Developing a Reliability-Based Waste Load Allocation Strategy for River-Reservoir Systems

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Abstract: Enhanced socioeconomic criteria and temporal changes in the topology of the system often require waste load reallocation (WLRA) in a river-reservoir system to sustain long-term water quality standards. In addition to climate and hydrological changes, hydrologic fragmentation and dam construction may significantly affect the waste-accepting capacity of the water body through changes in its physical, chemical, and even biological characteristics. Deterministic waste load allocation optimization designs are often bounded with a set of rigid constraints. These constraints do not allow any flexibility to account for uncertainties and the possibility of system failure. This paper presents a reliability-based waste load reallocation model in a complex river-reservoir system. We have linked a physical and surrogate simulation model with the Particle Swarm Optimization algorithm to present an efficient methodology for reallocating waste loads in a river-reservoir system with reliability constraints. Reliability requirements are addressed by different sets of constraints in three different formulations for the entire planning horizon. The problem, as defined, contains real and integer variables, and is formulated as a mixed-integer nonlinear programming problem. It finds the maximum values of monthly waste loads that may be discharged into the river-reservoir system under predefined reliability constraints. The surrogate model itself is refined using an online dynamic routine which makes it suitable for planning waste load allocation in multiperiod and high-dimensional system optimization under reliability-based water quality constraints. The proposed model is applied to the Karkheh river-reservoir system to illustrate its performance under various reliabilities. **DOI: 10.1061/(ASCE)WR.1943-5452.0000973.**

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Introduction

Any changes in the topology of water bodies and/or socioeconomic criteria will often require waste load reallocation (WLRA) in river-reservoir systems. A waste load reallocation (WLRA) model finds the required levels of pollutant treatments for different waste dischargers as a system's topology changes and/or as social and economic criteria are enhanced (Afshar and Masoumi 2016). To develop the best allocation strategy under new topological conditions, a WLRA model may couple an optimization algorithm with a physical water quality simulation model. Application of deterministic waste load allocation (WLA) models have been reported by Takyi and Lence (1999), Burn and Yulianti (2001), and, recently, Parmar and Keshari (2014). Fuzzy concepts and mathematics have widely been used to tackle the uncertainties in WLA models (Sasikumar and Mujumdar 2000; Ghosh and Mujumdar 2006; Saadatpour and Afshar 2007). In a recent work, Nikoo et al. (2013), used a fuzzy transformation technique for optimal allocation of water and waste load in rivers. Although earlier works have mainly dealt with single-objective frameworks (Burn and McBean 1985; Fujiwara et al. 1986), more recent researchers have emphasized multiple-objective optimization (Burn and Yulianti 2001; Yandamuri et al. 2006; Karmakar and Mujumdar 2006). A brief literature survey reveals that almost all previous research has tackled the WLA problem in river networks without any water augmentation or storage facilities.

In addition to climate and hydrological changes, hydrologic fragmentation and dam construction may significantly affect the waste-accepting capacity of a water body through changes in its physical, chemical, and even biological characteristics (Harmon et al. 2014; Friedl and Wuest 2002). Although use of one-dimensional (1D) simulation models may be sufficient for assessing water quality in rivers (Dai and Labadie 2001; Chaves and Kojiri 2005; Kerachian and Karamouz 2006), more detailed two- or three-dimensional (2D or 3D) models should be utilized for simulation of river-reservoir systems. Realizing the computational burden, use of 2D or 3D physical water quality simulation models in design optimization with water quality targets has not been addressed extensively in the literature. The issue may be even more complex and computationally expensive if uncertainties in reservoir inflow and waste load generation are embedded into the procedure.

Addressing water quality in a river-reservoir system, Kerachian and Karamouz (2007) combined a genetic algorithm with a conflict resolution technique to optimally operate a river-reservoir system in Iran. They simplified the system by using a simulation model for salinity and temporal stratification. Assuming a completely mixed storage node, a WLA model was proposed by Nikoo et al. (2014) for a river-reservoir system. The computational burden of a simulation-optimization (S-O) model which combines a process-based river-reservoir water quality model with an optimization algorithm has widely been addressed (Ostfeld and Salomons 2005;

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Castelletti et al. 2011). For given optimization algorithms, parallel computing, response surface methodology, and surrogate modeling are often recommended to manage the computational burden of large-scale S-O models (Emami Skardi et al. 2015). Surrogate models may be used to approximate the behavior of an original model while keeping the size and scope of the problem unchanged (Wagner 1995). A data driven metamodel may be used as a surrogate model to reduce the computational cost of a physical simulation model over a range of field-measured and/or synthetic data. The synthetic data is often produced by running the original simulation model for different scenarios. Metamodeling for the approximate solution of large-scale S-O problems has received increasing attention (Mousavi and Shourian 2010). Various metamodels have successfully replaced computationally-expensive simulation models for optimum design and operation of environmental and water resources systems (Wang and Shan 2006; Shourian et al. 2008; Zhang et al. 2009; Emami Skardi et al. 2015). However, replacing a 2D water quality model for simulation of a river-reservoir system with a surrogate model in an S-O framework has not been widely approached (Castelletti et al. 2009; Afshar and Masoumi 2016).

This paper presents an S-O model to derive a reliability-based waste load reallocation plan for a river-reservoir system. The planning model intends to present a methodology for refining the planning strategy for WLA in a river-reservoir system. It couples CE-QUAL-W2, a 2D physical water quality simulation model, with an improved version of the particle swarm optimization (PSO) algorithm to optimally reallocate waste loads in a river-reservoir system with reliability constraints. Reliability requirements are addressed by different sets of constraints. The model consists of real and integer variables, and hence is formulated as a mixed-integer nonlinear programming problem. The model assesses the consequences of any temporal and spatial waste load on the system under predefined reliability constraints. Spatial and temporal variation of selected state variables are estimated and refined, benefiting from a simulation and artificial neural network (ANN)-based surrogate model. The surrogate model itself is refined using an online dynamic routine. The proposed methodology may be suitable for any multiperiod S-O problem with water quality and quantity objectives. Application of the model and its performance is illustrated using data from the Karkheh river-reservoir for various reliabilities.

Reliability-Based Waste Load Allocation in River-Reservoir Systems

Reliability Concept

In a deterministic waste load allocation optimization, the designs are often bounded with a set of rigid constraints. Whereas reliable design intends to limit the chance of failure to within an allowable low level (Agarwal 2004), reliability-based optimum design (RBOD) identifies optimal design for a fixed failure probability. If justified, RBOD compromises between higher reliability and lower cost of the system. Compared to deterministic optimization, in RBOD formulation the critical modes of failure are replaced with a set of constraints addressing the probabilities of failures. Probability constraints may be used to address single or multiple measures of system sustainability, such as reliability, resilience, and vulnerability. These constraints may correspond to the failure probability of one single or the entire system's failure modes (Agarwal 2004). Reliability, resilience, and vulnerability (RRV) are often used as indices to assess the performance of water resources management policies in meeting predefined quality and/or quantity targets (Hashimoto et al. 1982).

Defining $\boldsymbol{S}$ and $\boldsymbol{U}$ as sets of satisfactory and unsatisfactory states, the system is in a satisfactory state if desired water quality conditions are met at all checkpoints during that period:

$$X_{i,t} \in S; \quad \forall\ i \tag{1}$$

where $X_{i,t}$ = pollution concentration at checkpoint i during period t. Based on this criterion, the system is in unsatisfactory condition if the target quality is not met at least at one single checkpoint. Here, we address a satisfactory state by $Y_t = 1$, and zero otherwise:

$$Y_t = \begin{cases} 1 & \text{if } X_{i,t} \in S; \quad \forall\ i \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

In a multiperiod problem with multiple checkpoints, the total number of observations will be equal to $C = i \times t$. Based on our definition of total number of temporal and spatial observations C, the reliability of the system in meeting the prespecified quality target is presented as

$$\text{Reliability } R^{(q)} = \frac{\sum_{t=1}^{TP} Y_t}{TP} \tag{3}$$

where TP = total simulation time; and superscript q stands for quality. This definition assumes the system is in unsatisfactory condition if it does not meet quality restrictions at all checkpoints. In other words, if the prespecified quality requirement is not met at a single checkpoint, a failure is registered for the entire system.

Model Structure

Reliability of waste load allocation may be defined as the probability that the allocated wastes to the dischargers will meet the required standards, i.e., provide the water quality requirements at all checkpoints in the specified period under the stated conditions. The problem is a nonlinear multiperiod optimization problem with a computationally-expensive simulation model. On a 3.4 GHz Pentium IV processor (Core i7-2600, Green Pars, Iran) with 8 GB RAM, each simulation run for 66 longitudinal segments and 55 layers (high-resolution setup) takes 160 min. For a low-resolution setup with only 19 longitudinal segments and 28 vertical layers, a simulation run is reduced to 23 min. Therefore, for tens of thousands of function evaluations in a simulation-optimization framework, the total computing time may theoretically exceed a few years. For the case example of this study with the proposed low-resolution setup, the computational time was reduced by more than 92%, whereas prediction accuracy was sacrificed by less than 4.8%.

Following the reliability concept, the WLA in a river-reservoir system may be treated as an RBOD in which the total waste loads reallocated to the dischargers may be maximized. Theoretically, the model may be formulated either as a single-objective problem under an imposed set of reliability constraints over the operation horizon, or formulated as a biobjective problem in which reliability is treated as another objective. The latter case may provide the whole spectrum of solution strategies impacting a system's reliability. Although its theoretical formulation is quite easy and straightforward, the solution would be extremely time-consuming. Reliability is a continuous variable and the resulting external archive (to store nondominated solutions) would be very large, which exponentially increases computational time. Even with the help of surrogate data-driven models, computer run time may exceed days or weeks, if convergence ever occurs. In fact, this is an ongoing

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research in our research group, and the required improvements in solution strategy and possible achievements may be reported subsequently. This paper uses the former approach, in which reliability is included as a set of constraints over the entire operation horizon.

In a river–reservoir system, the reliability constraints may be imposed on running segments of the system (the river), inside the reservoir, or both. These reliability constraints are imposed both in spatial and temporal scales. In the absence of nonpoint sources, the single-objective reliability-based WLRA in a river-reservoir system may be formulated as

$$\text{Maximize} \quad \text{Loading} = \sum_{i=1}^{D}\sum_{\tau=1}^{12} Load_{i,\tau} \tag{4}$$

Subject to

$$RS_t = RS_t^{(u)} + RS_t^{l} \quad t = 1,2,\ldots,TP \tag{5}$$

$$S_{t+1} = S_t + I_t - E_t - RK_t - RS_t \quad t = 1,2,\ldots,TP \tag{6}$$

$$S_{\min} \le S_t \le Cap \quad t = 1,2,\ldots,TP \tag{7}$$

$$RS_t \ge RE \quad t = 1,2,\ldots,TP \tag{8}$$

$$E_t = f(S_t, S_{t+1}, he_t) \quad t = 1,2,\ldots,TP \tag{9}$$

$$\text{Reliability } R^{(q)} = \frac{\sum_{t=1}^{TP} Y_t}{TP} \tag{10}$$

$$Y_t = \begin{cases} 1 & \text{if } C_{i,t} \in S_1 \text{ for } \forall\ i \\ 0 & \text{Otherwise} \end{cases} \quad t = 1,2,\ldots,TP \tag{11}$$

$$\boldsymbol{R}^{(q)} \ge \propto^{(q)} \tag{12}$$

$$C_{j,t} < \beta_{\text{quality}} \times C_{\text{standard}} \quad t = 1,2,\ldots,TP, \quad j = 1,2,\ldots,M \tag{13}$$

where $\boldsymbol{S_1}$ and $\boldsymbol{U_1}$ refer to satisfactory and unsatisfactory states for quality constraints, respectively; water released from the upper and lower intakes of the reservoir is represented by $RS_t^{(u)}$ and RS_t^{l}, respectively; $Load_{i,t}$ = allocated waste load to discharger i in period t (decision variable); $\propto^{(q)}$ refers to the required reliability levels for water quality; TP, D, and M = simulation period, number of point sources (dischargers), and the number of checkpoints, respectively; $C_{j,t}$ = concentration of phosphate at checkpoint j and month t; C_{standard} = standard value of phosphate concentration; Cap = reservoir full capacity; S_t refers to reservoir storage at the beginning of month t; and I_t, and E_t = volumetric inflow and evaporation to and from the reservoir. Monthly net evaporation height, controlled release, spill, and environmental flow are represented by he_t, RS_t, RK_t and RE, respectively. The last constraint [Eq. (13)] imposes another restriction on the upper bound of quality violation. Although we may accept failures defined by the reliability constraints, the concentration of the pollutant (i.e., phosphorous) in the failed periods is not allowed to exceed the prespecified percentage (β_{quality}). Loading may have monthly variations over the planning horizon; however, it is kept unchanged from one year to the next during the planning horizon.

This formulation, the F1 formulation, flags a success only if all checkpoints during the current period (day) fully satisfy the quality constraints. In other words, a failure will be flagged if a quality constraint violation is observed in one (or more) checkpoints. One may, however, define the reliability based on average quality parameters over all checkpoints. In this formulation, the F2 formulation, the average reliability for all checkpoints for any time step is calculated. In this case, at each time step, the reliability levels for all checkpoints are calculated individually and the average value is reported as the system's reliability. In the F2 formulation, failure at a single checkpoint may not fully account for the system's failure. In other words, it reduces the system's overall reliability per its observed reliability. In the F2 formulation, the definition of reliability [Eqs. (10) and (11)] is replaced with the following Eqs. (14) and (15):

$$Y_{i,t} = \begin{cases} 1, & \text{if } X_{i,t} \in S_1 \quad \forall\ t, i \\ 0, & \text{otherwise} \end{cases} \tag{14}$$

$$\text{Reliability } R^{(q)} = \left(\sum_{t=1}^{TP}\sum_{i=1}^{NC} Y_{i,t}\right) \Big/ C \tag{15}$$

To be in consistent with the existing conditions, we used the historical reservoir release by following the same reservoir operation policy.

Model Description and Development

As presented in Fig. 1, the proposed model integrates an optimization module, a process-based simulation model, and an efficient surrogate model. The optimization module uses a tailored version of the particle swarm optimization algorithm. To improve the convergence of the algorithm and preserve diversity to escape from local optima, fitness uniform selected strategy (FUSS) is used. In addition, as will be discussed subsequently, specific criteria were used to update the solutions in the archive. The system is carefully simulated using the CE-QUAL-W2 simulation model. The surrogate input-output (ANN) model is trained and retrained (as required) using data generated by running CE-QUAL-W2. The physical simulation model (CE-QUAL-W2) is recalled to generate new data if archive updating is required. The estimated values for state variables are used to evaluate the objective function and generate new trial solutions by the optimization module.

This study uses a modified PSO algorithm to develop an optimum waste load allocation under reliability constraints. In the PSO algorithm, the state of the ith particle in search space is addressed by its position X_i and velocity V_i in a multidimensional way. In a D-dimensional search space, the next position of each particle is addressed by its personal best experience ($p_{\text{best}(i)}$) and the global best experience of the swarm ($g_{\text{best}(i)}$)

$$X_i(t) = X_i(t-1) + V_i(t) \tag{16}$$

$$V_i(t) = W_{\text{inertia}}^{t} \cdot V_i(t-1) + C_1 \times r_1(t) \times (P_{\text{best}(i,t)} - X_i(t)) + C_2 \times r_2(t) \times (g_{\text{best}(t)} - X(t)) \tag{17}$$

where $X_i = (x_{i,1}, x_{i,2}, \ldots, x_{i,D})$; $V_i = (v_{i,1}, v_{i,2}, \ldots, v_{i,D})$; r_1 and r_2 = uniformly distributed random numbers [0, 1]; and C_1 and C_2 = tuning parameters that determine the relative weight of the cognitive and social components, respectively. The $g_{\text{best}(i)}$ and $p_{\text{best}(i)}$ represent global best and personal best for particle i in the t th iteration. The inertia weight W_{inertia}^{t} is assumed to decrease linearly as iterations increases (Eberhart and Shi 1998)

$$W_{\text{inertia}}^{t} = (W_1 - W_2) \times \frac{Mir - ir}{Mir} + W_2 \tag{18}$$

where Mir = allowed maximum number of iterations; and W_1 and W_2 = maximum and minimum values of inertia weight, respectively.

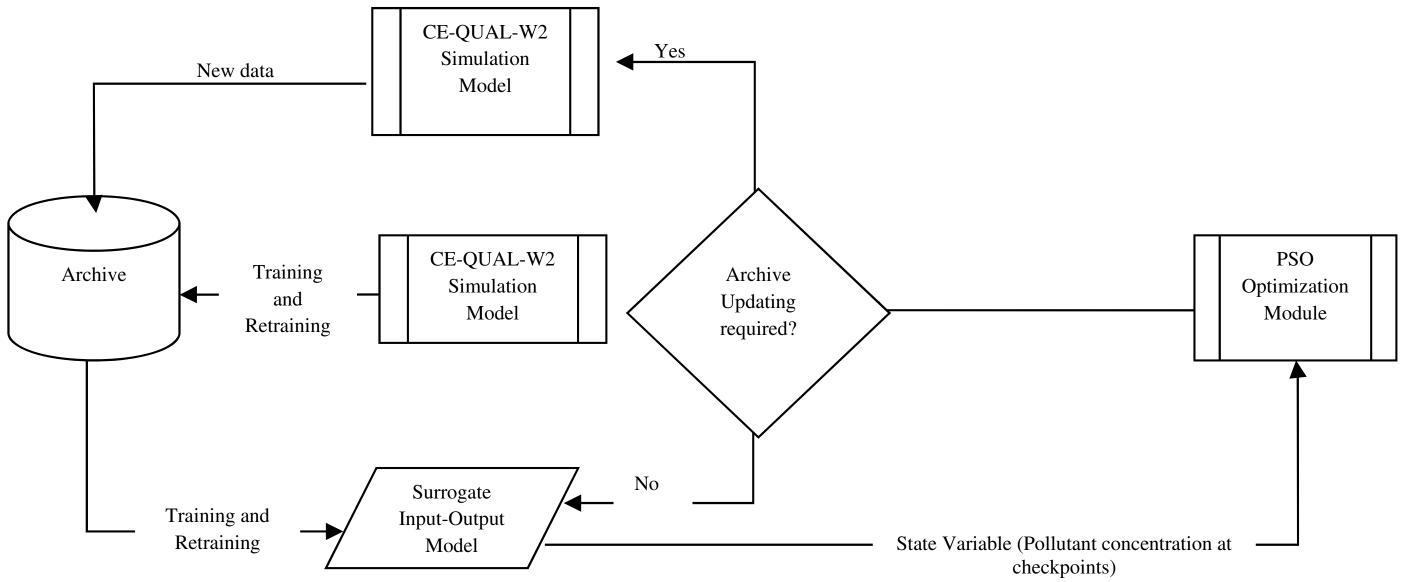

Fig. 1. Schematic presentation of the solution methodology.

Their values are tuned to make an appropriate balance between global and local search. This paper uses the random walk and fitness uniform selection strategies to improve the convergence of the algorithm and preserve diversity to escape from local optima (Cui et al. 2008).

Simulation and Optimization Modules

To simulate a complex river-reservoir system under different loading conditions a process-based water quality simulation model is often preferred. The very large number of function evaluations in a simulation-optimization problem may impose severe limitations on the use of computationally-expensive simulation models in a multiperiod problem. As the complexity and computational burden of a simulation model increases, its merit may diminish at the point at which the system's response to different excitations is to be estimated. The computational restrictions may be relaxed by using more efficient optimization algorithms or by reducing the simulation model's running time. The former approach reduces the number of function evaluations, while the latter approach may concentrate on parallel computing and/or the use of surrogate models (Emami Skardi et al. 2015). Aside from using an efficient PSO algorithm, this study benefits from a set of ANN models developed for different checkpoints, which significantly reduces the computational time of the physical simulation model (CE-QUAL-W2). Both CE-QUAL-W2 and the surrogate models are used interchangeably for the simulation of the system in a compromise between accuracy and computational time. The surrogate models are dynamically refined and filled with the newly-generated data as regions of sparse data in the feasible policy space are identified.

This study uses a professionally and academically appreciated CE-QUAL-W2 model to estimate the perfect response of a complex river-reservoir system (Cole and Wells 2008; Afshar 2013; Diogo et al. 2008; Gelda and Effler 2007). It assumes lateral homogeneity and therefore is highly recommended for relatively long and narrow water reservoirs with no major lateral sink or source terms. The system's operation rule and bathymetry data, outlet descriptions, meteorological data, initial conditions, and time series of inflow and water quality data form the main data requirements (Afshar et al. 2013).

This study uses an iterative routine for resampling and remodeling for validation and/or optimization (Fig. 2). To enhance model accuracy, the proposed scheme dynamically validates and refines the surrogate models as required [Fig. 2(b)] (Wang and Shan 2006). Afshar and Masoumi (2016) proposed and used the following two criteria to update the archived data:

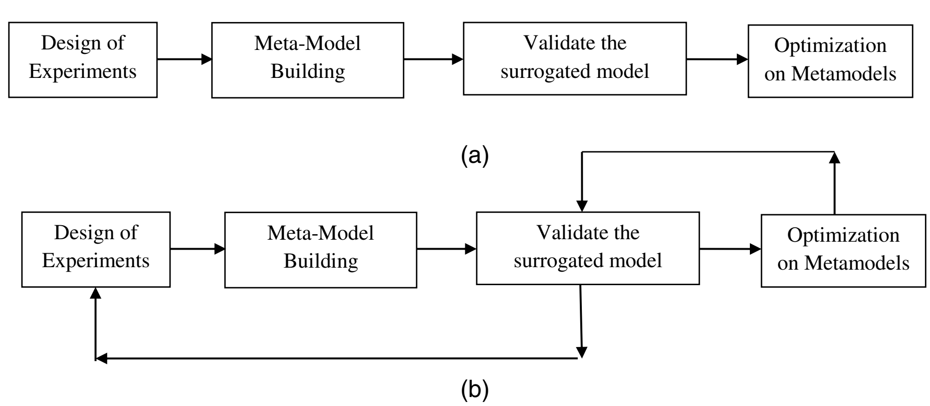

Fig. 2. Metamodel-based design optimization: (a) sequential structure; and (b) adaptive structure. (Adapted from Wang and Shan 2006.)

$$\text{if } \left(\sum_{i=1}^{NPL} \sum_{j=1}^{NTS} \frac{Z_{i,j}}{T} \right) \geq \alpha_1 Z_{i,j} = \begin{cases} 1 & \text{if } \left(\frac{|x_i^* - x_{i,j}^{\text{archive}}|}{x_i^*} \right) \geq \beta \quad \forall\ i \in NPL, \quad \forall\ j \in NTS \\ 0 & \text{otherwise} \end{cases} \tag{19}$$

$$f\left(\sum_{i=1}^{NPL} \sum_{j=1}^{NTS} \left(\frac{|x_i^* - x_{i,j}^{\text{archive}}|}{x_i^*} \right) \times \frac{1}{T} \right) \geq \alpha_2 \quad \forall\ i \in NPL, \quad \forall\ j \in NTS \tag{20}$$

where α_1, α_2, and β = precision measures specified by the user; $x_{i,j}^{\text{archive}}$ = ith component of the jth archived solution; and x_i^* = value of the ith component of the *gbest* solution, which refers to the best pollutant load (phosphate in this study) for the ith discharger from the beginning of the search process until the present iteration. The g_{best} solution is a vector whose elements x_i^* address the optimum waste load allocated to discharger i. As presented, g_{best} enters Eqs. (19) and (20) by its elements x_i^*, as they appear in the numerator and denominator of the equations.

The criteria in Eq. (19) show that the archive will be updated when the percent of the time that the normalized value of the difference between the generated data (x_i^*) and the archived data ($x_{i,j}^{\text{archive}}$) is greater than the prespecified value of α_1. Under the second criteria [Eq. (20)], the CE-QUAL-W2 model is recalled to refine the archived data if the average value of the difference between the generated data and the archived data for the total number of archived solutions (NTS) exceeds the prespecified value of α_2. If these conditions are met, the physical simulation model is called up to generate new data. The new data supplements the previous training data for surrogate model retraining.

To select the optimum strategy for any prespecified reliability level, we have used the fitness uniform selection strategy as introduced by Cui et al. (2008). Although higher fitness receives higher selection pressure in standard selection schemes, FUSS preserves diversity better than they do. When using FUSS, low populated fitness levels may effectively be favored (Cui et al. 2008). This study uses the same concept to develop an efficient optimization module (Afshar and Masoumi 2016).

Model Application

Case Study

To test the performance of the proposed modeling scheme in solving a reliability-based WLRA problem, we applied it to the Karkheh system in Iran (Iran Water and Power Development Company 2006). The 127-m-high multipurpose Karkheh dam has been under operation since 2001. With 5346.8 Mcm storage at normal water level, the reservoir release is used to irrigate 180,000 hectares of land and provide drinking water for nearby municipalities. At its normal level, surface area of the reservoir is 162 km^2 and its length is approximately 64 km. With a length to surface area ratio of 0.4, it may be categorized as a long reservoir. Use of laterally-averaged two-dimensional models is certainly a good choice for this reservoir, which has multiple outlets at different levels and historical stratification and significant depth variation of water quality parameters. Previous studies have revealed that the reservoir is susceptible to eutrophication, and phosphorus is the controlling constituent (Afshar and Saadatpour 2009). The data used in this study is mainly extracted from Afshar et al. (2012), Saadatpour (2012), Iran Water and Power Development Company (2006), and Afshar and Saadatpour (2009).

Model Setup

For successful application of the proposed approach, all three modules (CE_QUAL_W2, SM, and FUSS-PSO) had to be set up for future use. In other words, the tunable parameters of FUSS-PSO had to be identified, the simulation model had to be calibrated, and the surrogate models had to be tuned for increased computational efficiency and minimum redundancy and noise.

The Karkheh system, including the reservoir, upstream reach, and downstream reach, were divided into longitudinal and vertical segments with varying dimensions (Afshar and Masoumi 2016). Compromising between accuracy and computational cost, the river-reservoir system was segmented to 28 longitudinal layers and up to 18 vertical layers. The upstream (downstream) reach was subdivided into 14 (57) reaches with 5 (6) vertical layers (Afshar and Massoumi 2016). This study used the same calibration parameters reported by Afshar et al. (2013). The final calibration values for the most important parameters may be found elsewhere (Afshar et al. 2013).

Extensive trial and error procedures and reported values for tunable parameters were used to set up the optimization module (PSO). The model was set up for $W_1 = 0.9$, $W_2 = 0.4$, $C_1 = 0.6$, $C_2 = 0.4$, and population size of 50 with 200 iterations.

The surrogate models were structured with an appropriate number of input parameters to increase the computational efficiency and interpretability of the model while reducing redundancy and noise (Sindelar and Babuska 2004). The structure of the proposed ANN surrogate model included 33 neurons and one hidden layer. For a given source of pollutants, the response of the system was highly dependent on the position of the checkpoints. Therefore, the responses at different checkpoints were estimated with the surrogate models with varying input nodes (Table 1). Although only 12 and 14 input nodes were selected for checkpoints upstream and downstream of the reservoir, the inside of the reservoir was addressed by 43 input nodes. The input selection of the ANN model was accomplished by extracting a priori knowledge of the system being modeled and intensive sensitivity analyses (Saadatpour 2012). To identify the most important factors affecting phosphate concentration in the Karkheh reservoir's outflow, mutual information (MI) criteria were used. Mutual information measures provide information about the general dependence of random variables without making any assumptions about the nature of their underlying relationships. MI expresses the quantity of information one obtains on x by observing y (MacKay 2003). Input training data was mostly derived from the solution to the CE_QUAL_W2 model, which was assumed to be a reliable representative of the actual system under various conditions.

Table 1. Selected parameters in surrogate models

	Checkpoints		
Parameter	Upstream	Inside the reservoir	Downstream
Number of neurons in the hidden layer	33	33	33
Number of hidden layers	1	1	1
ANN type	Perceptron	Perceptron	Perceptron
Number of input nodes	12	43	14

The surrogate models for the reservoir and upstream and downstream reaches received common monthly data on wind speed, air and water temperature, concentration of water quality parameters in the natural flow [i.e., phosphate, nitrate, ammonium, total suspended solid (TSS), algae, dissolved oxygen (DO), and biochemical oxygen demand (BOD)], headwater and water diversions, and phosphate loading from all point sources. The surrogate model for the downstream reach received additional data on the reservoir water level and the portion of water released from the middle outlet.

The surrogate model, which estimates reservoir water quality responses to different excitations, was influenced by some additional parameters specific to the reservoir. For the Karkheh reservoir, the additional data consisted of reservoir water level, evaporation rate, the portion of the release from the upper outlet, and upstream diversions. However, the water quality data on natural inflow upstream from the reservoir, reservoir inflow, and phosphate loading from point sources were considered with different lag times ranging from 0 to 2 months. A total of seven major load dischargers were identified along the river upstream from the reservoir (Afshar and Masoumi 2016). This study allocated the maximum monthly phosphorus load to each discharger, which led to 84 decision variables.

The response of the system to different random pollutant loadings (initial trial solutions) was estimated with multiple runs of the CE-QUAL-W2 simulation model. The state variables (i.e., phosphorus concentration) at all monitored checkpoints were determined and saved in an external archive (Fig. 1). The archived information was used to train the surrogate model, which would later replace the physical model in the simulation-optimization process. This study initially archived 20 trial solutions, each addressing the temporal and spatial variation of phosphorus concentration due to a given loading scenario.

The training and validation of the surrogate model was conducted using 20 sets of 180 periods of data. The training of the ANN model was tested for various sets of input data ranging from 1 to 30 randomly generated data sets. We observed that increasing the input data sets from 20 to 30 made no major improvement in the accuracy of the outputs. The data for the first 156 periods were used for training, and the data for the last 24 periods was used for validation purposes. Computer processing time for these 20 trial solutions approached to 460 min on a 3.4 GHz Core i7-2600-CPU computer (Afshar and Masoumi 2016). Increasing the initial size of the archive (i.e., number of trial solutions) would certainly cause a relative increase in the required processing time.

Statistical measures reported previously show that the proposed surrogate model may effectively and efficiently be used to simulate hydrodynamic and water quality behaviors of the Karkheh system. This study used the same calibration and validation parameters and procedures (Afshar and Masoumi 2016) for deriving reliability-based solutions for waste load reallocation.

Discussion of the Results

In view of the long-term response of large reservoirs to input variations and the inherent stochasticity of natural inflow, a single period model based on the dries period will fail to address the response of the system to various excitations. In a river-reservoir system, water quality responses must be treated on a multiperiod basis with long-term pollutant loading. Compared to daily loading in total maximum daily load (TMDL) calculations, monthly or annual loads are often preferred in river-reservoir systems (USEPA 1999). Realizing the stochastic nature of inflow and the temporal variation of climatic parameters, long-term simulation of a system may be the most reliable approach for identification of system failures and their severity.

The Karkheh river-reservoir system was used to illustrate the performance of the proposed reliability-based approach. To exhibit the performance of the proposed approach and the effects of reliability constraints on the system's capacity to receive loads from the dischargers, three different cases were considered. All cases used the same basic data and model parameters for a 5,400-day (180-month) simulation period. The EPA states that phosphate concentrations in streams discharging into lakes or reservoirs should not exceed 0.05 mg/l. We set the same restriction on the checkpoints; however, we relaxed it by 20% for those checkpoints that might violate the general restriction in limited time steps as recommended by the local experts. Although the recommendations of local experts may have had no solid rationale, they provided insight into the reliability-based waste load allocation.

Case I used the F2 formulation with quality reliability of 1.2 ($\beta_{\text{quality}} = 1.2$). Case II used the F2 formulation but relaxed quality restrictions at single checkpoints (unrestricted $C_{\text{j,t}}$). Case III used the F1 formulation with $\beta_{\text{quality}} = 1.2$. The optimal allocation strategies were developed using data for 180 monthly periods with water quality reliabilities ranging from 0.95 to 0.80. For partial verification of the results, spatial distribution of the total maximum monthly load for Reliability $R^{(q)} = 1$ was checked against the results of original settings, in which the system was restricted to satisfy the prespecified quality constraints over the entire simulation period at all checkpoints (Afshar and Masoumi 2016). As expected, we obtained the same results and values for allocated waste load at different dischargers and associated state variables.

If the restriction on minimum quality requirement (constraint number 16) is relaxed, the system capacity may significantly exceed the original case. As presented in Table 2, for 95% reliability, the overall capacity of the system to receive phosphorus load may increase by 23% compared to the original case with restricted constraints (100% reliability). In-depth observations of the results show that checkpoints inside the reservoir are significantly more sensitive and reveal higher quality constraint violations. The downstream checkpoints, as compared to the upstream ones, have a significantly higher impact on total permissible waste loads by the dischargers. Checkpoints inside the reservoir are significantly more sensitive to reliability constraints and reveal higher quality constraint violations.

For Case I (F2 formulation, $\beta_{\text{quality}} = 1.2$), the maximum permissible waste load increased from 16 to 28% for reliability levels ranging from 95 to 80%, respectively (Table 2). In this case the rate of violation at all violated checkpoints was strictly limited to 20% of the standard value. In other words, under no circumstances should the phosphorus concentration exceed 0.06 mg/l, as addressed by Constraint Number 16 for $\beta_{\text{quality}} = 1.2$. The reliability level, however, was checked based on overall system performance as averaged at all checkpoints. Although minor violations at checkpoints 4, 14, and 15 were observed, the phosphorus concentration

Table 2. Increase in maximum permissible waste load allocation (%) with reliability constraints compared to restricted reliability of 100%

	Case I	Case II	Case III
Reliability (%)	F2 formulation, $\beta_{\text{quality}} = 1.2$	F2 formulation, Unrestricted $C_{\text{j,t}}$	F1 formulation, $\beta_{\text{quality}} = 1.2$
95	16	23	3
90	22	28	7
85	26	31	9
80	28	34	10.5

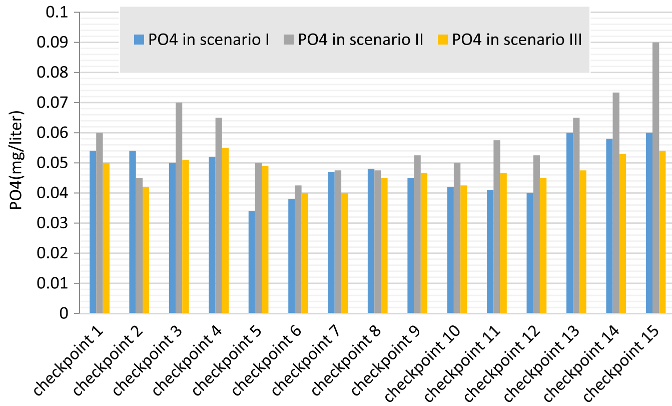

Fig. 3. Phosphorus concentration at different checkpoints on a critical day in a relatively dry year for a reliability level of 95%.

never exceeded 0.05 mg/l, as dictated by Constraint Number 16 for $\beta_{\text{quality}} = 1.2$. For Case III (F1 formulation, $\beta_{\text{quality}} = 1.2$), in which the reliability level was checked for all individual checkpoints, the maximum permissible waste load increased from 3 to 10.5% for reliability levels ranging from 95 to 80%, respectively (Table 2).

The spatial distribution of phosphorus concentrations at different checkpoints for Cases I, II, and III and a reliability level of 95% on a typical day in a relatively dry year is presented in Fig. 3. As expected, more frequent and larger quality violations from the predefined target value of 0.05 mg/l are observed for Case II compared to other cases. In fact, by relaxing the restriction on the rate of violation at violated checkpoints, the phosphorus concentration has gone up to 0.09 mg/l at Checkpoint 15, which corresponds to an 80% violation from the target value of 0.05 mg/l. This checkpoint is located at the most downstream segment of the river-reservoir system. For Case I (F2 formulation, $\beta_{\text{quality}} = 1.2$), although phosphorus concentration at 6 checkpoints exceeds the target value of 0.05 mg/l, none of them violates the restriction imposed by the upper bound of quality violation (β_{quality}) as addressed by Eq. (16). Again, most of the checkpoints with violations are located downstream from the reservoir (Checkpoints 13, 14, and 15). As expected, Case III is the most conservative, with restricted violations and a smaller increase in total maximum permissible waste load allocation under the given reliability. Aside from small violations of the target phosphorus concentration at three checkpoints, the quality constraints are fully satisfied at the remaining ones. As expected, except for Case II, we do not see any violations of the upper bound for quality violations for $\beta_{\text{quality}} = 1.2$.

The temporal variation of phosphorus concentrations at Checkpoint 1 upstream of the reservoir for all three cases is presented in Fig. 4. For Case I, (F2 formulation, $\beta_{\text{quality}} = 1.2$), the reliability level was checked based on overall system performance as averaged at all checkpoints; therefore, the prespecified reliability level of 95% is not necessarily strictly satisfied for all single checkpoints. The total number of months in which the target value of 0.05 mg/l is not strictly satisfied is approximated as 6 out of 180 months [Fig. 4(a)]. In other words, reliability level for this single checkpoint exceeds the prespecified level of 95%. The constraint violation never exceeds the value addressed by Constraint Number 16 for $\beta_{\text{quality}} = 1.2$.

For Case II (F2 formulation, unrestricted $C_{j,t}$), the temporal distribution of phosphorus concentrations at Checkpoint 1 reveals larger variations and violations from the upper bound of the quality constraint as addressed by Eq. (16). However, for a reliability level of 95%, the total number of months in which the target value of 0.05 mg/l is violated does not exceed 9 months for the entire simulation period of 180 months [Fig. 4(b)]. The rate of quality violations during some periods far exceeds the upper bound of 0.06 mg/l ($\beta_{\text{quality}} = 1.2$). This is clearly because we have replaced $\beta_{\text{quality}} = 1.2$ with unrestricted $C_{j,t}$, which relaxes the restriction on the upper bound.

For Case III (F1 formulation, $\beta_{\text{quality}} = 1.2$), there are no violations of the target quality during the entire simulation period of 180 months. Although some limited violations are permitted under the imposed reliability constraints, the quality constraints are fully satisfied. This can mainly be attributed to the severer quality conditions at the downstream checkpoints. In addition, Eq. (16) for $\beta_{\text{quality}} = 1.2$ is fully satisfied, with a reliability level of 100%. In other words, although there is some unused waste-receiving capacity at this checkpoint, its further utilization may result in constraint violations at checkpoints located further downstream [Fig. 4(c)].

The monthly distribution of concentrations at the most critical checkpoint downstream from the reservoir (Checkpoint 15) is presented in Fig. 5. For Case I, (F2 formulation, $\beta_{\text{quality}} = 1.2$), in which the system reliability level was checked based on overall system performance as averaged at all checkpoints, the upper bound on the quality constraint was restricted for all checkpoints as addressed by $\beta_{\text{quality}} = 1.2$. Therefore, the prespecified reliability level of 95% was not strictly satisfied at all single checkpoints. This is clearly observed at Checkpoint 15, located downstream from the reservoir. Although the overall reliability level of 95% is satisfied for the entire system, the total number of months in which 0.05 mg/l is not strictly satisfied at this checkpoint is approximated at 33 out of 180 months [Fig. 5(a)]. In other words, the reliability level for this single checkpoint is far less than the prespecified level of 95%. Again, in none of these periods has the constraint violation exceeded the prespecified value addressed by Constraint Number 16 for $\beta_{\text{quality}} = 1.2$.

As expected, for Case II (F2 formulation, unrestricted $C_{j,t}$), the temporal distribution of phosphorus concentrations at checkpoint 15 reveals larger variations and violations from the upper bound of quality constraint as addressed by Eq. (16). Although for reliability level of 95%, the total number of months in which the target value of 0.05 mg/l was violated is smaller (27 months) than that of Case I for the entire simulation period of 180 months, the rate of quality violations during some periods far exceeded the upper bound of 0.06 mg/l for $\beta_{\text{quality}} = 1.2$ [Fig. 5(b)]. This is clearly because we have replaced $\beta_{\text{quality}} = 1.2$ with unrestricted $C_{j,t}$, which relaxes the restriction on the upper bound.

For Case III (F1 formulation, $\beta_{\text{quality}} = 1.2$), in which the reliability level was checked for all individual checkpoints, no violations from the upper bound of the quality constraint for $\beta_{\text{quality}} = 1.2$ (0.06 mg/l) were observed. In other words, Eq. (16) for $\beta_{\text{quality}} = 1.2$ was fully satisfied, with a reliability level of 100%. As expected, there were only 9 months in which the target value of phosphorus concentration (i.e., 0.05 mg/l) was violated. For the remaining 171 periods, the phosphorus concentration remained below the target value of 0.05 mg/l [Fig. 5(c)]. This led to the prespecified reliability level of 95%. Case III is the most conservative and restricted reliability-based waste load reallocation to the river-reservoir system.

Checkpoints inside the reservoir behave differently in comparison to those upstream and/or downstream of the reservoir. For all three cases, most of the violations from target constraints were concentrated in the second half of the simulation period (Fig. 6). The gradual accumulation of phosphorus inside the reservoir seems to play a key role in this observation. Due to the large storage volume

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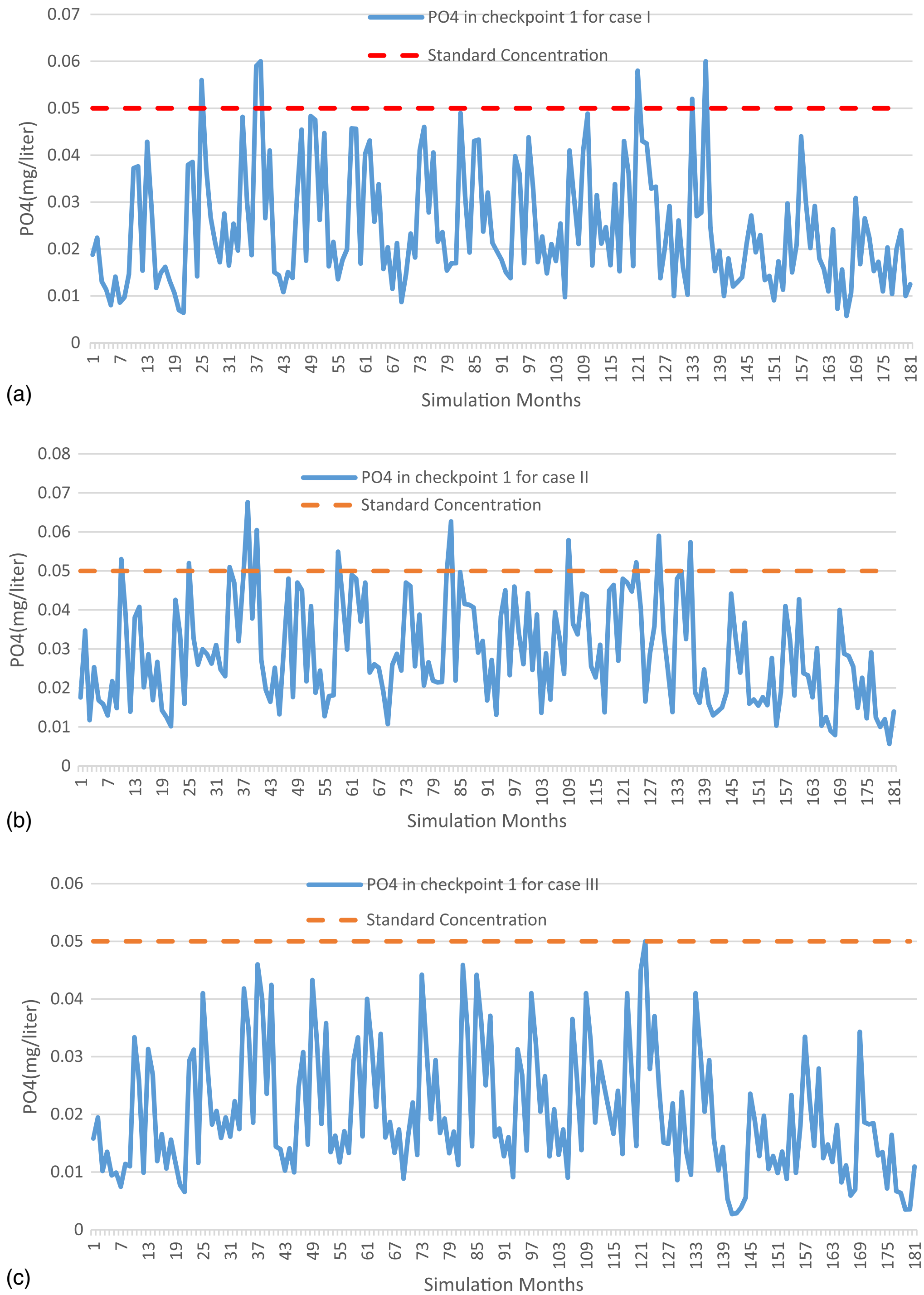

Fig. 4. Temporal variation of phosphorus concentrations at Checkpoint 1 for Cases (a) I; (b) II; and (c) III.

of the reservoir and the low initial phosphorus concentration within the reservoir, it took a few years before the phosphorus concentration reached a stable condition. Regardless of this general trend, in Case III, the total months with violations of the target phosphorus concentration did not exceed the limiting value of 9 months, leading to 95% reliability [Fig. 6(c)]. However, the behavior of Cases I and II was like the behavior discussed for Checkpoints 1 and 15. For Case I, the rate of quality violations was strictly restricted by 0.06 mg/l for $\beta_{\mathrm{quality}} = 1.2$ [Fig. 6(a)]. For Case II, the upper bound of the quality constraint was frequently violated because we relaxed the constraint by accepting unrestricted $C_{\mathrm{j,t}}$ [Fig. 6(b)].

Conclusion

Due to the inherent stochasticity of natural inflow and the long response time of large reservoirs to waste loads, a multiperiod model was used to address the response of a system to various excitations. The problem was formulated as a reliability-based multiperiod optimization problem. It was shown that adaptive use of the dynamically-refined surrogate model may extremely reduce the computational time required by physical simulation models in the simulation-optimization process.

To exhibit the performance of the proposed approach and the effects of reliability constraints on a system's capacity to receive

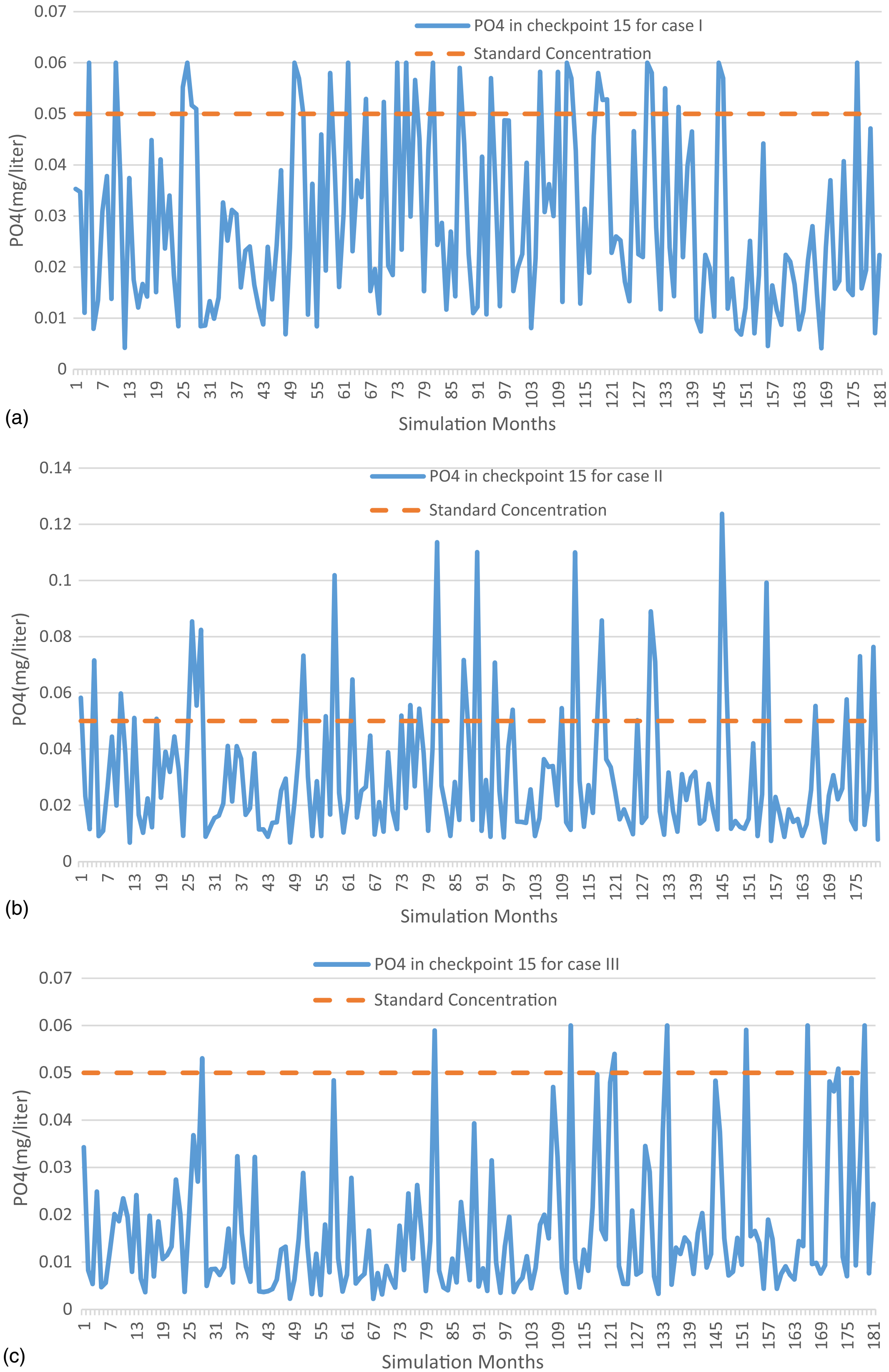

Fig. 5. Phosphorus concentration at Checkpoint 15 for Cases (a) I; (b) II; and (c) III.

loads from the dischargers, three different formulations were considered. The F1 formulation flagged quality constraint violations when they were observed in one (or more) checkpoints. In the F2 formulation, however, the reliability level was checked based on overall system performance as averaged at all checkpoints. In brief, for a 95% reliability level, the overall system capacity to receive phosphorus load for the F2 and F1 formulations increased by 16 and 3%, respectively. When the maximum rate of quality

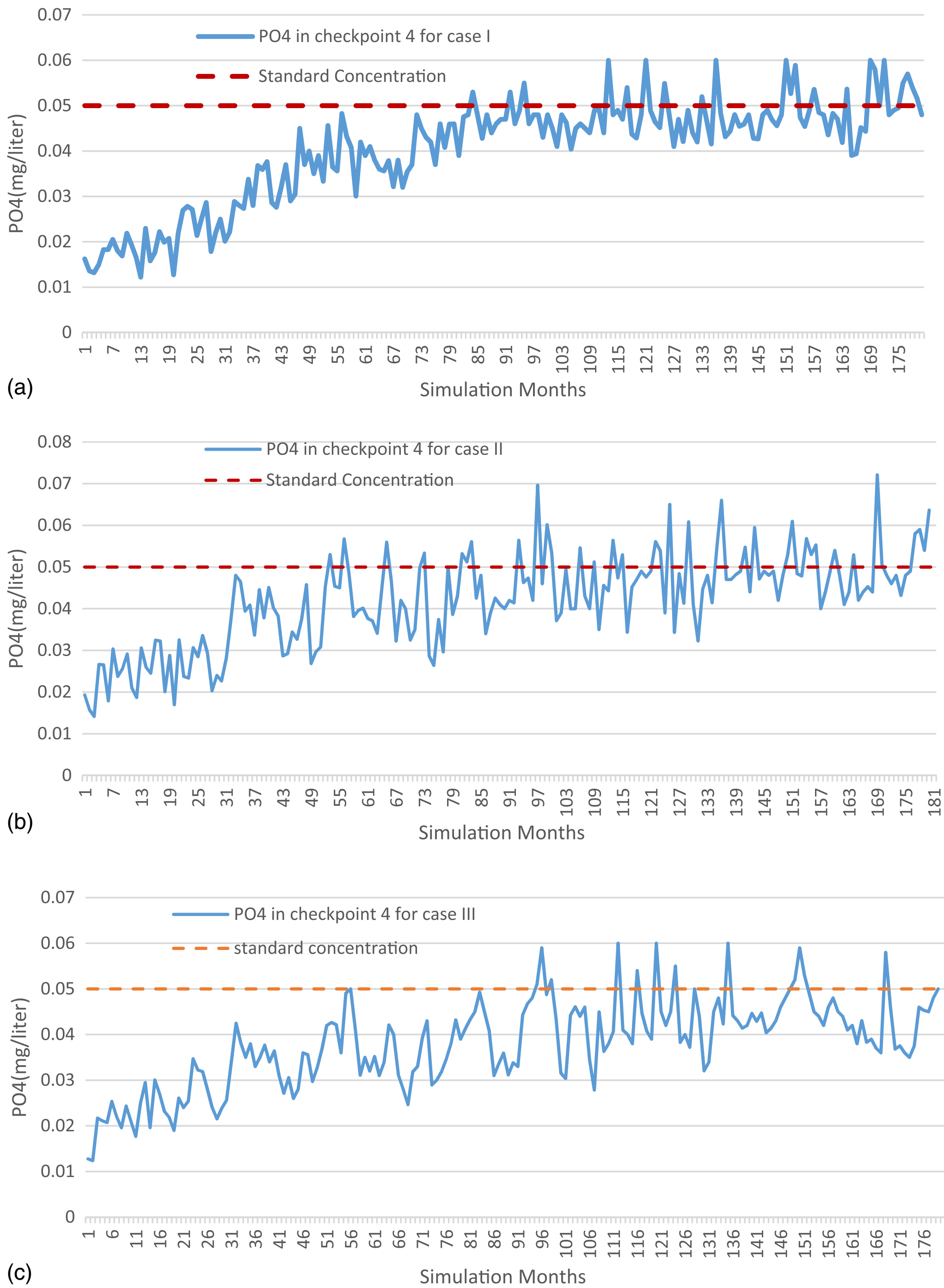

Fig. 6. Phosphorus concentrations at checkpoint 4 inside the reservoir for Cases (a) I; (b) II; and (c) III.

violations on individual checkpoints was relaxed, the maximum permissible load increased to 23% for the same overall reliability level. The increase in maximum permissible load was significantly higher for lower reliability levels. A tradeoff between the maximum load and the desired reliability level may help authorities develop long-term strategies.

The results show that checkpoints inside the reservoir are significantly more sensitive to reliability constraints and reveal higher quality constraint violations. The downstream checkpoints, compared to the upstream ones, had a significantly higher impact on total permissible waste loads by the dischargers. For checkpoints inside the reservoir, most of the violations from the target constraint were concentrated in the second half of the simulation period. The gradual accumulation of phosphorus inside the reservoir seems to play a key role in this observation. We believe that the large storage volume of the reservoir and the low initial phosphorus concentration within the reservoir played a key role in this observation. In fact, it took few years before phosphorus concentrations reached to a stable condition. We conclude that authorities may wish to partially relax quality constraints at some checkpoints during the entire management period for higher waste load allocation permits. Accounting for multiple pollutants and sustainability measures may improve the model's academic and professional benefits. The value of coupling this model with a watershed simulation model to include nonpoint sources may also be explored.

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