E-proceedings of the 38th IAHR World Congress
September 1-6, 2019, Panama City, Panama
doi:10.3850/38WC092019-1665

SIMULATION-OPTIMIZATION OF POLLUTANT SOURCE ALLOCATION IN THE KUCUK MENDERES RIVER BASIN

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ABSTRACT

Water quality models are important tools in supporting river basin scale decision-making and exploration of pollutant loading effects on the water quality of the receiving waterbody. Contemporary river basin management studies rely on the intensive use of modeling to evaluate pollutant source control strategies. To ensure that water quality standards are met in the receiving waterbody, a viable strategy is to appropriately allocate loadings to all point sources in the river basin such that good quality water status is achieved. The problem of source allocation can be effectively solved using a simulation-optimization approach. The objective of this study is to develop an approach to allocate pollutant point sources in a river basin. We present the interim results of a simulation-optimization approach to set effluent limits for the Küçük Menderes river basin which is located in Western Turkey. The approach is demonstrated on a sub-basin that receives discharges from three industrial sites, one domestic wastewater treatment plant and one tributary. The water quality model AQUATOX is used to determine time-variant concentrations in the main reach. The model is set up using arbitrary yet realistic values for hydraulic variables and point source loadings of one decaying pollutant. The optimum allocation of pollutant loadings to maintain a certain water quality standard is determined using the generalized-reduced-gradient method (GRG). We demonstrate that the simulation-optimization process simplifies when response coefficients and the principle of superposition are used to calculate the cumulative effect of pollutant loadings. We present also an example calculation of optimum source allocation.

Keywords: waste load allocation, modeling, water quality, AQUATOX, optimization, watershed management

1 INTRODUCTION

Water quality models are important tools in river basin management. They must reliably represent river basin and receiving water bodies to facilitate the exploration of cause and effect relationships between various pollutant sources and water quality. Contemporary river basin management studies rely on the intensive use of modeling to evaluate pollutant source control strategies. To ensure the protection of the aquatic environment and human health, pollutant concentrations in the receiving waterbody must meet certain water quality standards. For this purpose, one of the viable strategies is to appropriately allocate the total maximum daily load (TMDL) to all points sources in the river basin such that good quality water status can be maintained or is achieved in the future. The problem of load allocation, from here on referred to as source allocation, can be effectively solved using a simulation-optimization approach that is based on the use of a surface water quality model.

The objective of this study is to develop a water quality-based approach to allocate pollutant point sources in a watershed. The ultimate goal of the source allocation is to derive receiving water quality-based effluent limits for point sources in the Küçük Menderes River Basin (KMRB). This effort is a sub-task of an ongoing national-funded research project entitled "Identification of Receiving Waterbody Based Discharge Limits Küçük Menderes River Basin Case Study". Interim results of the continuing model development are presented in this conference paper.

2 DESCRIPTION OF STUDY BASIN

The KMRB is located in Western Turkey, between 37.94°- 38.37° N latitude and 27.15° – 28.42° longitude coordinates. The drainage area of the basin is 3377 km^2 and the length of the main reach of the river is 129 km with a mean discharge of 11.45 m^3/s (TUBITAK-MRC, 2010). River water quality in the basin is under significant environmental stress due to agriculture, husbandry and to a certain extent because of raw domestic and industrial wastewater discharges. According to the 2016 census data, the population is 480,000 which is estimated to generate 82,000 m^3 of domestic wastewater per day. The total wastewater discharge from industries is approximately 27,000 m^3/d. Consequently, the total wastewater discharge to surface water bodies in the basin is 109,000 m^3/d. A study reports that roughly 77% of the wastewater is discharged from treatment plants while the remainder is being released directly from the sewerage (MoEF, 2016).

3 METHODS

The approach is demonstrated on a sub-basin of the KMRB that receives discharges from three industrial sites, one domestic wastewater treatment plant and one tributary. The surface water quality model AQUATOX (Park et al., 2008) is used in this study to determine concentrations in the main reach. The AQUATOX model is a general ecological risk assessment tool that represents processes relevant to fate and transport of conventional water pollutants, nutrients, sediments, and toxic chemicals. It can be implemented as a simple model, as it is done in the present study, or as a complex food-web model that investigates pollutant effects on aquatic life forms. In this study, the model is set up using arbitrary yet realistic values for hydraulic variables and point source loadings of one decaying pollutant. Time-variant concentrations are tracked at three hypothetical observation points located on the main reach of the river.

Using the AQUATOX model as a simulator, the optimum allocation of pollutant loadings to maintain a target water quality standard, namely the environmental quality standard (EQS) as it is defined in the Water Framework Directive of the European Union, is calculated using the generalized-reduced-gradient method (GRG) method (Lasdon et al., 1978) with a penalty function. GRG is a numerical algorithm that is generally applied to solve smooth non-linear problems. Its implementation is simple and the application is available as an add-in of the spreadsheet software Microsoft Excel. After executing the optimization, the resulting total pollutant load yields actually the total maximum daily load (TMDL) (USEPA, 1991) without the margin of safety that is usually defined in the formal definition of the concept.

3.1 Simulation of River Water Quality

Water quality of the main reach is simulated using the AQUATOX model. The main reach is divided into 12 segments which are 1-km long and have a constant width of 15 m each. The cross-section of the river is assumed as rectangular and the flow depth is calculated using the flowrate continuity equation. Each segment is by definition an ideal completely-mixed reactor thereby assuming homogeneous physical and chemical conditions within the segment. Segments are linked together creating a one-dimensional, uniform cascading flow by neglecting dispersion between segments. The discharge in the main reach before the merging of the tributary and the point sources is assigned as 1.906 m^3/s. The tributary connects to the main reach with a discharge of 0.05 m^3/s. There are three point sources discharging wastewater to the main reach with a flow rate of 0.116 m^3/s each. An additional point source representing a domestic wastewater treatment plant is assigned a discharge rate of 0.093 m^3/s. The pollutant originating from the point sources is allowed to decay with a first-order rate constant of $k = 5.0\ d^{-1}$. All discharge rates and pollutant concentrations assigned to the tributary and point sources are arbitrary and do not rely on any kind of measurement. A flowchart of the simulated system is shown in Figure 1 and characteristics of the point sources, the tributary and the main reach is summarized in Table 1. These characteristics are used also in the setup of the AQUATOX model.

The temporal settings of the model are as follows; the total simulation time is set to 30 days considering sufficient time required to reach steady-state conditions in the system. The time step size is variable which is determined by the model by maintaining numerical stability. The convergence criterion is set to 0.001 as relative error and the results are reported in hourly time steps. The model determines the concentration time series for each segment. However, for the purpose of this study, concentrations at three observation points are tracked which are located in segments S5, S10, and S12. These observation points also serve as pilot points to obtain compliant concentrations with the water quality target (WQT). The last segment S12 represents at the same time the downstream boundary of the model.

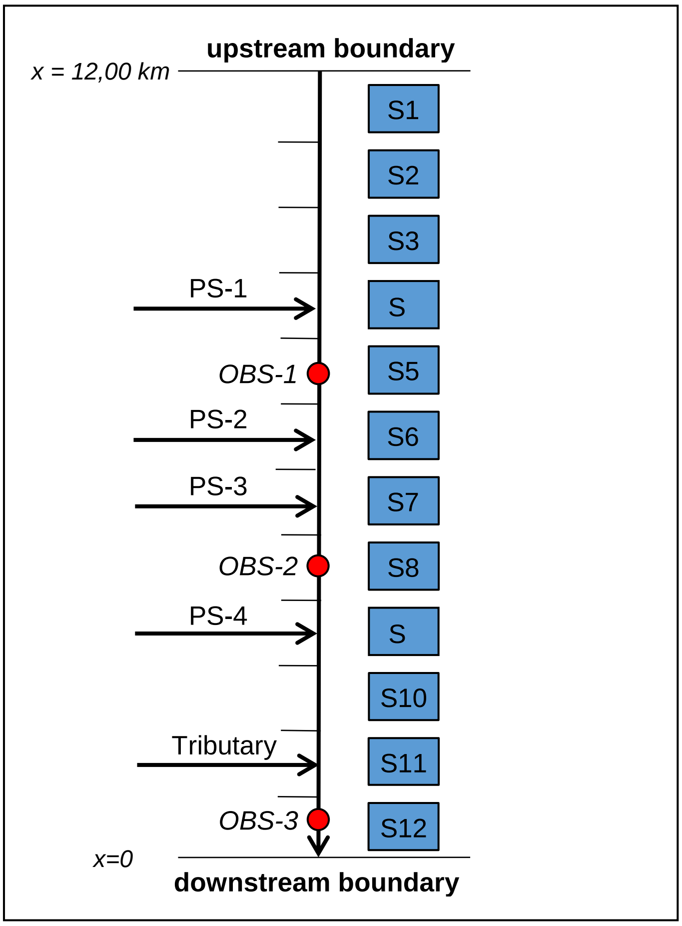

Figure 1. Segmentation and topology of the water quality model (PS: point source; OBS: observation point)

Table 1. Characteristics of the simulated river system

	Discharge Q (m^3/s)	Concentration of Decaying Pollutant C_i (mg/L)	Pollutant Load q_i (g/day)
Upstream Boundary of Main Reach	1.906	0.0	0.0
Tributary	0.05	50.0	2.16×10^5
PS-1 (domestic wastewater)	0.093	150.0	12×10^5
PS-2 (industrial wastewater)	0.116	100.0	10.0×10^5
PS-3 (industrial wastewater)	0.116	80.0	8.0×10^5
PS-4 (industrial wastewater)	0.116	60.0	6.0×10^5

3.2 Optimization Scheme

The problem of pollution load allocation among the point sources defined in the study area can be solved by using the following optimization equation:

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

subject to the following constraints:

$$q_i = C_i \times Q_i \quad ; \quad i = 1, 2, 3, \dots n_d \quad [2]$$

$$\bar{q} = \frac{1}{n_d}\sum_{i=1}^{n_d} q_i \qquad [3]$$

$$C_j(t) = \sum_{i=1}^{n_d} \alpha_{i,j}(t) \times q_i + C_j^0(t)$$
$$j = 1, 2, 3, \dots n_m \quad , \quad t = 1, 2, 3, \dots n_t \qquad [4]$$

$$\mathcal{C}_{\min} \le \mathcal{C}_i \le \mathcal{C}_{\max} \quad ; \quad i = 1, 2, 3, \dots n_d \qquad [5]$$

where Z is the value of the objective function to be maximized; n_d is the number of point sources; n_m is the number of observation points, n_t is the number of time steps in the total simulation period; q_i is the pollutant load which is obtained by multiplying the source concentration, $\mathcal{C}_i$ by the river flowrate, Q_i for the i^{th} source location; λ_1 and λ_2 are the penalty coefficients; $\bar{q}$ is the mean of the pollutants loads assigned to each source; $C_j(t)$ is the simulated pollutant concentration in the river water at j^{th} observation location and time t; $\tilde{C}$ is the WQS to be satisfied in the modeled river system; $C_j^0(t)$ is the background concentration in the river water at the j^{th} observation location and time t; $\alpha_{i,j}(t)$ is the concentration response coefficient which is used to calculate the pollutant concentration at the j^{th} observation location and time t due to a pollutant discharge from the i^{th} source location; and $\mathcal{C}_{\min}$ and $\mathcal{C}_{\max}$ are the lower and upper bounds of the pollutant concentrations discharged from the point sources.

As can be seen from the mathematical formulation given above, the objective of the presented approach is to maximize the total pollutant load discharged from every point source. This objective is constrained by means of two penalty functions. The first penalty function is represented by the second term in Eq. [1] and aims to obtain a fairly equal load allocation among the sources. According to this penalty term, the objective function is penalized, if the allocated loads deviate from their mean value. The second penalty function is given as the third term in Eq. [1] and is used to satisfy the given WQT requirement of the modeled water quality variable. According to this penalty term, if the calculated pollutant concentration at any observation point and time does not satisfy the condition of $C_j(t) < \tilde{C}$, in other words it does not meet the water quality standard, the solution gets a penalty value and the objective function is reduced. Both of these penalties are integrated into the objective function by using the penalty coefficients of λ_1 and λ_2. It should be noted that values of these penalty coefficients are arbitrary and can be determined by trial-and-error since there is no any systematic way to determine their exact values. In the general sense, higher values of these coefficients imply more effort to satisfy the associated constraint set.

Another important aspect of the presented approach is the simulation component. As indicated previously, normally, the water quality response of the KMRB to the generated pollutant discharge pattern is determined by simulating the given river system with the AQUATOX model, the simulator. It is important to note that AQUATOX is an independently operated water quality simulation model and therefore it is not possible to invoke it directly from within the optimization model to determine the resulting pollutant concentrations. Therefore, instead of executing the simulator externally for each optimization iteration, the simulation-optimization process is simplified by using indirect means to determine river water concentrations and subsequently making use of the superposition of solutions principle. First, a concentration response matrix (CRM) is calculated by directly using AQUATOX model outputs. The elements of the CRM are calculated based on

$$\alpha_{i,j}(t) = \partial\left(C_j(t) - C_j^0(t)\right)/\partial q_i \qquad [6]$$

The use of CRM is formulated in Eq. [4] and it can be directly used to determine the pollutant concentrations for any source pollutant load at any given observation point and time. Elements of the CRM are obtained by executing the AQUATOX model separately for each point source so that only one point source is active in the system. Here, the discharge load can be set arbitrarily. After obtaining the CRM, pollutant concentrations at any location along the river can be determined for any source load value. Furthermore, just by defining the pollutant loads for the sources, individual solutions for each point source discharge can now be superimposed to obtain the cumulative effect of all point sources without executing AQUATOX. The superposition is warranted due to the linearity of the water quality model.

4 RESULTS

To obtain the CRM, the AQUATOX model is executed separately for each point source discharging a pollutant concentration of 100 mg/L one at a time. Using the CRM and superposition, pollutant concentrations at each observation point are determined for the case when all point sources are active. The assigned discharge concentrations are provided in Table 1. Resulting concentrations at the observation points are presented in Table 2. For verification, the same concentrations are obtained with the AQUATOX model using exactly the same source loadings. As a result, the total pollutant load entering the river system from all point sources is 3.82×10^6 g/day. The WQT is exceeded at OBS-2 and OBS-3 while it is met at the most upstream observation point.

Table 2. Resulting pollutant concentrations at observation points after 30 days and WQT values

	$C_j(30)$ before allocation mg/L	$C_j(30)$ after allocation mg/L	WQT $(\tilde{C})$ mg/L
OBS-1	6.04	2.33	
OBS-2	12.43	5.82	8
OBS-3	12.35	8.00	

To reduce the total load and to maintain the water quality standard, the source allocation problem is solved. The pollutant source allocation problem is formulated using the formulation given above and is solved with the GRG method by implementing C_i $(i = 1, 2, 3, \ldots n_d)$ concentration values as the decision variables. Before the search process, the initial values of C_i are taken as 0 for each source location. Furthermore, the lower and upper bounds of them are taken as $C_{\min} = 0$ and $C_{\max} = 1000$ mg/L, respectively. Note that before the execution of the optimization, some trials are conducted to determine the penalty coefficients. Trial runs yield the use of $\lambda_1 = 10^0$ and $\lambda_2 = 10^8$ for the search process. After executing the optimization the solution convergence plot given in Figure 2 is obtained. As can be seen, both objective function and total pollutant load values are zero at the beginning of the search process since the initial source concentrations are used as 0. After the 6th iteration, both of them is increased by the GRG method and this improvement proceeds until the 24th iteration where the search process is terminated. Eventually, the total load from all pollutant sources is maximized. In this solution, the default termination criterion of the GRG solver is used. For the objective function value at the 24th iteration, the obtained model results are shown in Table 3 where it is evident that allocated pollutant loads are almost equally distributed among the point sources by virtue of the first penalty term in Eq. [1]. Based on the optimized pollutant load allocation, the resulting output concentrations and the corresponding WQT values are provided in Table 2. The simulated concentration profile along the river main reach is presented in Figure 3. Overall, the concentrations at all observation points are lower than the WQT value. However, the pollutant concentration exceeds the WQT in segment S11 of the river. Since there is no observation point defined in this segment, it cannot be considered in the optimization process. In addition, the total load is reduced to 2.31×10^6 g/day which is the maximum possible allowed without compromising the WQT value at any of the observation points. At OBS-3, the calculated concentration is equal to the WQT threshold which can be expected since OBS-3 is the last observation point on the river main reach, thereby reflecting the cumulative effect of all upstream pollutant sources. The source allocation problem is adequately solved by meeting WQT requirements, maximizing the total discharge load and distributing the load equally among the sources.

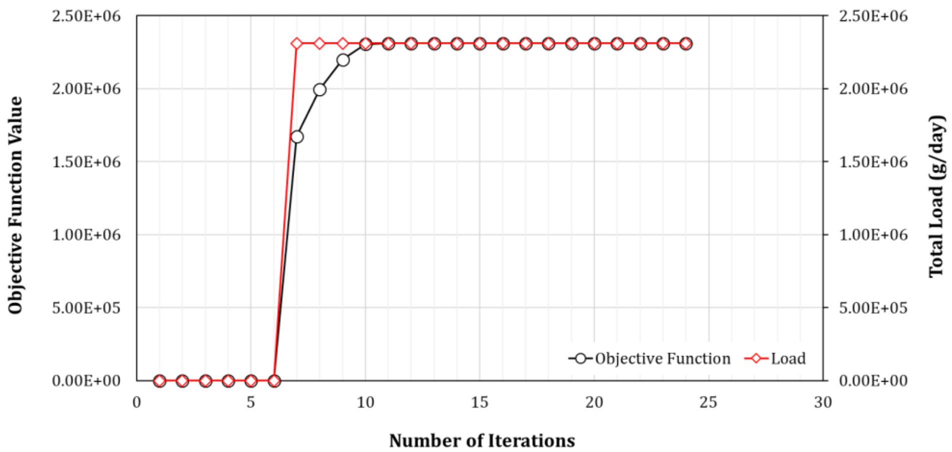

Figure 2. Convergence plots of the proposed solution approach

Table 3. Allocated pollutant concentrations and loads of the point sources

	C_i mg/L	q_i g/day	$\bar{q}$ g/day
Tributary	106.97	462,129.25	
PS-1	57.77	462,129.47	
PS-2	46.21	462,129.41	462,129.37
PS-3	46.21	462,129.38	
PS-4	46.21	462,129.32	

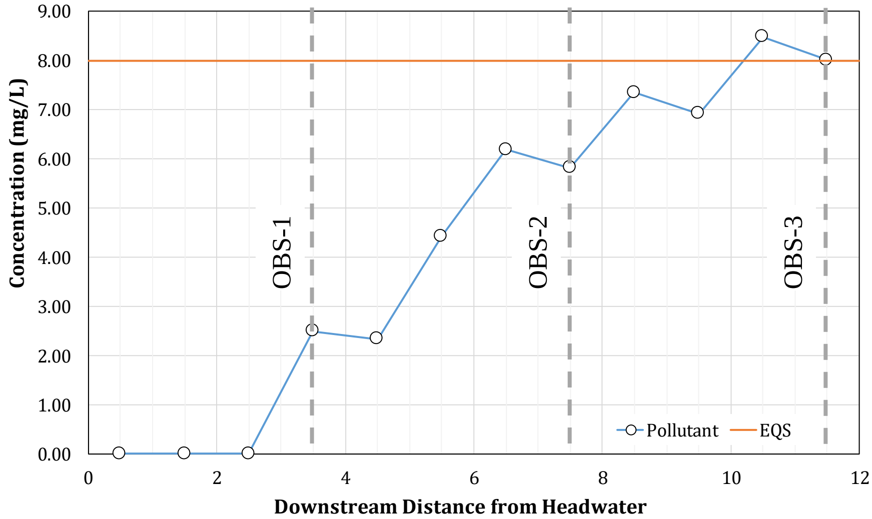

Figure 3. Pollutant concentration profile for the main reach after optimized allocation of point sources

5 CONCLUSIONS

A simulation-optimization approach to allocate point sources in a river basin yields a pollutant load distribution that complies with water quality standards of the receiving waterbody. We demonstrate that the simulation-optimization process simplifies when concentration response coefficients and the principle of superposition are used to calculate the cumulative effect of pollutant loadings without actually executing the simulator. We present also an example calculation for the KRMB that results in the optimum allocation of loadings for each point source in the sub-watershed. This study is the first step towards the development of waterbody-based discharge limits for the entire KMRB. The framework presented here will be extended to other sub-basins while field data will constitute the input of the allocation studies. The goal for future studies is to improve the optimization scheme such that the distribution of the total maximum daily load among point sources can be further adjusted by defining the wastewater treatment process related constraints. This adjustment is expected to lead possibly to more realistic source allocations.

ACKNOWLEDGEMENTS

This study is funded by the Scientific and Technological Research Council of Turkey (TUBITAK) under project number 116Y413/116Y414/116Y415.

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