of recordings for maximum discharge times.

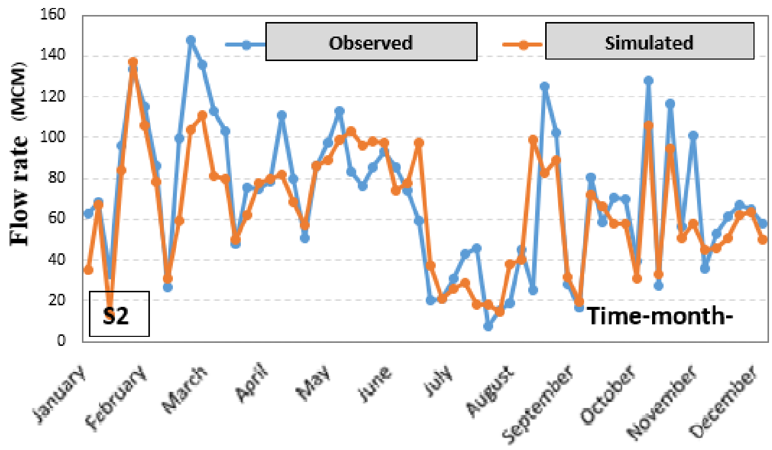
Table 11. Effective parameters in the calibration.

Location	Total Roughness Coefficient	Obstacle Roughness Coefficient	Cross Section Change Coefficient	Channel Level Coefficient	Granulation Coefficient
Sediment bed	0.033	0	0.01	0	0.028
Wall	0.053	0.005	0	0	0.028

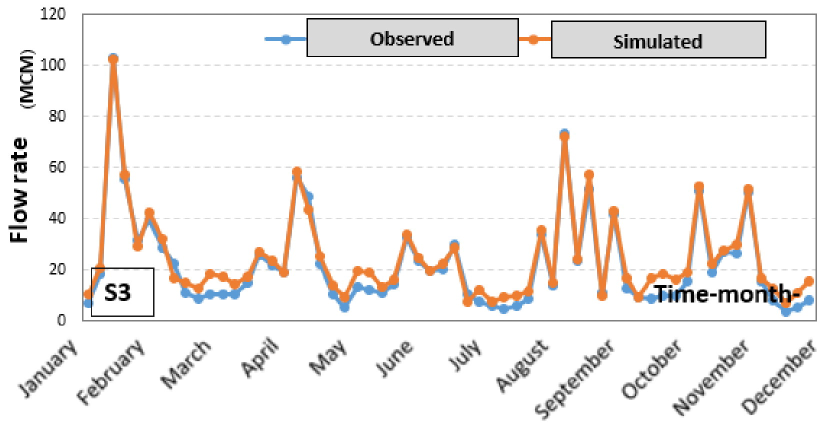


(**a**)

Figure 11. *Cont.*



(**b**)



(**c**)

Figure 11. Parameter Q for the QUAL2KW model during calibration for stations (**a**) S1; (**b**) S2; and (**c**) S3.

At the beginning of the Jarahi River and after the confluence of the Allah and Maroon Rivers, the water temperature decreased significantly during all months due to the increase in the Allah River water discharge. After the intersection, this decrease was between 2 and 8 °C depending on the season. Towards the end of the Jarahi river, due to the addition of municipal sewage and agricultural effluents with high temperatures, as well as changes in physical and hydraulic river characteristics including a sharp decrease in the slope of the high flow path, the water temperature rose gradually, reaching 37 °C.

5. Conclusions and Recommendations

Concerning the end of the Jarahi River in particular, for most of the warm months of the year, the concentration of DO was relatively reduced compared to the intersection with the Maroon River, but in most of the cold months of the year, this trend was reversed. The reason for this change in approach is the severe fluctuations in the river flow in hot and cold months of the year, especially the difference in discharge in the dry years with low rainfall and the wet years with high rainfall.

Water quality parameters determined at the monitoring stations and the calibration results of the QUAL2KW model for the Maroon and Jarahi Rivers indicated from a qualitative perspective that the EC ascended along the Maroon River reaching 1750 mms/cm. The DO concentration depends primarily on the flow rate of the river.

Agriculture and urban sewage contamination input to the river was responsible for the BOD reaching a maximum of about 7.9 mg/L at approximately 300 km from the end of the Jarahi river. The maximum concentration of BOD at Behbahan station was 113.5 mg/L but decreased thereafter.

The calibrated values with GA showed the best optimization for the model calibration. The QUAL2KW water quality model provided a reliable simulation of the water quality for a large catchment area with only sparse data. The model will help to better manage and exploit the surface water in catchments such as the Maroon and Jarahi basin, which is monitored by only three stations. Concerning the Jarahi River, the concentration of BOD did not change significantly in the low-water-months of the year but did change significantly in the high-water-months. The rate decreased towards the end of the river. The EC changes in the Maroon River can be explained by a 10% decrease in the flow.

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