

A Novel Wastewater Load Allocation Approach for River Basins Using Simulation-Optimization Models

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Abstract

In this study, a new wastewater load allocation approach using a linked simulation-optimization model is proposed to determine the receiving body-based discharge limits by considering the discharge standards used by the European Union Water Framework Directive. By using the proposed approach, wastewater loads of point sources can be determined in such a way that the parameters exceeding the water quality targets (WQT) in receiving water bodies meet the relevant WQT. The simulation part is used to determine pollutant concentrations throughout the river system using the AQUATOX water quality simulation model. However, since AQUATOX is an independent simulation model and its source code is not publicly available, it is not possible to execute it with the optimization model for the generated load combinations. Therefore, a concentration-response matrix (CRM) is developed as a surrogate water simulation model by using the outputs of the AQUATOX model. After this process, the developed CRM is integrated into an optimization model where the heuristic differential evolution (DE) optimization approach is used. The performance of the proposed simulation-optimization approach is evaluated on a sub-watershed of the Kucuk Menderes River Basin by considering different waste load allocation scenarios for the CBOD₅ water quality parameter. The results showed that the proposed simulation-optimization approach can effectively allocate the wastewater loads among different point sources by considering the WQT values of the CBOD₅ parameter.

Keywords: Wastewater; load allocation; simulation-optimization

1. Introduction

Wastewater load allocation (WLA) is an important component of water quality management and plays a key role to obtain satisfactory water quality in river basins. Treated and untreated wastewater discharges contribute to the deterioration of river water quality, which can cause lethal effects on aquatic life. Therefore, a considerable number of published studies exist on solutions to control wastewater discharge loads and increase water quality through water

resources planning and management (Boose, 2002; Jia and Culver, 2006; Deng et al., 2010; Su et al., 2018; Afshar et al., 2018). These studies generally use trial-and-error based approaches to meet the relevant water quality standards; however, it is not practical to obtain solutions for multiple pollutant sources (Boose, 2002). Recently, most WLA studies have only been carried out to determine the quantity of reducing pollution levels at the sources by simulation-optimization model until obtaining satisfactory water quality and maximum discharge load considering the economic efficiency of production facilities (Burn and Yulianti, 2001; Cho et al., 2004; Jia and Culver, 2006; Deng et al., 2010; Zou et al., 2010, Han et al., 2011; Afshar and Masaumi, 2016; Afshar et al., 2018; Saadatpour et al., 2019; Su et al., 2019). Thus, many studies involving simulation-optimization models can be found in the scientific literature. Among them, Deininger (1965) first employed simulation-optimization models where linear programming based deterministic optimization approach was used to improve the water quality by considering the dissolved oxygen concentration in the river system. Similarly, Reville et al. (1968) used linear programming to obtain pollutant loads that result in satisfactory water quality in river system. On the other hand, Liebman and Lynn (1966) and Klemetson and Grenny (1985) used dynamic programming to minimize wastewater management costs.

Note that in the conducted studies, the water quality processes in river systems were simulated with different simulation models such as QUAL2E (Burn and Yulianti, 2001; Parmar and Keshari, 2014; Saadatpour and Afshar, 2007), QUAL2K (Saadatpour et al., 2019), CE-QUAL (Afshar et al., 2018), WASP4 (Cardwell and Ellis, 1993), etc. These water quality simulation models have been combined with both heuristic and deterministic optimization approaches. In those approaches, pollutant loads were equally allocated (equality approach) among the point sources, no matter which simulation and optimization models are used (Burn and Yulianti, 2001; Cho et al., 2004; Afshar and Masaumi, 2016; Afshar et al., 2018; Saadatpour et al., 2019). Although this equity approach seems quite reasonable for points sources with similar characteristics, it may not be reasonable to allocate the same pollutant loads to sources that have different characteristics and capacities. In 2020, an unequally load allocation approach have been suggested to overcome with this problem in the literature and this approach have been used with deterministic GRG optimization technique (Sadak et al., 2020).

In this study, a novel simulation-optimization approach is proposed for allocating the wastewater discharge loads considering water quality targets (WQTs). In contrast to most previous studies, waste loads are allocated among point sources by assigning different allocation weights for each source. In the simulation part of the proposed approach, carbonaceous biochemical oxygen demand (CBOD₅) is considered the main water quality parameter, and the AQUATOX (Park et al., 2008) model is used to simulate the fate and transport of this parameter in the river system. It should be noted that the water quality model should be executed separately in an iterative fashion for each scenario that was generated by the optimization model. However, AQUATOX is an independent simulation model, and it cannot be executed directly from the optimization model for the generated load allocation scenarios. Therefore, a concentration-response-matrix approach (CRM) is developed that is based on the resulting concentration of the discharged pollutant in the river. CRM is basically a surrogate water quality model that provides the change in pollutant concentration in the river for unit load discharges. The surrogate water quality model approach based on CRM was originally developed to solve groundwater problems by Gorelick (1982a, 1982b), but Su et al. (2019) and Sadak et al. (2020, 2022) have used it to solve surface water quality problems. This developed CRM-based surrogate model is then combined with a heuristic optimization model where the DE optimization approach is used. The performance of the proposed simulation-optimization approach is evaluated on a sub-watershed of the Kucuk Menderes River Basin

by considering different waste load allocation scenarios. The identified results indicated that the proposed simulation-optimization model can successfully allocate the pollutant loads by considering different load allocation weights.

2. Problem Definition

The problem of waste load allocation by means of the proposed simulation-optimization approach can be defined by the conceptual example given in Figure 1, where concentration curves are intended to show just increases in concentrations, and do not reflect the real outcome of an advection-dispersion process.

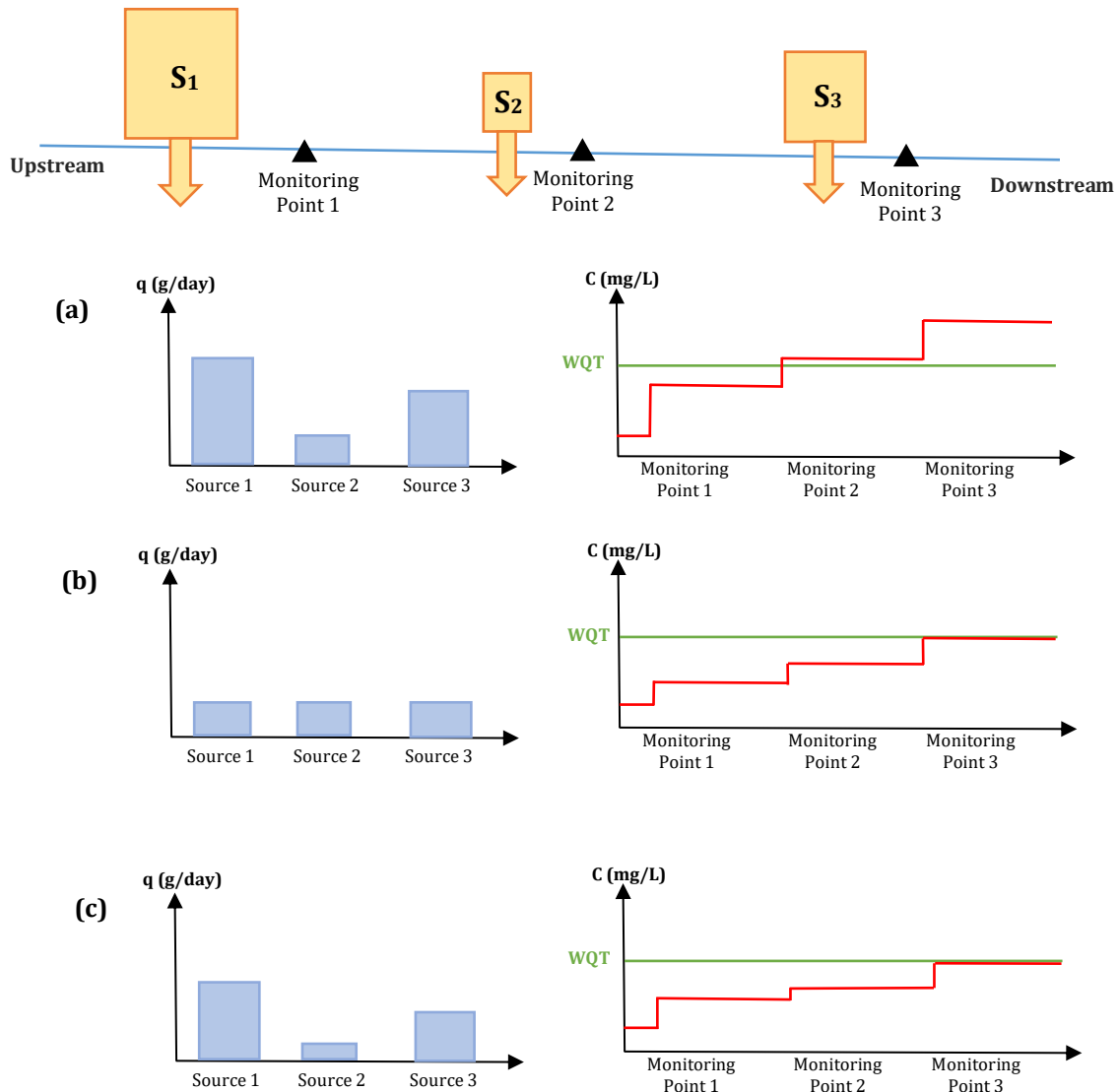


Figure 1. A conceptual model of wastewater load allocation (a) before allocation, b) equal allocation approach, c) proposed allocation approach

As can be seen from the conceptual example, there are three pollutant point sources in the river system. The influence of these source locations on the receiving water body can be measured by concentrations at three monitoring points, each located downstream of a source. Figure 1(a) represents a case where no allocation plan is followed by the decision-makers. In this case, each source discharges the pollutant without considering the WQT in the receiving water body, therefore WQTs are not satisfied at the second and third monitoring points. In Figure 1(b), the optimization approach has been applied by considering the equality approach

such that all the sources have the same pollutant loads. As shown, WQT limits are satisfied for all the monitoring points. On the other hand, in Figure 1(c), the pollutant loads are allocated using weights that are proportional to initial load allocations. As can be seen, the final loads are allocated proportionally to the initial condition while satisfying the WQT at all monitoring locations. Similarly, it is possible to assign different load allocation weights to different locations depending on their relative load allocation importance to each other. The following section explains how this proposed load allocation procedure is mathematically applied to the solution of the problem.

2.1. Proposed Simulation-Optimization Approach

The objective of the optimization model is to maximize the total pollutant loads at the source locations subject to WQTs at the monitoring points. Mathematically, this optimization objective can be formulated as in Eq (1): ($i = 1, 2, 3, \dots, n_d$; $j = 1, 2, 3, \dots, n_m$; $t = 1, 2, 3, \dots, n_t$):

$$Z = \max \left\{ \sum_{i=1}^{n_d} (q_i - \lambda_1 \times (q_i - \omega_i \times q^*)^2) - \lambda_2 \times \sum_{j=1}^{n_m} \sum_{t=1}^{n_t} (C_j(t) - \tilde{C})^2 \right\} \quad (1)$$

subject to Eq (2), Eq (3), Eq (4), Eq (5) and Eq (6):

$$q_i = C_i \times Q_i \quad (2)$$

$$q^* = \frac{\sum_{i=1}^{n_d} q_i}{\sum_{i=1}^{n_d} \omega_i} \quad (3)$$

$$C_j(t) = \sum_{i=1}^{n_d} \alpha_{i,j}(t) \times q_i + C_j^0(t) \quad (4)$$

$$C_{\min} \leq C_i \leq C_{\max} \quad (5)$$

$$\alpha_{i,j}(t) = \frac{\partial (\hat{c}_j(t) - c_j^0(t))}{\partial q_i} \quad (6)$$

where, n_d is the number of point sources, n_m is the number of monitoring points, n_t is the time step and q_i is the load of the i^{th} point sources, Z is the objective function value to be maximized, λ_1 is the first penalty coefficient, which maintains the weighted load allocation among pollution sources, λ_2 is the second penalty coefficient that ensures highest possible load discharges from the point sources, ω_i is the load allocation weight of point sources, q^* is the allocated load, which ensures that the load of the pollutant is allocated among the source locations at desired levels (q^* equals to the mean of q_i , if ω_i values are all equal to 1), $C_j(t)$ is the concentration of the j^{th} pollutant calculated by the response-matrix and \tilde{C} is the WQT for the CBOD₅ parameter, C_{\min} and C_{\max} are the minimum and maximum CBOD₅ concentrations.

As can be seen from Equation 1, the objective function of the optimization model includes two penalty functions. The first penalty function is used to allocate the pollutant loads among the source locations proportionally with the given load allocation weights (ω_i). The second penalty function is used to ensure that the differences between the simulated pollutant concentration and WQT value are minimized. Note that the optimization formulation given above also includes the components of the CRM-based surrogate model. The proposed CRM based surrogate model is based on the principle of linear superposition which requires of linear relationship between the input and output data. It can also be used to simulate the fate and transport of the multiple water quality parameters. The elements of CRM are calculated by executing the AQUATOX water quality simulation model for unit load discharges from the source locations. After each model execution, the resulting pollutant concentrations at the monitoring points are saved. The background concentrations are then subtracted from the simulated concentrations to obtain an independent response of the system for the given unit loadings. The calculated CRM can then be used as a surrogate water quality simulation model and integrated into the optimization model for solving the WLA problem. Detailed information regarding the proposed CRM-based water quality simulation model can be found in Sadak (2019). Note that all solutions are conducted using the differential evolution (DE) approach in the optimization model. DE is an evolutionary-based heuristic optimization approach and has similar computational steps with the genetic algorithm (GA) where the natural evolution process is simulated through mutation, selection, and crossover operations. Despite their similarities, there are some differences such as most GA applications consider the binary coding system whereas DE considers real number coding systems. Furthermore, each candidate solution in GA is subjected to the genetic evolution process if the associated probability of that process is satisfied whereas each candidate solution in DE is subjected to those processes without considering any probability. Compared to other heuristic optimization algorithms, DE is relatively easy to employ and is less prone to get stuck in local optimums which is one of the reasons it is used to solve the WLA problems in this study.

3. Study Area

The applicability of the proposed simulation-optimization approach is evaluated by considering hypothetical but realistic water quality parameters on a tributary of a sub-watershed of the Kucuk Menderes River Basin (KMRB). The KMRB is located in the western part of Turkiye (Figure 2) and lies between $38^{\circ} 41' 05''$ and $37^{\circ} 24' 08''$ N latitudes and $28^{\circ} 24' 36''$ and $26^{\circ} 11' 48''$ E longitudes. The main river reach of the basin has a mean discharge of $11.45 \text{ m}^3/\text{s}$ and nearly 130 km length that originates from the Kiraz region and together with other tributaries, it discharges all the carrying water to the Aegean Sea. In particular, the city of Izmir, which is the third largest city in Turkiye, is located in the lower basin. Therefore, the water quality of the Kucuk Menderes River is prone to serious environmental stresses since industrial and agricultural activities are very dominant around Izmir.

Figure 2 also includes the location of this tributary which is called the Ilica Stream. Note that this hypothetical example includes 5 point sources, and the impact of these sources is recorded at three monitoring points. Locations of the point sources and monitoring points are given in Figure 3. Among the point sources shown in Figure 3, S_1 represents a domestic wastewater treatment plant, S_2 is considered as a point source representing the mass influx from the tributary, Uladi Stream. The remaining three sources (S_{3-5}) represent the discharge locations of the industrial facilities in the region. After defining the point sources and monitoring locations, the fate and transport of the CBOD_5 water quality parameter is simulated by using the AQUATOX simulation model. This study is one of the outputs of the TUBITAK research project, and data related to the study area were obtained due to detailed field studies. As

mentioned earlier, a hypothetical water quality model has been created using real field measurement and pollutant point sources.

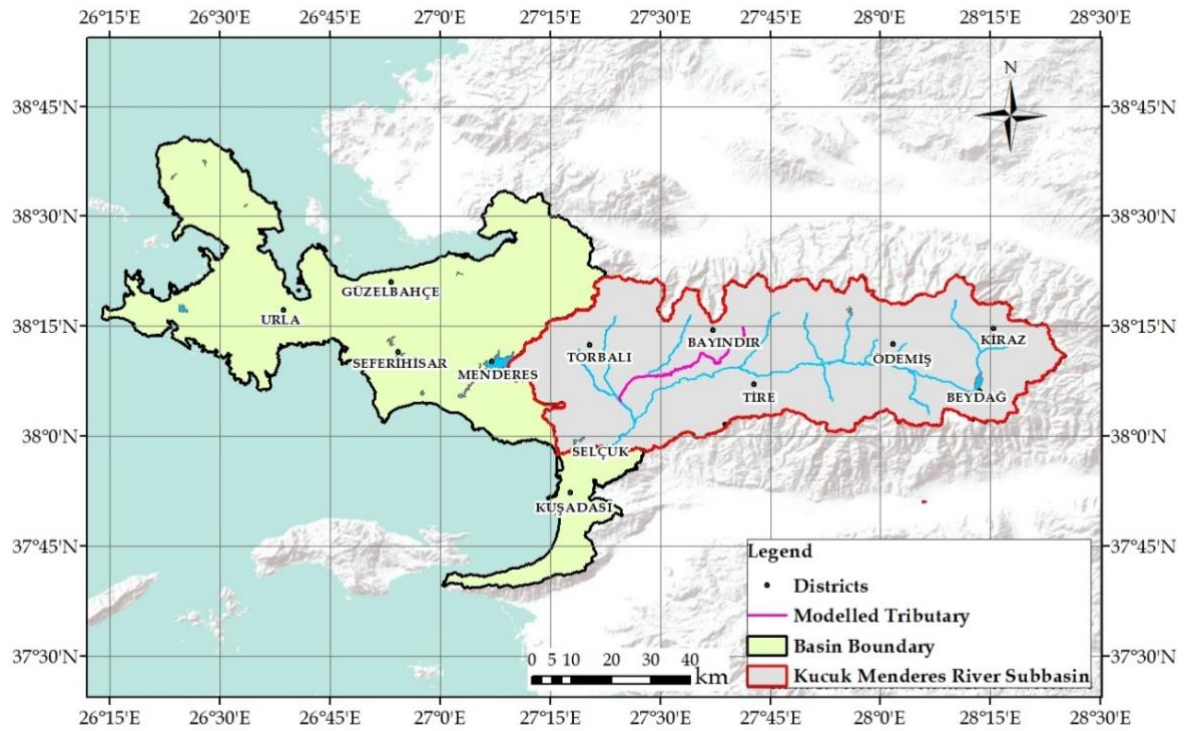


Figure 1. The Kucuk Menderes River and its basin boundary

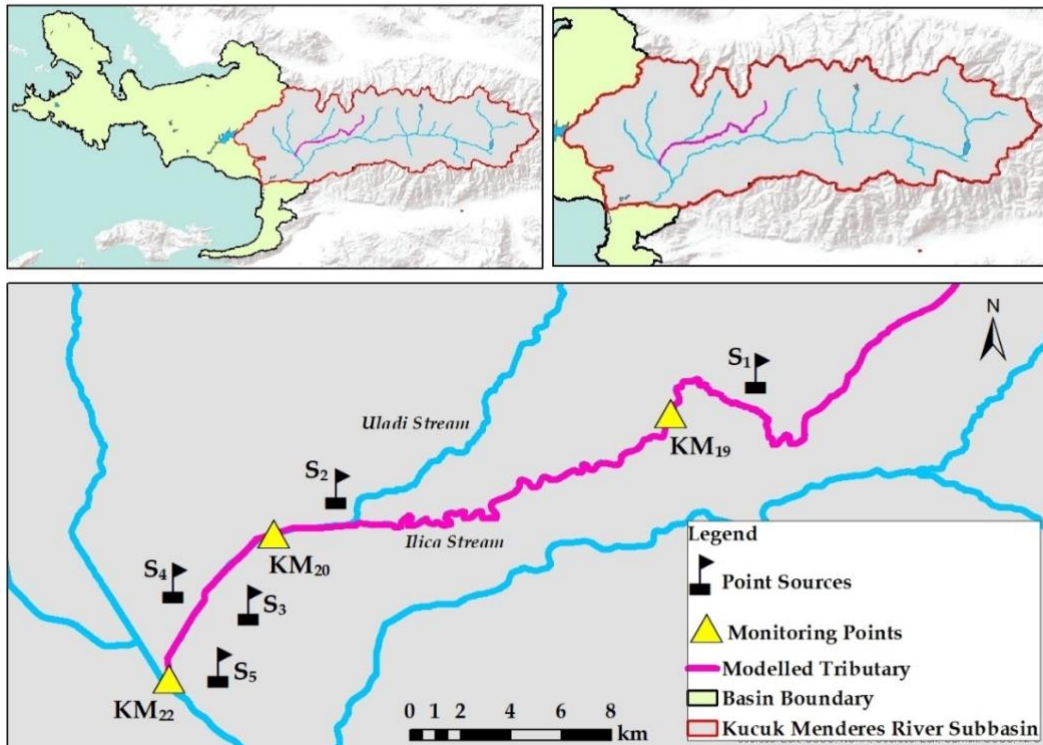


Figure 2. Application study area on the Kucuk Menderes river sub-basin

4. Model Application

As explained previously, the proposed simulation-optimization approach aims to allocate the pollutant loads among the source locations based on the given load allocation weights. To this aim, four different hypothetical load allocation scenarios have been considered to evaluate the applicability of the proposed load allocation scheme (Table 1). In the first scenario, the load allocation weights are taken as 1 for all the sources. In the other scenarios, different load allocation weights are considered for the point sources to evaluate if the pollutant loads are proportionally allocated among the source locations or not. For all the scenarios, the following site characteristics were used: Number of sources: $n_d = 5$ (S_1, S_2, S_3, S_4, S_5); Number of pollutants: $n_c = 1$ (organic matter in the form of suspended and dissolved detritus); Number of monitoring points: $n_m = 3$ (KM-19, KM-20, KM-22); Number of time steps: $n_t = 30$ days. Note that the penalty coefficients of λ_1 and λ_2 have been selected as 1 and 10^9 , respectively according to previous trials. Furthermore, the WQT for the model output CBOD_5 was selected as $\tilde{C} = 8$ mg/L considering environmental quality standards for the optimization process.

Table 1. The load allocation coefficients (ω_i) for each scenario

Sources	Scenario 1	Scenario 2	Scenario 3	Scenario 4
S_1	1	2	1	2
S_2 (Tributary)	1	1	1	1
S_3	1	1	1.5	1
S_4	1	1	1	2
S_5	1	1	2.5	3

5. Results

Application results of the simulation-optimization approach for Scenario 1 - 4 are summarized in Figure 4. It is evident that the proposed approach allocates the total pollutant loads among point sources proportionally with the given load allocation weights. For example, since the load allocation weights in Scenario 1 are the same, all the sources get the same pollutant loads as expected by the optimization model. For Scenario 2, since only the first source has a weight of 2 whereas the others have 1, the first source location gets two times greater pollutant loads than the others in the basin. Note that all of these load allocation weights are hypothetically generated for evaluating the applicability of the proposed simulation-optimization approach.

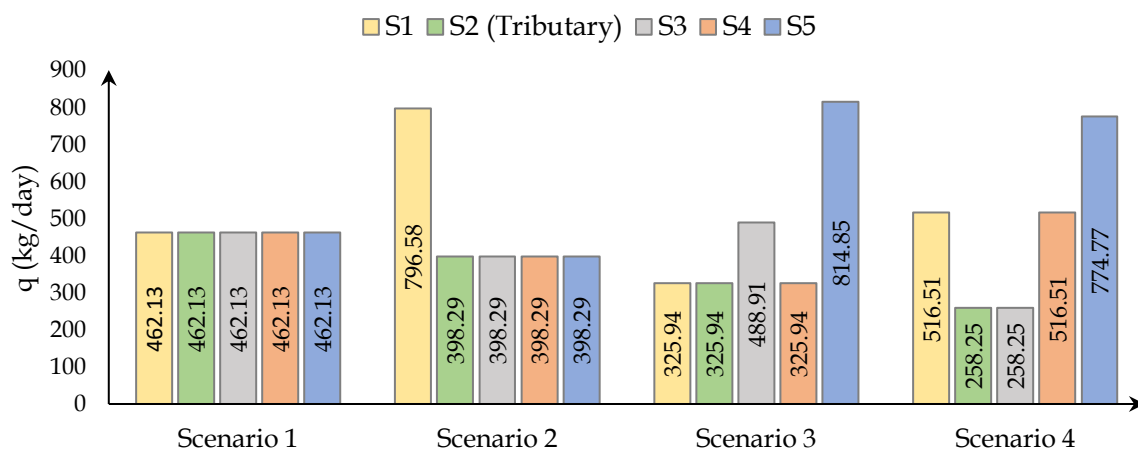


Figure 4. Simulation-optimization model results for each scenario

Another important result of the simulation-optimization model is the CBOD_5 concentrations which, it should be lower than 8 mg/L throughout the river system for the satisfactory water

quality. For the output CBOD₅ concentrations, comparison of the post allocation final calculated values at the monitoring points with the corresponding WQT is given in Table 2. As can be seen for all the scenarios, the calculated CBOD₅ concentrations are lower than the WQT at KM-19 and 20. On the other hand, the CBOD₅ concentration is equal to the WQT at monitoring point KM-20, which is an expected result since KM-20 is located in the downstream reach of the tributary. This also means that the simulation-optimization approach allocates the maximum amount reasonable load among the sources.

Table 2. Resulting CBOD₅ concentrations for the obtained load allocations of each scenario

\tilde{C} (mg/L)	CBOD ₅ concentrations in the stream after load allocation			
	$C_j(30)$ (mg/L)			
	Scenario 1	Scenario 2	Scenario 3	Scenario 4
KM-19	2.33	4.01	1.64	2.60
KM-20	5.82	6.51	4.80	5.40
KM-22	8.00	8.00	8.00	8.00

6. Conclusions

In this study, a simulation-optimization approach is proposed for solving the WLA problems in river basins. The proposed approach aims to allocate the pollutants loads among the sources by considering environmental WQT values in the receiving water body. Furthermore, this proposed approach considers the load allocation weights for all the point sources to allocate the total loads as to be proportional to the provided weights. This is one of the most important contributions of this study since the proposed approach suggests controlling the load allocations at certain levels for all the source locations. To simulate the fate and transport of the pollutants in river systems, a new CRM-based surrogate water quality simulation approach is also developed which is the other important contribution in this study. This developed CRM-based surrogate model is integrated with a DE-based optimization model. The performance of the proposed simulation-optimization approach is evaluated on a sub-watershed of the Kucuk Menderes river basin in Turkiye by considering different waste load allocation scenarios. Identified results indicated that the proposed simulation-optimization approach can successfully allocate pollutant loads by considering the provided load allocation weights and by satisfying the WQT values for all the monitoring points.

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Author Statement

The authors have contributed to this paper in this manner:

Derya Sadak: Development of the simulation-optimization approaches, programming, manuscript preparation; M. Tamer Ayvaz: Development of the simulation-optimization approaches, programming, evaluation of the results, manuscript preparation; Alper Elçi: Building of the water quality simulation model, evaluation of the results, manuscript preparation; Mehmet Dilaver: Evaluation of the results, manuscript preparation; Selma Ayaz: Evaluation of the results, manuscript preparation.

Conflict of Interest

There is no conflict of interest for this study.

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