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Uncertainty Analysis of River Water Quality Based on Stochastic Optimization of Waste Load Allocation Using the Generalized Likelihood Uncertainty Estimation Method

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Abstract

The aim of this study is to improve the water quality of rivers while satisfying the interests of pollution sources and environmental protection agencies (EPA). For this purpose, a stochastic integrated simulation–optimization approach is developed for waste load allocation (WLA) in a river system. The water quality simulation model (QULA2Kw) is coupled with an evolutionary optimization model (multi-objective imperialist competition algorithm (MOICA)) to minimize wastewater treatment costs and biochemical oxygen demand (BOD) violations of the standard level. The applicability of the approach is demonstrated by the case study of the Dez River in Iran. The stochastic model (ARIMA) is used to forecast the headwater from 2022 to 2025. The influence of the uncertainty of the stochastic parameters (headwater, oxidation rate, point source inflow, abstraction, and point source concentration) is evaluated by the Generalized Likelihood Uncertainty Estimation (GLUE) model. The results showed that the point source inflow uncertainty is higher than other parameters. The results of optimal WLA under the uncertainties showed that the dissolved oxygen (DO) uncertainty bound was narrower than the BOD. The solutions in Pareto fronts showed the contradiction between polluters and environmentalists' interests, and according to the waste load criterion, using this methodology not only improved the river water quality but also there were least violations of standards along the river.

Keywords GLUE · MOICA · Prediction · QUAL2Kw · Uncertainty · Water quality

1 Introduction

Rivers are important and major sources of water supply for industry, urban consumption, and agricultural uses (Babamiri et al. 2021). The water quality of rivers could be significantly impacted by human activities, such as urbanization and industrialization (Hu et al. 2018; Meng et al. 2017). The entry of nutrients and biodegradable pollutants into rivers, including sanitary wastewater, agricultural, and industrial residues, can significantly reduce

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water quality and pollute it (Zhang et al. 2015). Therefore, proper water quality management in river systems is necessary and inevitable to maintain the health of rivers and human life (Ebrahimi and Khorram (2021)). Simulation or numerical modeling of river water quality is the initial step in river water quality management. The QUAL2Kw model is widely regarded as one of the most comprehensive models for simulating river water quality. Numerous studies have utilized this model to assess river water quality (Gikas 2014; Pashmchi et al. 2022).

Different management practices have been developed to maintain and improve water quality. These methods can be divided into two main categories: i) controlling the total pollutant emission amount related to water carrying capacity; and ii) employing technologies for water quality improvement in accordance with ecological restoration engineering (Yang et al. 2015). Generally, these two groups were rarely combined into an integrated water environmental management system, leading to various complexities. These complexities include trade-offs between optimizing treatment technology, waste load allocation, and system cost in water quality management. Faced with these challenges, several optimization techniques were developed for economically and environmentally sustainable water management (Nikoo et al. 2016). Optimizing waste load allocation (WLA), which refers to determining the allowable amount of waste load discharged into a river by different pollution sources, is recognized as an effective approach for river water quality management (Mahjouri and Bizhani-Manzar 2013; Moridi 2019). This approach aims to meet water quality standards while acknowledging that the treatment level and cost may not necessarily be satisfactory for the dischargers. Several optimization techniques have been developed for economically and environmentally sustainable water management (Zare Farjoudi et al. 2021). Evolutionary Algorithms (EA) and classical optimization methods are two common approaches. However, the EA optimization method can be applied equally to linear or nonlinear constraints and objectives, as well as to time-separable or non-separable objectives. It has shown better performance in reaching Pareto fronts faster (Aghasian et al. 2019; Moridi 2019).

In this vein, Yandamuri et al. (2006) developed a multi-objective optimization framework for optimal WLA in rivers using the Nondominated Sorting Genetic Algorithm-II (NSGA-II). Their results showed that the sort of detailed information obtained from such multi-objective modeling helps decision-makers decide whether the extra cost to be incurred to achieve the incremental degree of equity is justified. Liu et al. (2014) evaluated the influence of different objectives of NSGA-II in an integrated model, such as maximizing economic benefit, pollutant discharge, and minimizing water deficiency. The efficiency of the model in analyzing the interaction between water and wastewater allocation indicated the importance of reducing chemical oxygen demand (COD) in the river. Feizi Ashtiani et al. (2015) used the Multi-Objective Particle Swarm Optimization (MOPSO) algorithm to minimize the pollutant treatment costs in the river WLA regarding environmental standard violations and inequity criteria. Their results indicated that the approach can be used well for multi-objective optimization, even in comparison with NSGA-II.

To date, several algorithms have been developed for optimizing water resources systems, including genetic algorithms (GA) (Azari et al. 2018; Jalili et al. 2022), particle swarm optimization (PSO) (Nagesh Kumar and Janga Reddy 2007; Noory et al. 2012; Muronda et al. 2021), honey bee mating (Haddad et al. 2006), ant colony optimization (Kumar and Reddy 2006), simulated annealing (Georgiou et al. 2006), and imperialist competition algorithm (Afshar et al. 2015). The imperialist competition algorithm (ICA), a relatively new evolutionary algorithm proposed by Atashpaz-Gargari and Lucas (2007), has been successfully applied to various single-objective engineering problems (Yousefi et al. (2011); Talatahari et al. (2012); Hosseini-Moghari et al. (2015)), but few attempts have been made to utilize it in the area of multi-objective optimization. Enayatifar et al. (2013) developed a multi-objective optimization based on ICA (MOICA) and demonstrated its effectiveness on several benchmark functions. The results were compared with those of NSGA-II and MOPSO, proving to be better or at least on par. Nazari and Deihimi (2017) developed fuzzy multi-objective optimization based on ICA. The comparison with NSGA-II and MOPSO showed that MOICA is a more effective and reliable multi-objective solver covering the actual Pareto fronts. Babamiri et al. (2022) used the MOICA algorithm for optimal operation of reservoir-river systems based on quantitative and qualitative water management. Their results showed the algorithm's reasonable accuracy and high speed.

Optimized solutions are vulnerable to failure because decision-making in water resource quality management usually involves many factors with high uncertainties (e.g., runoff conditions, point source pollution, water demand growth, climatic forces, and model parameters) (Liu et al. 2014). Therefore, stochastic optimization models are essential to involve various sources of uncertainty in modeling and decision-making. In this regard, many researchers have carried out studies. For example, Nikoo et al. (2016) used a fuzzy optimization model to determine WLA policies with cooperative and non-cooperative approaches. The results showed the effectiveness of the methodology and its fairness in reallocating treatment costs to dischargers. Meng et al. (2017) developed a two-stage stochastic programming (TSP) model to support regional waste load (COD and NH_3-N) allocation. Their results helped establish a rational discharge permit system for each pollution unit under water quality targets and provided a basis for the production plans of these pollution units. Zare Farjoudi et al. (2021) applied a simulation–optimization approach to minimize wastewater treatment costs and dissolved oxygen violations from the standard level in the Zarjoub River, Iran. The uncertainty in river inflow was considered by Latin hypercube sampling to provide more realistic insights to decision-makers. Furthermore, studies have been conducted on the uncertainty of river water quality simulation, such as those by Wu et al. (2020), Zhang and Li (2021), Ebrahimi and Khorram (2021), Juwana et al. (2022), and Rahat et al. (2023).

Therefore, it is crucial to consider uncertainty in optimization to determine the optimal range of decision variables for making the best decisions. To date, several uncertainty analysis methods have been developed in hydrosystem analysis, including the generalized likelihood uncertainty estimation method (GLUE), which is one of the common methods in uncertainty analysis (Blasone et al. (2008), Beven and Binley (2014), and Dai et al. (2018)). This technique has received much attention and has been applied to a variety of problems in water resources management due to its simplicity and few required assumptions when used in practical applications (Beven and Binley 2014). The technique can handle input uncertainty, structural uncertainty, parameter uncertainty, and response uncertainty since it is connected to parameters and illustrates all uncertainties and impacts of the co-variation of parameter values on model performance indirectly (Beven et al. 2007). It has also been used to represent prediction uncertainty within the context of Monte Carlo (MC) analysis coupled with Bayesian estimation and propagation of uncertainty (Blasone et al. 2008). Using this method, studies have been carried out on uncertainty analysis of water quality management, such as Mannina (2011), Gong et al. (2011), Chen et al. (2014), Gerkani Nezhad Moshizi et al. (2023), and Zhong et al. (2023).

Stochastic models, which use statistical descriptions of stream flow and forecast processes instead of applying a specific streamflow sequence to determine operating policies, have recently gained widespread approval (Babamiri et al. 2022). Autoregressive integrated moving average (ARIMA) models are particularly popular, as they can efficiently predict a value in a response time series as a linear combination of past observations and easily accommodate seasonality (Szeląg et al. 2019). These models are considered the best statistical linear type of models for runoff prediction and have been widely employed in studies on modeling streamflow time series by various researchers (Muronda et al. 2021). Studies conducted so far on stochastic optimization of WLA in the river system are limited; however, none has addressed or investigated the uncertainty of river water pollution based on optimal conditions of WLA using the GLUE method. Therefore, this study aims to develop a framework that links the MOICA with the body of a qualitative (QUAL2K) model to optimize the WLA for dischargers along the Dez River in Iran. So, it can provide optimal solutions for system allocation and ensure the maintenance of the quality of the river according to the world's standards. It discusses and analyzes the impact of uncertainty on the acceptable levels of water quality parameters and attempts to accomplish it with the GLUE technique and a simulation-based optimization approach.

2 Material and Methods

2.1 Study Area

The Dez River is one of the most important river systems in Iran, playing a vital role in providing water for agricultural and industrial usage in the southwestern provinces. The Dez River Basin is located between 48° 10′—50° 21′ eastern longitude and 31° 34′—34° 17′ northern latitude, spanning a length of 215 km. This basin has an average elevation of 1603 m and an area of approximately 21720 km2, which is divided upstream and downstream by the Dez Dam. The study area has a semi-arid climate with an annual precipitation of 252.38 mm, an annual temperature of 25.1 °C, and an annual pan evaporation of approximately 2035 mm. Consequently, the average water inflow to the reservoir is 152 m3/s (http://www.irimo.ir). The river flows from north to south, and the present study focuses on the downstream part with a length of 173.78 km. Figure 1 shows the location of the study area (4355 km^2), plains, rivers, hydrometric stations, point sources of pollution, and withdrawals of the river in the study area. Recently, the water quality of the river has deteriorated due to the discharge of domestic wastewater and agricultural runoff. Therefore, this research attempts to allocate a specific waste load to point sources in order to meet the standard BOD concentration at the control point.

2.2 Stochastic Modeling of River Flow

This study modeled streamflow time series using the Autoregressive Integrated Moving Average (ARIMA (p, d, q)). The model was then used to predict the Dez River head flow at Dezful station for the future period of 2022–2025.The most common method in time series modeling is the autoregressive moving average (ARMA)-based approach, such as the autoregressive integrated moving average (ARIMA) and seasonal ARIMA (SARIMA). The formulation of SARIMA (p,d,q)(P,D,Q) is a complete stochastic model with differencing and seasonality as described in Box and Jenkins (1976).

The ARIMA model was developed for each month using the AIC, RMSE, and ACF tests for the flow forecasts. Thus, the structure of the ARIMA model for each month was shown in Table 1.

Figure 2 shows the historical and predicted inflow time series in Dezful station.

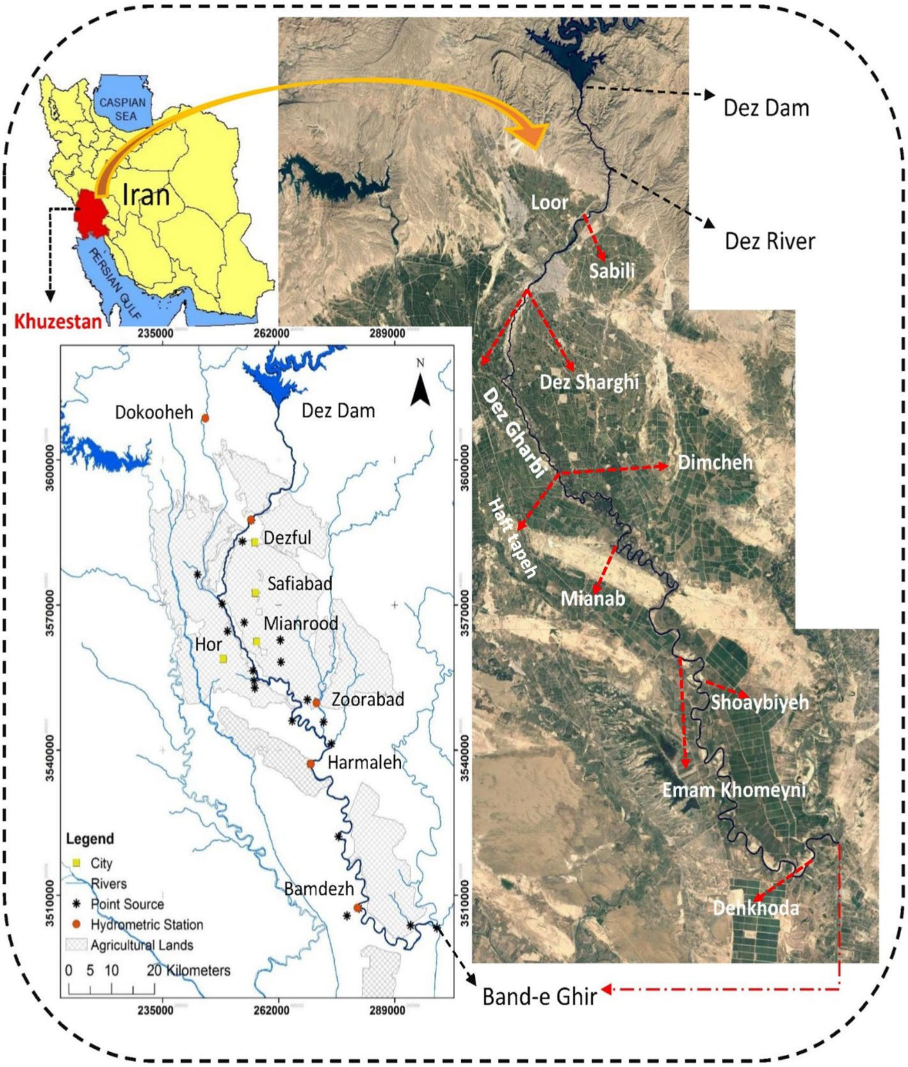

Fig. 1 Location of the study area in Iran and Khuzestan province

2.3 Water Quality Simulation Model (QUAL2Kw)

QUAL2Kw is a 1D water quality simulation model that numerically solves the governing differential equations of constant river flow and advection–dispersion. These equations take into account the effects of advection–dispersion, dilution, constituent reactions, and interactions, as well as sources or sinks. In QUAL2Kw, the general mass balance equation for all constituent concentrations in the ith River reach can be written as (Chapra et al. 2008):

$$\frac{\partial C}{\partial t} = \frac{\partial (AD\frac{\partial C}{\partial x})}{A\partial x} - \frac{\partial (AUC)}{A\partial x} - \frac{dC}{dt} + \frac{S_C}{V} \quad (1)$$

Table 1 The ARIMA models developed in Dez dam site for different months

Month	Model	AIC	RMSE (m^3/s)
January	ARIMA (1,1,1)	27.12	1.43
February	ARIMA (2,1,1)	38.26	1.26
March	ARIMA (2,0,1)	18.76	1.21
April	ARIMA (1,0,1)	25.44	1.62
May	ARIMA (2,1,1)	34.92	1.08
June	ARIMA (2,1,1)	38.22	1.52
July	ARIMA (1,1,1)	29.13	1.27
August	ARIMA (1,0,1)	24.42	1.54
September	ARIMA (1,0,1)	27.27	0.35
October	ARIMA (1,1,1)	33.21	2.92
November	ARIMA (1,0,1)	30.39	1.41
December	ARIMA (1,0,1)	25.41	1.40

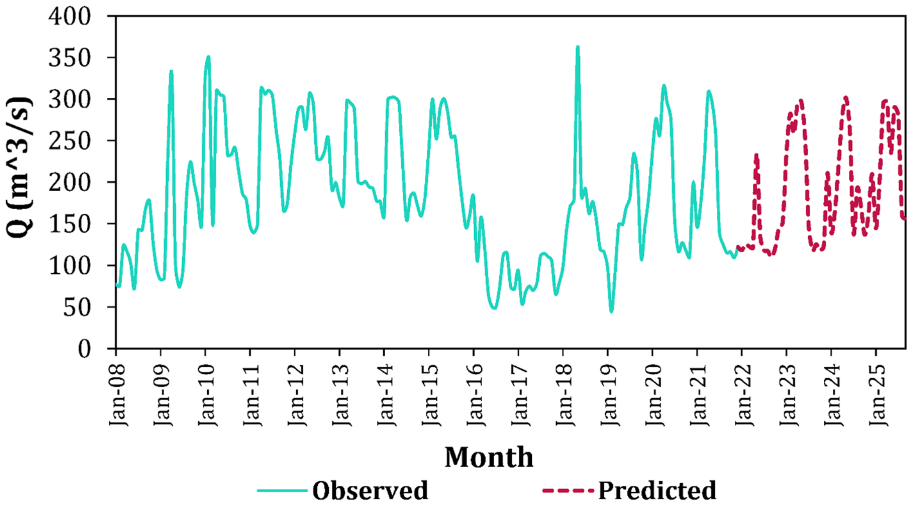

Fig. 2 Historical and predicted inflow (2022 to 2025) in the Dez dam station

where C: concentration of the specific parameter; v: volume of water in the river reach; U: mean water velocity in the reach; D: diffusion coefficient; A: river estuary section area; S_C: external sinks or sources of the C element; *t*: time (day); and *x*: the distance of each reach from the origin (here, Dez dam) along the river in the flow direction.

The QUAL2Kw model minimizes the sum of differences between observational and computational results using fitness relationships, for which the RMSE relation is most applicable. The genetic algorithm then uses the fitness result for automatic model calibration. The validated model is re-run with a new set of information to measure the error rate between the calculations and the observations in the validation phase.

2.4 Data and Pollution Sources

Many parameters are required for river water quality simulation, including hydraulic data in fragments (headwater flow, river bottom slope, riverside slope, river bottom width, and Manning coefficient), meteorological data (temperature, wind speed, dew point temperature, solar radiation, and cloud cover percentage), and water quality of point sources and nonpoint sources (DO, BOD, and surface water inflow). The detailed requirements can be found in Chapra et al. (2008).

Khuzestan Water and Power Authority (KWPA) and Khuzestan Department of Environment (KDOE) are the two main authorities for Dez River water quality monitoring and supervision (KWPA 2001). Hydrometric and quality data from Dezful, Harmaleh, and Bamdezh stations were collected from KWPA, and wastewater discharge (point sources) was gathered from KDOE. Table 2 represents the average of quantitative and qualitative characteristics corresponding to the most important sources of pollutants in the study area. Moreover, hydrodynamic data were obtained from the Dezab Engineering Company (www.dezab.com).

Table 2 Average discharge and monthly wastewater of point sources pollutants along the Dez River

Pollutant Sources	**Name**	**Distance from upstream (Dez dam) (km)**	**Q (m^3/s)**	**T (°C)**	**DO (mg/L)**	**BOD (mg/L)**
Urban wastewater	Dezful	8.6	2.4	28	3.4	94.2
	Safiabad	26.6	0.4	24	4.7	20.8
	Hor	37.5	0.5	24	5.2	23.8
	Mianrood	40.3	0.6	24	4.8	25.6
Industrial wastewater	P Mahi	23.2	5.2	24	2.5	22.1
	K Hafttapeh	38	1.8	26	4	110.6
	Kagz Pars	69.2	0.6	28	2.2	150.3
Agricultural drainage	Loor	4.7	1.3	16	6.2	3.8
	Sabzab	23.5	3	24	8.1	4.2
	Banehasan	31.4	1.3	26	7.6	3.2
	Sagari	33.2	4.2	23	8.7	3.7
	Haftapeh	43.3	1.3	25	7.6	2.4
	Salimeh	55	2.8	24	6	3.3
	Tapdarin	55.4	1.2	26	7.4	4.2
	Atij	65.2	2.3	25	6.9	4.3
	Mianab	107.5	3.5	29	3.1	2.8
	Kharvar	134.7	2.2	31	3.5	5.5
	Shoabiye	167.9	11.1	27	7.2	7.3
Hydrometric Station	Dezful	6.5	174.9	18.2	8.6	3.6
	Harmaleh	81.5	123.4	28.6	5.5	3.5
	Bamdezh	136.6	116.9	29.7	4.8	3.8

2.5 Generalized Likelihood Uncertainty Estimation (GLUE)

In GLUE, parameter uncertainty accounts for all sources of uncertainty, i.e., input uncertainty, structural uncertainty, parameter uncertainty, and response uncertainty, because ‘‘the likelihood measure value is associated with a parameter set and implicitly reflects all these sources of error and any effects of the covariation of parameter values on model performance’’ (Choi and Beven 2007). In this study, the GLUE analysis was performed as follows:

1. The Monte Carlo method was used to generate a large number (103) of parameter set for the model. Each parameter value was randomly drawn from the ranges presented in Table 3 randomly. Figure 3 shows the probabilistic distributions of the five selected stochastic parameters.
2. The exponential criterion (L) was calculated based on the simulated BOD and DO values from the QUAL2Kw model. The inverse error variance (Mantovan and Todini 2006) was used as the exponential criterion:

$$L = \left[\sum_{j=1}^{n} \frac{(O_j - Y(\theta_j))^2}{n-2} \right]^{-1} \tag{2}$$

   where θ_j is the jth set of parameters O_j the measured values, $Y(\theta_j)$ the model output for the jth parameter set, and n is the number of parameters sets. Larger values of L indicate greater agreement between simulated $Y(\theta_j)$ and actual O_j.
3. Taking into account the acceptable threshold (ASR), the set of parameters that lead to better model performance (the set of acceptable parameters) is separated from the other set of parameters. In other words, by descending sorting the L values together with the set of parameters (θ_j, for j = 1,2,….,n) associated with them, a fixed percentage of parameters led to a higher-performance model are selected as the set of acceptable parameters. In this study, the acceptable threshold is set as a percentage of the number of samplers (n) by 1%.
4. Finally, the model output uncertainty is evaluated by calculating the exponential weights for the set of acceptable parameters (θ) (Muronda et al. 2021).

$$P_i = \frac{L_i}{\sum_{i=1}^{n} L_i} \text{for i } = 1, 2, \ldots .., \text{n} \tag{3}$$

   where P_i is the probability or weight of the likelihood corresponding to the ith parameter set, and n is the number of acceptable parameter sets. The sum of the weights in

Table 3 Variation Ranges of Model Parameters used in the present study

Parameter	Unit	Lower limit	Upper limit
Headwater flow	m^3/s	112	298
Oxidation rate	day^{-1}	0	5
Point sources inflow	mg/l	89	148
Abstraction	m^3/s	72	208
Point sources concentration	mg/l	9	21

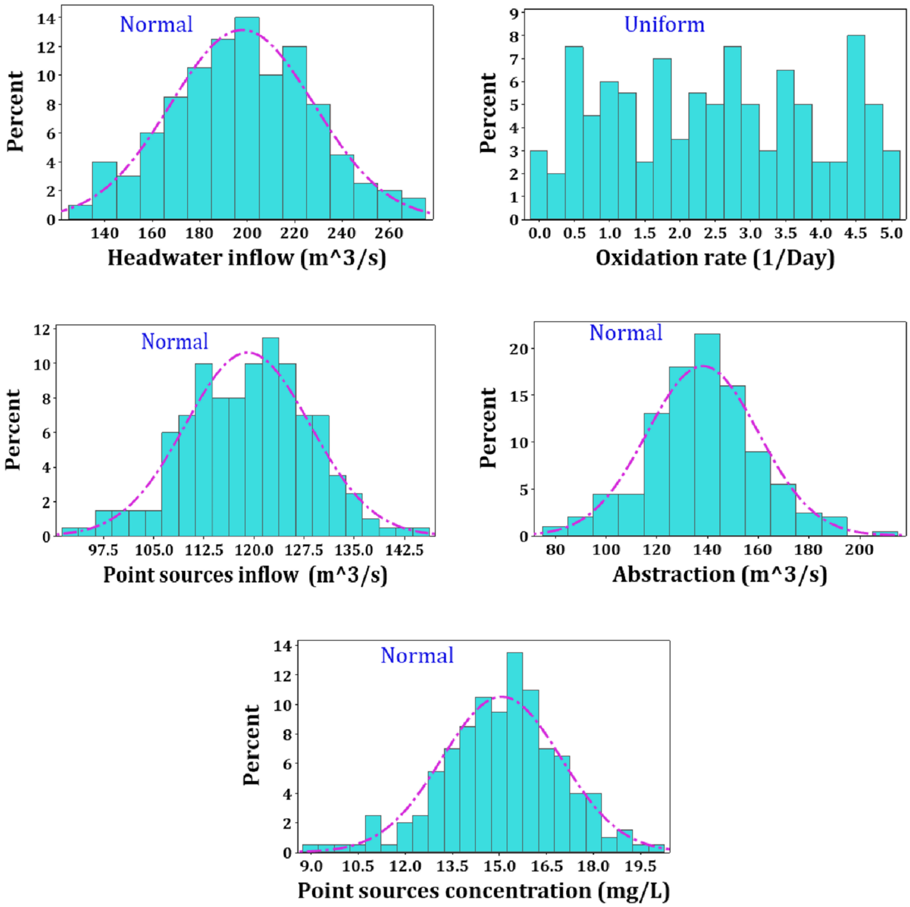

Fig. 3 Statistical distribution of parameters generated using the Monte Carlo simulation technique

the denominator is equal to 1. Indeed, these values (i.e., the weights) form the probability density function (PDF). Then, a 95% confidence interval (95CI) is extracted for the simulated model output.

The simulations beyond the upper and lower limits of about 2.5% are marked as outliers. Therefor, the remaining sets are considered the certainty range of 95CI. The certainty range obtained in the GLUE method approximately reflects all types of sources of error in the modeling process. This range shows the existence of uncertainties in model prediction (Blasone et al. 2008).

2.6 Multi-Objective Optimization (MOICA)

The imperialist competition algorithm (ICA) is an example of population-based algorithms (Enayatifar et al. 2013). The algorithm has been inspired by the idea of dividing countries into imperialists and colonies. Individuals in the ICA are called countries. Countries are within different parts of the problem space, which are called empires. The strongest country in an empire is called the imperialist, and other countries within that empire are named colonies. Iterations are called decades in ICA. Imperialists tend to attract colonies toward themselves in every decade (Atashpaz-Gargari and Lucas 2007). The MOICA was used in this study. In this method, rather than finding the lowest-cost associated countries as in the original algorithm, the non-dominated solutions are to be found. All countries on the Pareto-optimal front are considered to have the first rank. The imperialist countries are selected from this set, which could greatly impact the coverage and diversity of solutions. This impact is more significant when optimization has a high number of objectives. In the original ICA, each country is assigned a power based on the objective function, but, in the multi-objective method, the power of each country should be based on all objectives (Enayatifar et al. 2013).

2.7 Objective Functions

The purpose of this study is to improve the water quality parameter by minimizing treatment costs, removing pollutants, and minimizing BOD violations from the standard level in river water. Therefore, minimizing the total annual treatment cost and the BOD violation from the standard level is the objective function, as written in Eqs. (4) and (5). The Eq. (4) refers to the first objective function that minimizes the treatment cost of all dischargers. The first assumption of this research is that dischargers have to pay the treatment cost, and the treatment plant construction is paid for by the government. Also, Eq. (5) presents the objective function of improving the river water quality variable (BOD). It minimizes the BOD violation from the standard level (equal to 5 mg/l, here) at the checkpoint of the river. The constraint of the problem is formulated in Eq. (6) and shows that the optimized dischargeable BOD must be a portion of the initial BOD concentration.

$$\text{Min (treatment cost)} = \sum_{n=1}^{N} c_n t_n \tag{4}$$

$$\text{Min (BOD violation)} = \sum_{n=1}^{N} (BOD_{cp} - BOD_{standard})^2 \tag{5}$$

Subjected to:

$$BOD_n^{optimal\ discharged} = \alpha_n (BOD_n^{initial}) \tag{6}$$

where N = the number of dischargers/decision variables; c_n = treatment cost coefficient for each discharger based on $Q_n * BOD_n^{initial}$; Q_n = inflow of discharger n; $BOD_n^{initial}$ = the initial BOD of discharger n before optimization; t_n = treatment level of discharger n; BOD_{cp} = BOD concentration at checkpoint; $BOD_{standard}$ = standard concentration of BOD in the river; $BOD_n^{optimal\ discharged}$ = BOD concentration of discharger after optimization process of polluter n. In this study, α_n is the decision variable of the simulation–optimization model and represents the percentage of BOD allowed to be discharged n after optimization process.

There are three major polluters along the Dez river (Dezful urban sewage, K-Hafttapeh industrial wastewater, and Kaghaz-Pars industrial wastewater), and if their pollution is controlled, the amount of pollution in the Dez river will be within the standard level of Class 1B (BOD = 5 mg/l), so the decision variables are the treatment amount of these pollutants.

Table 4 Coefficient of treatment cost for dischargers

Discharger	c_i (1000$)
Dezful	158.6
K Hafttapeh	141.03
Kagaz Pars	235.06

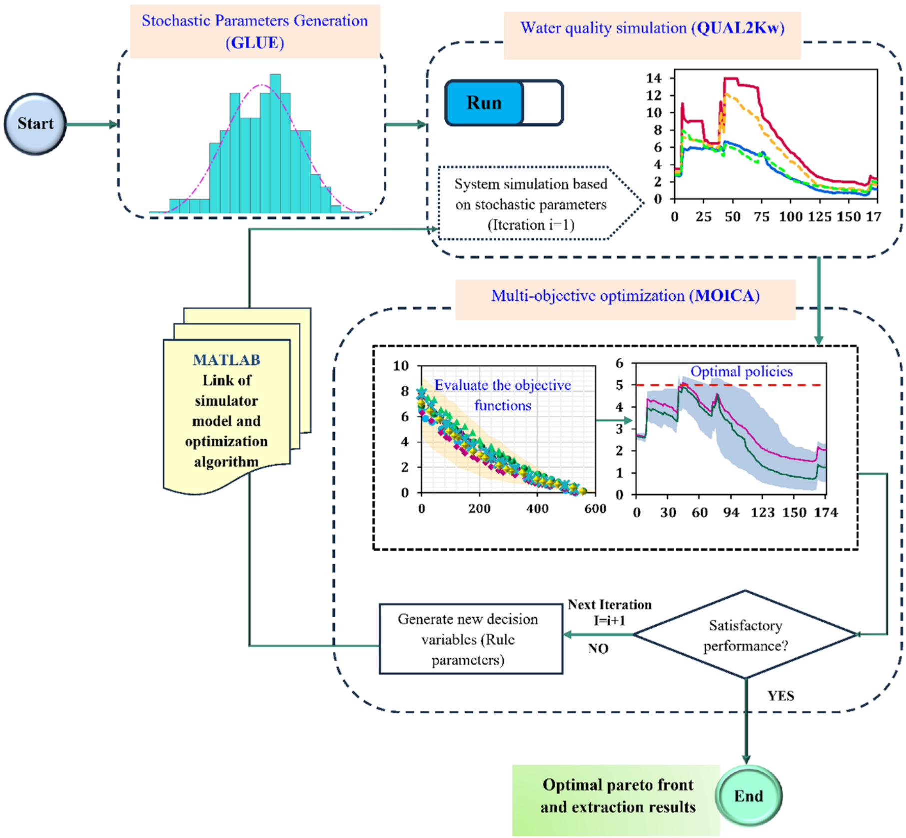

Fig. 4 Stochastic Simulation–Optimization Modeling Framework

The coefficients of the treatment cost in Table 4 are calculated based on the research done by Estalaki et al. (2015).

2.8 Stochastic Simulation–Optimization Modeling Framework

Figure 4 provides an overview of the methodology. First, data is prepared and entered into QUAL2Kw. Calibration and verification of the model are then carried out. Stochastic parameters are generated using the GLUE technique, with a normal distribution function applied for the stochastic approach. The two-objective optimization model minimizes both "total treatment cost" and "BOD violation of the standard level at the checkpoint." Once a calibrated model is reached, QUAL2Kw is linked to the optimization algorithm MOICA. In this proposed structure, decision variables are generated by MOICA in each iteration, and these variables are used to determine pollution loads in QUAL2Kw. After running the model based on these variables, the results are evaluated, and objective functions (Eqs. 5 and 6) are calculated. If the objective functions are not met, new variables are introduced into the simulation model by applying new management conditions, and then the objective functions are retested. This cycle is repeated until optimal values are reached. Each optimization cycle is executed for a series of random data generated by the GLUE method, and an uncertainty band is obtained from the number of runs taken.

3 Results

3.1 Model Calibration and Validation (QUAL2Kw)

The model was calibrated using monitoring data from three stations: Dezful, Harmaleh, and Bamdezh (Fig. 1). Field data from the dry and wet seasons of 2020 and the wet season of 2021 were used for model calibration, while data from the dry season of 2021 was used for model validation. The RMS value (calculated as the sum of RMSE, MAE, and SE) was used to evaluate the simulation results, as shown in Fig. 5. A lower RMS value indicates better performance for QUAL2Kw. The simulation showed very good R values for all parameters. Overall, the DO parameter had the highest RMS value in the wet season of 2021 for calibration (RMSE = 0.8137, MAE = 0.7835, SE = 0.134, and RMS = 1.9112). The range of SE (15.3–31.4%) calculated from the present simulation was an indicator of how well the validated model performed. For BOD calibration, the highest RMS value was 1.724 in the wet season of 2020, while for validation, the RMS value was 1.488.

Figure 6 shows the changes in DO and BOD levels along the Dez river for the years 2020 and 2021 during both wet and dry seasons under existing conditions. The figure shows that the BOD level during dry seasons increased from 5.68 to 23.5 km. Subsequently, the BOD concentration decreased from 23.5 to 39.68 km with a slight change due to the river's self-purification, resulting in a decrease of 2.98 mg/l within this range. However, from 39.68 to

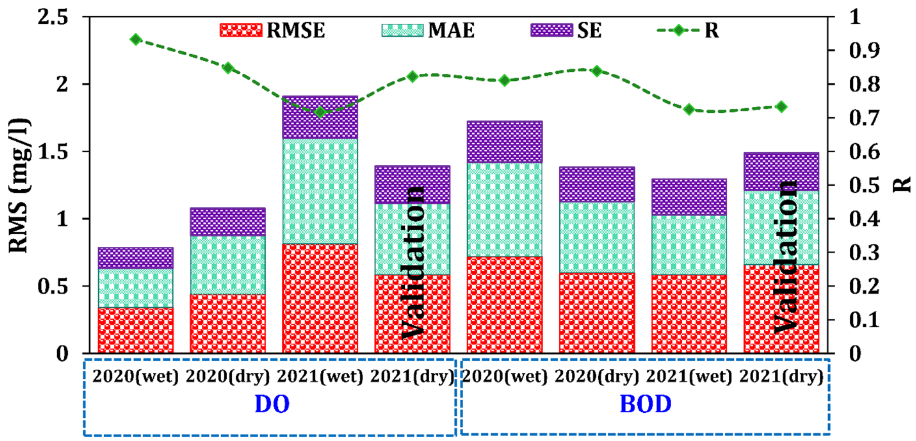

Fig. 5 Statistical indices for calibration and validation of QUAL2Kw model

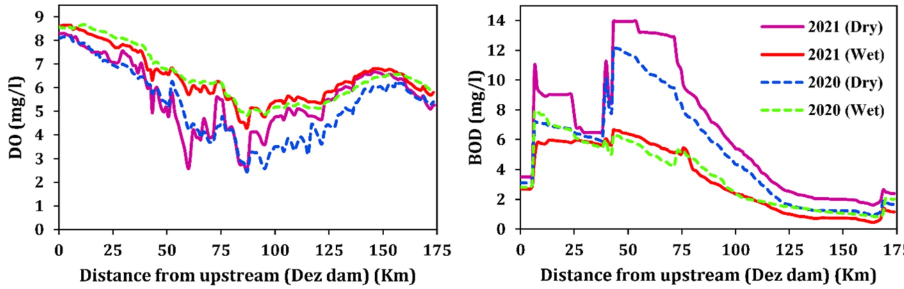

Fig. 6 BOD and DO diagrams for existing condition along the Dez River in wet and dry seasons (2020 and 2021)

71.49 km, the BOD level increased significantly due to the substantial discharge of urban and industrial sewage and agricultural effluents, along with a decrease in river flow in the headwater and an increase in harvesting from the river for agricultural purposes during dry seasons. From 71.49 km to the end of the river, the concentration of BOD reduced strikingly due to the self-purification of the river. For example, this amount of concentration decreased by 10.87 mg/l in the dry season of 2021. Along the Dez River and the discussed intervals, as the BOD increases, the DO value decreases. In other words, DO changes along the river are similar to BOD but vice versa. In the wet season along the river, the BOD concentration value is not as high as in the dry season. A slight increase can be seen in the range of 4.52 43.30 km due to the entry of pollution. From 43.30 km to the end of the river, as in the dry season, there is a significant decrease owing to the self-purification of the river (for example, in 2021, the BOD concentration reduced by 5.09 mg/l). In the wet season, the BOD concentration is reduced due to the increase in the flow of the headwaters and the decrease in the harvest of the river for agricultural purposes. As can be seen from the figure, the concentration of DO in the whole length of the river has increased compared to the dry season in the same proportion.

3.2 The Results of the Implementation of the Linked Stochastic Simulation-Optimization Model

3.2.1 Uncertainty Interval of Pareto Fronts Based on MOICA

As mentioned, the MOICA was utilized for the optimization procedure. In this process, a multi-objective function was used to optimize three decision variables, which were the discharge amounts of each of the three pollutants into the river. It was determined that the initial population should be at least triple the number of decision variables, resulting in an initial population of 9. The results showed that in lower repetitions, both objective functions experienced significant changes, while in higher iterations, the coverage function's variation amplitude was fixed, and the model focused on reducing violations from the permissible values of qualitative parameters. It was estimated that approximately 400 algorithm repetitions were required to achieve convergence, and the simulation–optimization linked model was implemented 3600 times. In the MOICA algorithm, the best solutions in each repetition were selected based on the assessment of the objective functions and stored as an optimal repository to move to the next step. Finally, the optimal Pareto-optimal front curve was attained in the last iteration between the optimization objectives. The optimization procedure mentioned above was implemented for a series of random data points (headwater flow, oxidation rate, point source inflow, abstraction, and point source concentration), generated by the GLUE method. To reach the optimization uncertainty band, the optimization method should be implemented for 1000 random data series that have been generated. Figure 7 shows the graph of the Pareto front interval, where the points offer the optimal solutions of the model for years from 2022 to 2025 in dry and wet seasons, and the axes represent the number of objective functions. The best solutions (the interval marked) with the lowest cost of treatment and the lowest violation from the permitted values of the qualitative parameter (BOD) were selected according to the evaluation of the objective functions, and the results of its implementation (the 1000 best optimal solutions) were evaluated in the qualitative model (QUAL2Kw).

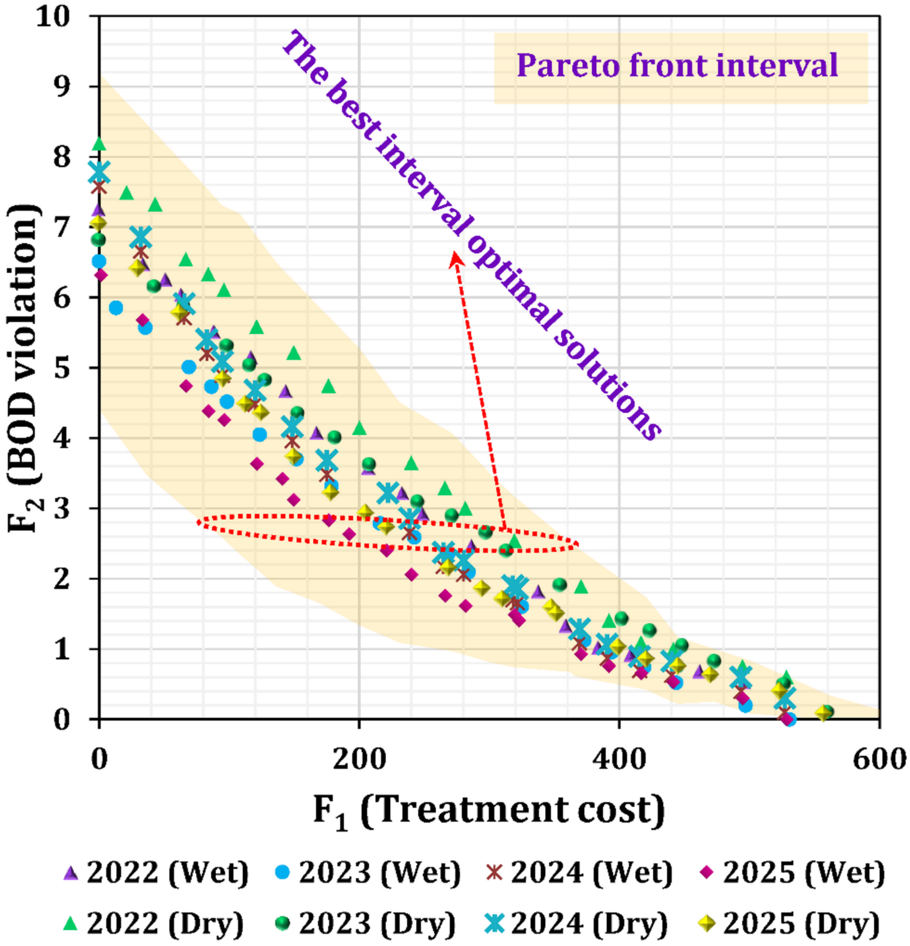

Fig. 7 The interval of Pareto optimal front based on objective functions (in thee 400 iteration)

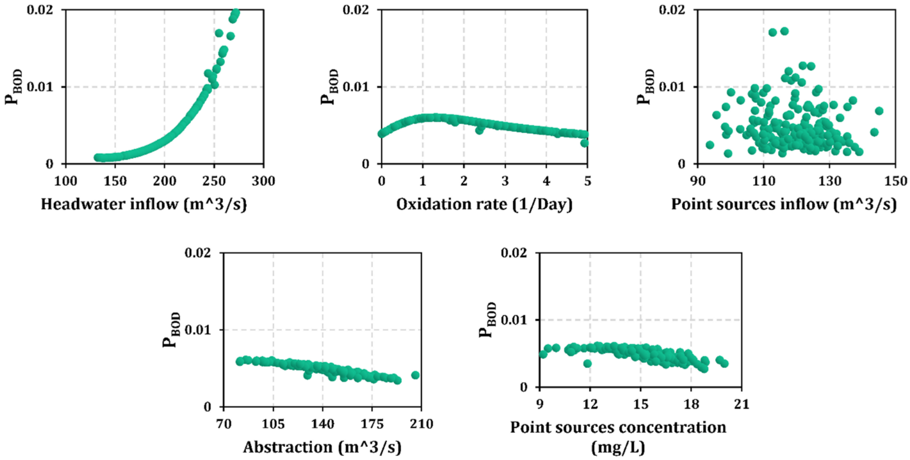

Fig. 8 Scatter plots of BOD probability (P_i) and stochastic parameters

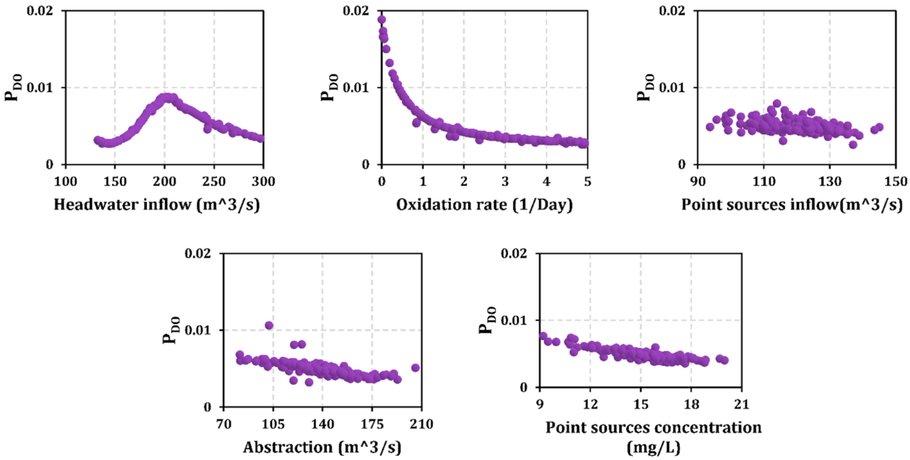

Fig. 9 Scatter plots of DO probability (P_i) and stochastic parameters

3.2.2 Uncertainty and Sensitivity Analysis of Linked Model

As discussed in the study's methodology, the GLUE method was employed, and the Monte Carlo procedure was used to generate large input stochastic parameter values for the linked simulation–optimization model. The parameters for the model were drawn from the ranges shown in Table 3. The linked model's performance was evaluated for each parameter set by comparing it with the measured data. Figures 8 and 9 show the scatter plots for the probability or weight of the likelihood (P_i) of BOD and DO, respectively, based on each of the parameter values sampled in the model. A dot in these figures represents one run of the model with the randomly selected monthly value within the selected boundaries. The shape of the distribution indicates the degree of uncertainty of the estimates, which sharp and peaked distributions associated with well-defined parameters, while flat distributions indicate more parameter uncertainty. The scatter plots enable one to pin down a model state variable, the most sensitive parameters, and the associated release. As can be seen in Figs. 8 and 9, for BOD and DO, the uncertainty of point sources's inflow is higher than for other parameters. Analysis of the sensitivity of BOD and DO to the parameters shows that BOD is more influenced by headwater's inflow than other parameters, while DO is more sensitive to the oxidation rate than other parameters.

3.2.3 Uncertainty Bounds of Pollutant Prediction Based on Optimization

Figures 10 and 11 show the pollutant-discharge prediction bounds for the BOD and DO parameters along the Dez River, based on optimal conditions from 2022 to 2025. As shown in Fig. 10, the maximum BOD concentration in the reach between 39 and 94 km along the river is slightly higher than the level of the class 1B standard for all years. In 2022, during the dry season along the river from 25.87 km to 110.38 km, the BOD concentration exceeds the level of the class 1B standard (5 mg/l), but for other years in both wet and dry seasons, the BOD concentration lies within the range of the class 1B limit. As seen in Fig. 11, the DO concentration value in the reach between 77 and 126 km along the river is lower than the permitted value of class 1B for all years. The amount of pollution in the river is much lower than the current conditions (without optimizing the discharge of pollution into the river), and the quality of the river water has improved to an acceptable level. Simultaneously, the amount of DO in the river has increased.

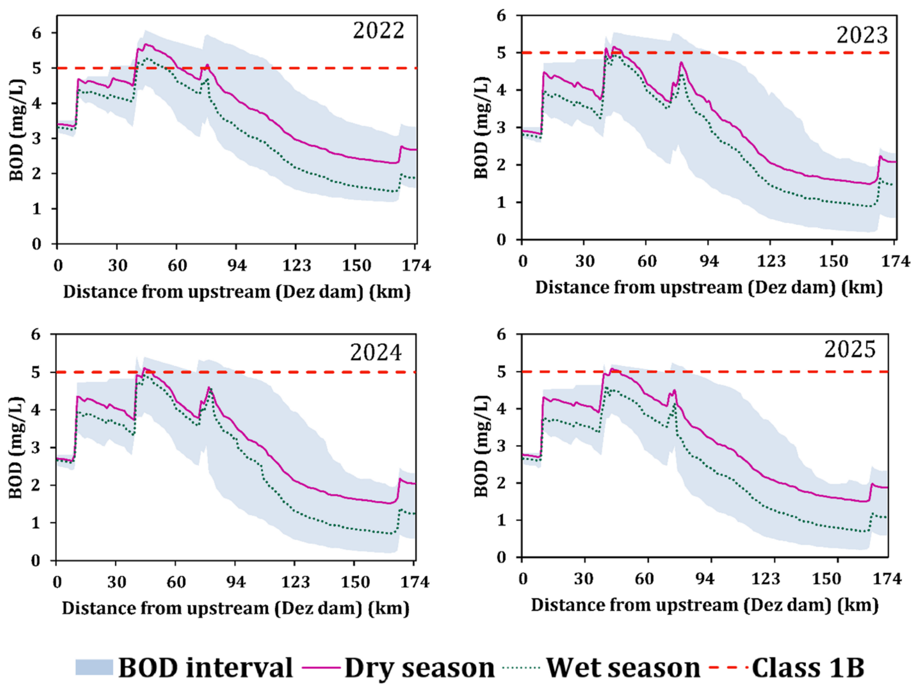

Fig. 10 Uncertainty bounds of BOD along the Dez River from 2022 to 2025

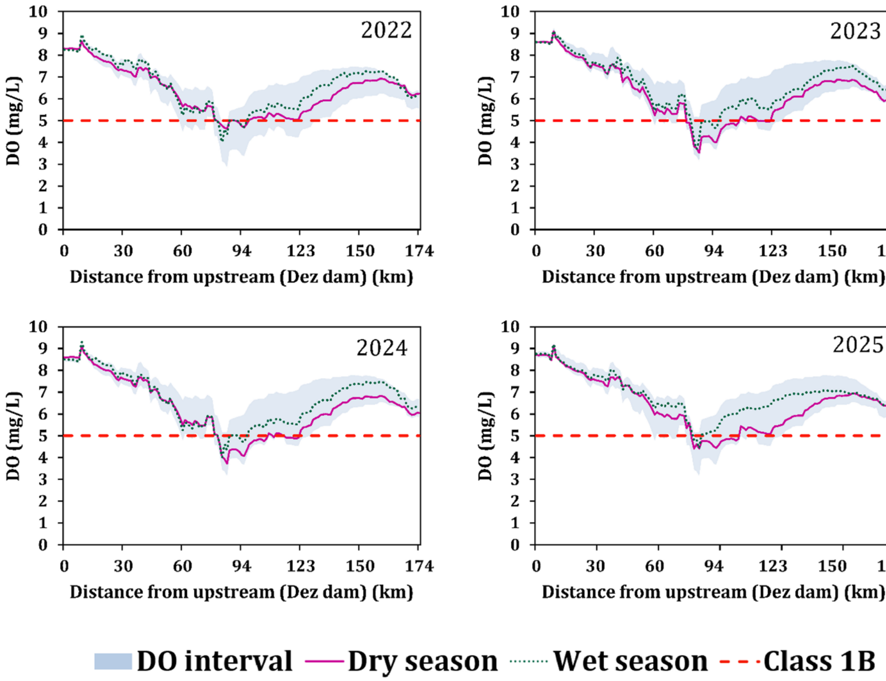

Fig. 11 Uncertainty bounds of DO along the Dez River from 2022 to 2025

The maximum values of BOD concentration at seven outflow points or canals of water harvesting along the Dez River are shown in Table 5. According to Table 5, the maximum value of BOD concentration will be higher than the limit of class 1B in all years (2022 to 2025) at outfall points 3 and 4. The highest value will be in 2022 at the outfall 4 (5.81 mg/l). In other canals, the maximum BOD concentration does not exceed the class 1B limit in all years. Also, the lowest maximum BOD concentration will be in 2025 at the outflow point of 7.

Table 5 Maximum BOD (mg/l) in water outflow points from 2022 to 2025

Demand site	Outflow	Distance from upstream (km)	2022	2023	2024	2025
Sabili	Outflow 1	4.4	3.52	3.01	2.81	2.74
Dez Sharghi	Outflow 2	10.8	4.67	4.72	4.55	4.52
Dez Gharbi						
Dimcheh	Outflow 3	39.2	5.56	5.41	5.21	5.03
Haftapeh						
Mianab	Outflow 4	73.5	5.81	5.51	5.28	5.11
Emamkhomeini	Outflow 5	96.4	5.52	4.96	4.93	4.76
Shoaybiyeh	Outflow 6	140.7	3.61	2.61	2.59	2.43
Dehkhoda	Outflow 7	165.7	3.06	1.94	1.94	1.91

The minimum values of DO concentration at water outflow points along the Dez River are given in Table 6. The results show that only in canal 5, the concentration of DO will be lower than the limit of class 1B in all years. For other water harvesting canals, the DO concentration value will be good, in other words, the minimum concentration of DO will be more than 5 mg/l.

Table 7 presents the percentage of pollution reduction and treatment costs in wet and dry seasons for the years 2022–2025 along the river. The percentage of treatment in dry seasons is in the range of 26.4% to 29.4%, while in wet seasons is in the range of 13.24% to 15.53%. The highest treatment cost for the dry season of 2022 is 320.19 (1000$). In general, the treatment cost in the wet season is about equal to one third of the treatment cost in the dry season.

4 Discussion

In the studies related to river water quality simulation, it is shown that the QUAL2Kw model provides reasonable results for simulation (Babamiri et al. 2021; Zare Farjoudi et al. 2021; Dasilva and Albuquerque Alves 2016). In this study, the QUAL2Kw model was also used to simulate the water quality of the Dez River. The results of calibration and verification of the model indicated that the model had high accuracy. To optimize water management projects, the use of meta-heuristic algorithms has been proposed by many researchers (Babamiri and Marofi 2021; Zeinali et al. 2020; Muronda et al. 2021). The MOICA algorithm was used to optimize the waste load allocation to the river, which has shown the higher accuracy of the algorithm compared to NSGAII and MOPSO (Enayatifar et al. 2013); Nazari and Deihimi 2017). The results of the linked QUAL2Kw model and the MOICA algorithm for waste load allocation in the study indicated that the developed model was satisfactory. The uncertainty band of water quality along the Dez River, calculated using the GLUE method, indicates whether water pollution will exceed the standard level in the future. Understanding this uncertainty regarding pollution along the river under optimal conditions allows for the maintenance of river water quality at the standard level. It also shows how the uncertainty in the waste load allocation to the river affects the performance of the optimization model. Crucially, it shows how different sources of uncertainty influence the changes in pollution along the river. In addition, studies investigating

Table 6 Minimum DO (mg/l) concentration in water outflow points from 2022 to 2025

Demand site	Outflow	Distance from upstream (km)	2022	2023	2024	2025
Sabili	Outflow 1	4.4	8.21	8.51	8.31	8.52
Dez Sharghi	Outflow 2	10.8	7.99	8.32	8.31	8.33
Dez Gharbi						
Dimcheh	Outflow 3	39.2	6.91	7.22	7.21	7.25
Haftapeh						
Mianab	Outflow 4	73.5	5.17	5.47	5.48	5.49
Emamkhomeini	Outflow 5	96.4	3.68	3.88	3.98	3.88
Shoaybiyeh	Outflow 6	140.7	5.68	5.95	5.94	5.91
Dehkhoda	Outflow 7	165.7	5.99	6.31	6.31	6.38

Table 7 The total waste load allocation (WLA) and purification costs along the Dez River

Year	Dry Season				Wet Season			
	Initial Load (Ton/Day)	**Allocated Load (Ton/Day)**	**Reducd Load %**	**Cost (1000$)**	**Initial Load (Ton/Day)**	**Allocated Load (Ton/Day)**	**Reduced Load %**	**Cost (1000$)**
2022	103354.82	72968.51	29.40	320.19	57183.61	49608.13	13.24	79.82
2023	81958.53	58994.69	26.41	299.35	55467.59	47640.56	14.11	102.03
2024	88746.32	63503.32	28.44	305.07	52714.12	44653.77	15.29	97.41
2025	83245.75	61242.23	26.43	301.35	56452.95	47685.81	15.53	120.07

uncertainty using the GLUE method have demonstrated its ability to accurately generate the uncertainty band, as shown by Mannina (2011), Muronda et al. (2021), and Gerkani Nezhad Moshizi et al. (2023).

5 Conclusions

The data collected from the quality monitoring stations along the Dez River indicated that the river is in a critical state of pollution, particularly in terms of BOD levels, which are primarily caused by the release of urban and industrial wastewater. This study also showed that there is no clear plan for controlling the concentration of this parameter. Therefore, it is necessary to use an optimal model that maintains the water quality at the standard level along the river. The two objectives of controlling the river water quality within the standard level and the treatment costs of pollutants were considered. The proposed method also investigated optimization while considering the uncertainty of stochastic parameters. The results showed that: 1) the GLUE method obtains uncertainty bands with high accuracy; 2) the sensitivity of BOD to headwater is greater than other stochastic parameters; and 3) the average cost of treatment in the wet season is about one-third of the cost in the dry season. Overall, this work offers a successful approach to demonstrate that the water quality along the river has improved with low treatment costs, and only minor violations of water quality standards for the river have occurred, especially in agricultural water withdrawing sites.

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Availability of Data, Material, and Code Data and codes will be available upon request of the journal to them.

Declarations

The authors have agreed on submitting this article, and it is not currently under any consideration for reviewing in other journals simultaneously.

Consent to Participate The authors voluntarily agreed to participate in this research study.

Consent for Publication The authors approved the publication of this study.

Conflicts of Interest The authors declare no conflict of interest.

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