Reservoir operation under accidental MTBE pollution: A graph-based conflict resolution framework considering spatial-temporal-quantitative uncertainties

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ABSTRACT

Given the hazardous effects of sudden dam reservoir contamination — as might occur upon the intrusion of the fuel additive methyl tert-butyl ether (MTBE) — the contaminant’s effect on the quality of allocated waters requires careful study. Employed to determine optimal reservoir operational rules in the case of sudden MTBE pollution, a risk-based simulation-optimization model was developed to simultaneously minimize unsatisfied water demand, the risk of violations of water quality standards, and the reservoir recovery time. Risks were assessed by considering various often-neglected pollution scenarios as a combination of location, quantity, and the season of pollution intrusion. The appropriateness of operational rules proved to depend upon thermal conditions and MTBE intrusion properties, confirming the necessity of considering location-quantity-season uncertainties. Social and regional conditions also occupied a dominant role in determining the level of satisfaction achieved under different water allocation strategies. Accordingly, by considering environmental conditions and local rules, a graph model for conflict resolution was established and used to reach a set of compromise operational rules. The developed framework could serve as a guide for water utilities to determine efficient reservoir operational rules after a sudden contaminant intrusion.

1. Introduction

Dam construction is a common solution to cope with year-round agricultural and domestic water demands, especially in areas subject to a hot and dry climate. Generally, dam reservoir water withdrawals are scheduled according to specific operational rules that depend on environmental conditions, quantity and quality of available water, and dam characteristics (e.g., Kerachian and Karamouz, 2006; Ashofteh et al., 2015; Poursahabi et al., 2020). Among these influencing factors, the danger of large dam reservoirs being intentionally or accidentally subjected to pollutant intrusion is of the utmost importance. Pollutant intrusion accidents most commonly occur as a result of human error, e.g., failure in the transportation of hazardous chemicals (Li et al., 2014). A sudden toxic chemical discharge into the Rhine River from a chemical warehouse fire via fire-fighting water runoff in 1986 (Giger 2009), the accidental contamination of Kyrgyzstan’s Lake Issyk-Kul and Barksoon River with sodium cyanide, spilled near the Kumtor gold mine in May 1998 (Pannier, 1998), pollution of Cayuga Inlet Creek (West Danby, NY) with diesel oil following a train derailment (Lytle and Peckarsky 2001), and a spill of arsenic-rich tailings from a pyrite mine in southern Spain (Kraus and Wiegand 2006), are only a few examples of sudden chemical contamination causing serious damage to aquatic life and contributing to ecosystem degradation. This issue is rather more critical in developing countries. For example, on March 4, 2003, a truck accident released 30,400 L of methyl tert-butyl ether (MTBE) into the Khalife-Tarkhan River (near Sanandaj, Upper Ghashghai River basin, Kordestan, Iran). The spill...
reached the Gheshlagh Reservoir within 24 hr, thereby limiting access to safe water and restricting water allocations (Afshar et al., 2017). Since pollutant intrusion accidents can lead to highly hazardous and acutely critical situations with highly undesirable consequences, even slight probabilities of contamination should be considered. In addition to employing physical barriers such as protective guard rails for accident prevention, appropriate operational responses must also be provided when these accidents do occur.

Several studies have employed modified optimization algorithms (Haddad et al., 2008; Afshar et al., 2011) to provide operational response strategies that balance concerns regarding freshwater quality and the quantity of water available to meet demands (Chaves et al., 2003; Kerachian and Karamouz, 2007; Castelletti et al., 2014; Azadi et al., 2016). Accordingly, it is critical that the operational rules developed and implemented in response to a reservoir’s sudden pollution and decline in water quality should be valid and effective. A range of simulation-optimization models has been applied to determine standard reservoir operational rules and allocate stored water according to water quality-quantity limitations (Liu et al., 2020; Nourani et al., 2020). While operational rules to manage sudden water contamination incidents in reservoirs are essential to avoid adverse effects on the health of water consumers, they have not been broadly studied (Saadatpour and Afshar, 2013; Shokri et al., 2014; Haddad et al., 2014; 2015; Amirkani et al., 2016). A pollution intrusion response management model was developed by Saadatpour and Afshar (2013) to simultaneously minimize reservoir recovery time and reduce water quality standard violations for different injection masses and locations, but it neglected the effects of intrusion timing. However, it is acknowledged that seasonal changes in water temperature, wind speed, reservoir surface area, and hydraulic conditions can theoretically affect both reservoir dynamics and the fate of pollutants within surface water bodies (Stocking and Kavanaugh, 2000). Assuming the possibility of injections in each of four seasons, Shokri et al. (2014) and Amirkani et al. (2016) demonstrated an apparent seasonality effect on the operational rules developed for a volatile pollutant spill. For example, the numerical experiment designed by Shokri et al. (2014) showed that, in terms of pollutant duration and maximum concentration, the intrusion of a volatile pollutant in spring offered fewer risks than at other times. While studies investigating the effect of different climatic conditions occurring with seasonal changes (Tahir et al., 2008; Ashofteh et al., 2015), or various pollutant characteristics (e.g., mass and intrusion location; Saadatpour and Afshar, 2013) have successfully generated optimal operational rules appropriate to a particular single factor, uncertainties arising from the simultaneous and potentially synergistic effects of
multiple factors have not been investigated. To reduce the risk of applying inefficient operational rules in the case of unavoidable incidents, these uncertainties should clearly be addressed in the process of determining optimization model objectives.

A further key issue in the case of sudden reservoir pollution is the type of pollutant involved. Since the transport of petrol (gasoline) is common in various parts of the world, it is important that the intrusion of various petrol additives, such as methyl tert-butyl ether (MTBE; IUPAC: 2-Methoxy-2-methylpropane), into bodies of water receive particular attention. However, among pollutants threatening the quality of surface water bodies such as dam reservoirs, MTBE intrusion has garnered limited attention (Amirkani et al., 2016; Shokri et al., 2014). Shokri et al. (2014) added the capacity to simulate the fate and transport of MTBE to the existing two-dimensional, laterally-integrated hydrodynamics and transport reservoir simulation model, CE-QUAL-W2. This capacity was included in the modified version of the CE-QUAL-W2 model and was shown to be reliable in a subsequent study (Afshar et al., 2017). Nonetheless, the performance of operational rules after MTBE intrusion has not been extensively investigated.

Reliable operational rules should be compatible with social and regional conditions, including stakeholders’ demands and goals (Daneshmand et al., 2014). In most previous studies (e.g., Kerachian and Karamouz, 2006 and 2007; Shirangi et al., 2008; Haddad et al., 2014; Yang et al., 2014), operational rules were obtained from simulation/simulation-optimization models with conflicting goals. In such cases, attempts were made to resolve existing conflicts over selecting operational rules using conflict-resolution methods such as Young or Nash bargaining theories. Among conflict resolution methods, the graph model for conflict resolution (GMCR) has demonstrated an inherent superiority in the analysis of the strategic aspects of water disputes (Dowlatabadi et al., 2020; Moosel et al., 2021; Wu et al., 2019; Madani and Hipel, 2007). By modifying classical game theory, GMCR has achieved an uncomplicated flexible structure that requires only minimal information to model and analyze the strategic conflicts/disputes between decision-makers with multiple conflicting objectives. Despite the necessity to consider local rules and the priorities of influential decision-makers, the implementation of GMCR has yet to be considered in selecting optimal compromise reservoir operational rules.

In the present study, a multi-objective simulation-optimization model was developed to determine optimal dam water withdrawals (a.k.a. “operational rules”) from reservoir outlets under sudden MTBE pollution. This was carried out by simultaneously minimizing unsatisfied water demand, the risk of frequency-magnitude violations of water quality standards, and the risk of modified reservoir recovery time (RRT). The developed model sought to address the shortcomings of previous studies and drive progress in establishing operational rules by taking advantage of the following approaches:

- Including uncertainties related to climatic conditions and pollutant characteristics by considering various pollutant intrusion scenarios,
- Assessing uncertainties arising from the potential synergistic effects of different climatic conditions and various pollutant characteristics,
- Addressing uncertainties by determining optimization model objectives for the worst-case scenarios, using the conditional value at risk (CVaR),
- Determining the compromise operational rule among the Pareto-front solutions with the help of conflict-resolution models, using the GMCR + decision support system.

To facilitate the modeling process and provide a comprehensive framework, the following procedures were implemented:

- Repeated executions of the calibrated CE-QUAL-W2 water quality and hydrodynamic model in a MATLAB® environment, drawing upon thousands of input–output sets to train and validate the surrogate model,
- Replacement of the simulation model by a surrogate model thanks to a combined principal component analysis-multilayer perceptron (PCA-MLP) artificial neural network, serving to reduce the model’s runtime and computational burden,
- Coupling optimization and surrogate models in the MATLAB® environment to determine the optimal reservoir operational rules under sudden MTBE pollution.

2. Methodology

A detailed explanation of the proposed model’s main methodological steps in determining optimal reservoir operational rules is illustrated schematically in Fig. 1. The proposed multi-objective framework (Fig. 1) includes five steps: (i) developing pollution scenarios, (ii) running a reservoir simulation, (iii) replacing the calibrated CE-QUAL-W2 simulation model with an appropriate reservoir surrogate model, (iv) determining optimal reservoir operational rules, and (v) determining the compromise operational rule. These steps are thoroughly discussed in the following sections.

2.1. Development of pollution scenarios

To include the uncertainties related to the pollutant’s fate and transport through the reservoir, operational rules were developed that considered different pollution scenarios. Based on a priori knowledge of the processes affecting the fate of MTBE in reservoirs and sensitivity analyses, pollutant intrusion time, pollutant quantity, and intrusion location were identified as parameters of influence. Accordingly, three pollutant concentrations (low, medium, and high), three intrusion sites within the reservoir (adjacent to the reservoir outlets, in the middle of the reservoir, and farthest from the outlets), and four intrusion times (first day of summer, spring, fall, and winter) were factored to establish 36 (3 × 3 × 4) different pollution scenarios (Fig. 2). Within this framework, the possibility of pollutant intrusion within any season served to address the seasonality effects on thermal conditions (i.e., air and water temperature), reservoir surface area (interchangeably used
with reservoir level), wind speed, water demands, and reservoir inflows. The three pollutant intrusion locations were selected to acknowledge the variability of reservoir response to the intrusion location and provide a reliable general optimization model. The selection of intrusion locations well-distributed across the reservoir’s expanse, rather than at high-risk intrusion locations alone, was considered in developing the numerical experiment in this study.

These scenarios shed light on how changes in water temperature, wind speed, and reservoir surface area might affect the fate of MTBE. Drawing upon the observations of Stocking and Kavanaugh (2000), who evaluated the impact of several environmental variables on the fate of MTBE in standing waters, one can postulate that water temperature and wind speed increases might accelerate the elimination of MTBE by increasing the rate of MTBE volatilization and decreasing its half-life. On the other hand, an increase in reservoir surface area would decelerate the elimination of MTBE by decreasing the rate of MTBE volatilization.

### 2.2. Reservoir simulation

Several processes, including volatilization, advection, biodegradation, photodestruction, adsorption, and abiotic degradation, are involved in deciding the fate of MTBE in standing water (Stocking and Kavanaugh, 2000). However, given the physicochemical properties of MTBE (i.e., a high tendency to dissolve in aqueous media, a relatively low Henry’s constant, and low adsorption to sediments) and its attendant behaviour in a body of water, many of these processes were insignificant or slow, leaving volatilization, advection, and decay processes as the preeminent pathways of MTBE elimination (Afshar et al., 2017). Accordingly, MTBE can be classified as a generic constituent that does not interact significantly with any of the water quality state variables and hydrodynamics (Wells, 2019).

A well-known two-dimensional, laterally-averaged, hydrodynamics and water quality simulation model, CE-QUAL-W2, has been widely used to model both vertical and horizontal pollutant propagation in reservoirs and lakes (Kim and Kim, 2006; Yu et al., 2010; Soleimani et al., 2016; Heidarzadeh and Nejad, 2017; Azadi et al. 2019; Burigato et al., 2019; Wells, 2019). Considering MTBE as a volatile generic constituent, the CE-QUAL-W2 model takes into account changes in MTBE concentrations caused by spilling of MTBE into the lake, vertical mixing of the water body, discharge of MTBE through reservoir outfalls, surface exchange of MTBE from the reservoir surface, and decay processes (Fig. 3).

Here, the CE-QUAL-W2 simulation model was calibrated and employed to determine the MTBE concentration at reservoir outlets over a 70-day simulation period for different magnitudes, locations, and timings of MTBE intrusion. The simulation period of 70 days was adjusted to equal the maximum RRT of the various pollution scenarios. Recognizing the ability of the CE-QUAL-W2 model to simulate thermal stratification in reservoirs (Gelda et al., 1998; Rangel-Peraza et al., 2012), this model was also used to estimate the temperature of different layers of the reservoir. Using the data regarding topography, inflow, weather, stream temperatures, and release values, the CE-QUAL-W2 model was calibrated in two stages: (i) reservoir geometry calibration, and (ii) reservoir hydrodynamic calibration.

To define and calibrate the finite difference model for the reservoir, information regarding reservoir geometry was gathered from a topographic map of the region and a viable volume-area-elevation diagram for the dam’s reservoir. These served, respectively, to determine the bathymetric cross-sections and evaluate the volume-area-elevation curve generated by the reservoir model. As the calibration of reservoir hydrodynamic features was sensitive to depth-temperature profiles and reservoir water surface elevation, monthly vertical temperature profiles and daily Water Surface Elevation (WSE) information was employed in the calibration of the developed reservoir hydrodynamic model.

With respect to the fate and transport of MTBE, a modified source/sink equation, which considered MTBE surface exchanges and biodegradation processes, including volatilization and absorption from the top layer (water surface) and possible zero- or first-order decay processes (Eq. (1)), was solved by the model in the form (Wells, 2019):

$$S_{\text{vol}} = -k_{d}S_{g}^{(T-20)} - k_{d}S_{g}^{(T-20)} \theta_{g} - \frac{1}{h_{RT}}K_{\text{GLF}}CGKLFG_{\text{RT}}$$

where,

- $S_{\text{vol}}$ is the source/sink term for the volatile generic constituent concentration,
- $k_{d}$ is the zero-order decay coefficient (g m⁻³ s⁻¹ at 20 °C),
- $\theta_{g}$ is the temperature correction factor (with a typical range of 1.02–1.05 (Heald et al., 2005)),
- $T$ is water temperature (°C),
- $k_{1}$ is the first-order decay coefficient (s⁻¹ at 20 °C),
- $G_{\text{RT}}$ is the volatile generic constituent concentration,
- $K_{\text{GLF}}$ is the reaeration coefficient for oxygen,
- $CGKLFG_{\text{RT}}$ is the unitless user-defined gas transfer factor (0.776 for MTBE), and
- $h_{RT}$ is depth of the surface layer computational cell (m).

As the focus was to develop a surrogate-based optimization model rather than one drawing upon a calibrated CE-QUAL-W2 model, zero-order decay was neglected, while first-order decay was determined using a $k_{1}$ coefficient value of:

$$k_{1} = \frac{\ln 2}{h_{5}}$$

where, $h_{5}$ is the MTBE half-life (Heald et al., 2005). In the present context, the value of 0.5 was assumed to be 28 days. The correction formulation presented by Elmore and West (1961) served to adjust the reaeration and first-order decay coefficients for other temperatures. In this regard, the temperature correction factor ($\theta_{g}$) was adjusted to 1.024, according to Wells (2019). Moreover, as suggested by O’Connor (1983), the reaeration coefficient, as a function of wind speed, was considered to determine the wind effects on MTBE evaporation from the top layer.

### 2.3. Reservoir surrogate model

Generally speaking, the implementation of CE-QUAL-W2 has been accompanied by considerable computational burdens. This limitation worsened when recurrent simulations were required, such as within simulation-optimization frameworks for fitness evaluations (Saatapour et al., 2020). To address the simulation-optimization model runtime concerns, the calibrated CE-QUAL-W2 simulation model was replaced by a modified version of the PCA-MLP surrogate model introduced by Vanda et al. (2021). Based on their proposed framework, principal component analysis (PCA) was coupled with a multilayer perceptron architecture (MLP) artificial neural network (ANN) model to assess the operational responses to pollution intrusion scenarios. Traditionally, a large dataset of inputs and outputs, procured by
repeated execution of the developed simulation model, is required to train and validate the ANN-based surrogate models. However, the redundant information in datasets prepared in this manner would not only potentially prevent the ANN model from accurately detecting the relationship between the input and output datasets, but might also result in an imprecise and time-consuming surrogate model. Within this framework, the PCA tool, therefore, served to: (i) reduce the dimensions of input and output data, (ii) reduce the model complexity brought about by high dimensionality, and (iii) minimize the overfitting risk of the MLP surrogate model.

### 2.3.1. Development of the PCA-MLP model

In accordance with Vanda et al. (2021), the two matrices of daily release strategies and their associated daily pollution concentration levels at reservoir outlets, whose dimensions had been reduced using the PCA tool, were respectively introduced to the MLP model as input and output matrices. However, given that reservoir response can vary significantly according to the time, location, and magnitude of the pollution intrusion, the use of such input–output data to train the MLP model was not applicable here. To address this, a representative training PCA tool, were respectively introduced to the MLP model as input and output matrices. However, given that reservoir response can vary significantly according to the time, location, and magnitude of the pollution intrusion, the use of such input–output data to train the MLP model was not applicable here. To address this, a representative training dataset was established, in which potential combinations of the four factors of time, location, and magnitude of the pollution intrusion, as well as daily release strategies were included. To do so, 500 different operational rules (release strategies) for discharging water from two reservoir outlets, applied over a 70-day period (a 140 × 500 matrix), were generated individually for each of the four seasons. This allowed the inclusion of seasonal effects on initial reservoir storage and daily reservoir inflow, making it possible to evaluate the feasibility of operational rules regarding reservoir capacity and the law of continuity on a daily basis (Karamouz et al., 2003). The 3 magnitudes and 3 locations of pollution intrusion were then combined with each release strategy generated, resulting in 18,000 [(500 × 500 × 500 × 500) × 3 × 3] possible scenarios.

Each possible pollutant intrusion scenario was introduced to the MLP model through a vector including 140 daily releases and four characteristics of the intrusion scenario (i.e., the values of air temperature, location, quantity, and time of pollutant intrusion). This led to a 144 × 18000 matrix representing the MLP input dataset. To estimate seasonal pollution concentrations at reservoir outlets under all scenarios (i.e., 500 × 3 × 3), the CE-QUAL-W2 model was forced with 500 associated release scenarios, 3 quantities, and 3 locations of pollution intrusion. This process was repeated for four seasons (i.e., the four different times of pollutant intrusion), resulting in a 140 × 18000 matrix of MTBE concentration levels, considering the 70-day simulation period and the two reservoir outlets. This generated two matrices, one of 144 × 18000 and another of 140 × 18000, representing the input and output datasets, respectively.

As an MLP neural network model may be subject to overfitting if trained with such a large input–output dataset (Vanda et al., 2021), the size of the input–output dataset must be reduced while maintaining critical information. This necessity was met due to: (i) the development of two distinct MLP models, one for each outlet, and (ii) the use of the PCA tool (for more detail, see Supplementary Material, Section S.2). The MLP model for each outlet (hereafter referred to as PCA-MLP) was then trained and validated against the prepared input-target dataset (see Supplementary Material, Section S.2), included within the optimization model. This served to determine MTBE concentrations at reservoir outlets under all pollution scenarios.

### 2.4. Optimal reservoir operational rules

Using a Non-Dominant Sorting Genetic Algorithm (NSGA-II) (Oeh et al., 2002), coupled with fixed PCA-MLP surrogate models, a three-objective optimization model was developed to determine optimal reservoir operational rules. A fast and elitist multi-objective genetic algorithm, NSGA-II employs standard genetic algorithm parameters (e.g., population size, operator probabilities, etc.) to determine a trade-off curve among conflicting objectives (Shrestha and Rode, 2008). To obtain optimal reservoir operational rules, three objective functions were prepared:

1. To satisfy agricultural water demand, the unsatisfied water demand (Z₁) was minimized:

   \[ Z₁ = \text{Minimize}(\text{UnD}) \]  

   where, \( \text{UnD} \) is the seasonal maximum unsatisfied water demand, calculated using Eqs. (S7) to (S10), Section S.3, Supplementary Material.

2. To maintain the quality of water released for downstream consumption, the risk of frequency-magnitude violations of water quality standards (Z₂) was also minimized:

   \[ Z₂ = \text{Minimize}(\text{CVaR}_{\text{RRT}}) \]  

   where, \( \text{CVaR}_{\text{RRT}} \) is the conditional value at risk (CVaR) of the standard quality violation at a confidence level of 0.05 (g m⁻³), determined based on the pollution scenarios’ calculated frequency-magnitude violations of water quality standards [Eqs. (S12) and (S13), Section S.3, Supplementary Material]. The frequency-magnitude violations were obtained by combining the relative frequency (i.e., the number of standard violations to the total simulation period) and magnitude (i.e., the magnitude of standard violations to the total MTBE intrusion mass) violations with different weights [Eqs (S14) to (S18), Section S.3, Supplementary Material].

3. To ensure that hydropower generation can proceed at maximum capacity as soon as possible, the risk of modified RRT (Z₃) was minimized:

   \[ Z₃ = \text{Minimize}(\text{CVaR}_{\text{RRT}^M}) \]  

   where, \( \text{CVaR}_{\text{RRT}^M} \) is the CVaR of modified RRT at a confidence level of 0.05, calculated as a function of the losses of modified RRT across the pollution scenarios. The losses of modified RRT were determined by assessing the maximum RRT of each outlet, and the difference in total MTBE intrusion and discharged mass, for all the pollution scenarios [Eq. (S20) to (S25), Section S.3, Supplementary Material].

Considering MTBE’s high capacity to volatilize from the water surface face, it can be instructive to explain the importance of including an objective function based on quality restrictions (i.e., Z₂) within the framework of this study. Although by nature MTBE will volatilize from the water surface, its low Henry’s Law constant and high aqueous solubility would lead it to more readily dissolve in water than volatilize. When released in rivers and streams, this property increases its persistence and mobility in the environment, such that its half-life in rivers and streams can exceed one day (Squillace et al., 1996). For instance, following the introduction of MTBE into Massachusetts’ Merrimack River (January 28, 2000), elevated levels of MTBE were detected in the river water for several days (US EPA, 2008). Hence, for a river-reservoir system where a pollutant has been spilled into an upstream reservoir, introducing an objective function based on quality restrictions is essential to ensure the attainment and maintenance of downstream water quality standards.

### 2.5. Compromise operational rule

The GMCR theory is typically modeled with GMCR-II and GMCR + decision support systems. Hipel et al. (1997) first explored a strategic groundwater contamination conflict using GMCR-II. Since then, many studies have employed these decision support systems and highlighted their capacity to aid in the investigation of the often challenging disputes over water resource allocation (e.g., Kassab et al., 2006; Kilgour and Hipel, 2005; Kinsara et al., 2015; Liu et al., 2017). The GMCR +
Fig. 4. Location of the Narmab dam reservoir within Golestan Province, Iran.

Fig. 5. The (a) longitudinal profile and (b) plan view of the 16 segments of the Narmab dam reservoir representing the MTBE concentration on the 278th Julian-day (fall season), two days after the intrusion of 300 m$^3$ pollutant from segment #9. The double arrow represents the pollutant intrusion location.
A decision support system was employed in the present study to determine a compromise operational rule among optimal rules. Local/governmental stakeholders were considered decision-makers, and their options, based on their priorities and goals, were identified as a conflict model. The feasibility, reversibility, and prioritization of options were then specified to analyze the model. Finally, the stability of the desired resolution was examined based on general metarationality (GMR), Nash stability (Nash), symmetric metarationality (SMR), and sequential stability (SEQ) solution concepts (Nash, 1951; Howard, 1971; Takahashi et al., 1984; Kinsara, 2018).

3. Case study

The efficiency of the developed model was tested against data from the Narmab dam in Golestan province, Iran. Constructed to meet the growing agricultural and domestic water demands of the cities of Minoo Dasht, Azad Shahr, and Gonbad Kavoos, the Narmab dam supplies water to a cultivated area of 190 km\(^2\), as well as generating hydroelectric power. At an average level, the Narmab dam reservoir holds 115.43 \times 10^6 m^3 of water (Sedghamiz et al., 2018) (Fig. 4).

The CE-QUAL-W2 simulation model of the Narmab dam reservoir considered 23 layers and 16 segments in simulating the fate and transport of MTBE within the dam reservoir (Fig. 5). The simulation model was calibrated using the data mentioned in Section 2.2, collected over a full year (2012) by the Golestan Province Regional Water Agency. Seasonal thermal conditions and other climatic parameters were taken from established values for different climate periods in the study area.

Addressing a multi-dimensional issue with several objectives, the present study developed compromise operational rules for the Narmab dam, minimizing unsatisfied water demand, violations of water quality standards, and modified RRT for its reservoir under sudden pollution intrusion, thereby meeting the respective and sometimes-competing priorities of the Ministries of Agriculture, Environment, and Energy regarding the quantity and quality of water released. In one such scenario, the Ministry of Agriculture wished to see agricultural water demands met all year long under any circumstance. In contrast, the Department of the Environment insisted on minimizing environmental pollution, preferring the time-consuming process of within-reservoir pollution control rather than the release of polluted water. Beyond these water quality-magnitude conflicts, the Ministry of Energy, which operates the hydroelectric power plant, preferred the shortest possible reservoir recovery to generate electricity, with the dam at full capacity as often as possible. This conflict was further explored using the developed GMCR.

4. Results and discussion

The proposed simulation–optimization model determined optimal operational rules by assessing different values of daily releases from reservoir outlets for 36 different pollution scenarios (as illustrated in Fig. 2). Including uncertainties, the model minimized the risk of modified RRT and frequency-magnitude violations of water quality standards after the sudden intrusion of MTBE by coupling the optimization model with the validated PCA-MLP surrogate model. Fig. 6 shows the 12 Pareto-front solutions produced by NSGA-II for a population size of 1,520 after reaching the specified maximum number (200) of generations.

Values of RRT ranged between 0.6 and 0.9 (Fig. 6), where 0 \leq RRT \leq 1.0, and RRT = 0 and RRT = 1.0, respectively, represent a lack of MTBE contamination in water discharged from reservoir outlets and no reservoir recovery after 70 days of imposed reservoir recovery operational rules. The same ranges were followed for the risk of frequency-magnitude violations of water quality standards.

Setting out compromise reservoir operational rules based solely on the Pareto-front solutions was a challenging issue given the conflict between the Ministries of Agriculture, Energy, and Environment regarding two aspects of RRT and the quantity of water discharged from reservoir outlets (Fig. 6). The decision variables corresponding to the Pareto-front solutions served to determine three affecting parameters.
from each decision-maker’s point of view, taking advantage of the post-processing capability provided in the optimization model. One of the affecting parameters was labeled “modified RRT,” which imposed the Ministry of Energy functions’ direct effect. The “released MTBE” and “satisfied water demand,” of major concern for the Ministries of Environment and Agriculture, respectively, were also introduced as affecting parameters.

The cumulative values of the decision variables (daily operational rules) over 70 days of the simulation are shown in Fig. 7. The RRT risk values for the Pareto-front solutions revealed that the determined operational rules were all capable of completely removing the MTBE pollution in less than 70 days. Consequently, the wide range of cumulative water release values under the operational rules indicated that water releases were not the only factor in MTBE pollution elimination, but that, considering the volatility of MTBE, thermal conditions might also exert potential effects. Thermal conditions, wind speed, and reservoir surface vary seasonally; accordingly, any operational rules determined through this process would only be reliable when seasonal performances are assessed. Furthermore, the time to reach the peak pollutant concentration at reservoir outlets, the maximum pollutant concentration, and the RRT values of each operational rule might be affected by the reservoir configuration’s role in the elimination of pollution, which would be significantly different given different pollutant intrusion locations (Vanda et al., 2021).

Optimal reservoir operational rules were divided into three categories: “Evaporation-based Rule,” “Evapo-release-based Rule,” and “Release-based Rule” for low, medium, and high releases, respectively (Fig. 7). The release-based rule attempted to control MTBE pollution by massive flow releases; this might pose serious hazards to the environment. In contrast, the evaporation-based rule required closing the reservoir outlets and employing the reservoir’s capacity to control the MTBE pollution through MTBE volatilization. The RRT values of each
category, as average values of all solutions in the category\(^1\), are shown in Fig. 8.

The fate of MTBE after spilling into surface water strongly depends on specific site characteristics that control chemical processes as well as physical and biological ones. In terms of the duration of pollutant presence and its maximum concentration, intrusion during the warmer season was expected to be less hazardous than in other seasons, regardless of the reservoir operational rules (Shokri et al., 2014; Stocking and Kavanaugh, 2000). Indeed, in the present case, the RRT was significantly shorter during the warmer seasons (spring and summer) than in the fall or winter (Fig. 8). Moreover, in spring and summer, the RRTs of evaporation-based and evapo-release-based rules were substantially shorter (usually zero) than those of the release-based rule. In contrast, the relative duration of RRTs was distinctly longer in the colder seasons. At first glance, these results may seem surprising as release-based rules would apparently benefit from both volatilization and contaminated water release; however, the high longitudinal transfer rate and vertical mixing of the water body under release-based rules transferred MTBE to the underlying reservoir layers, which significantly reduced the possibility of MTBE removal by volatilization and resulted in a rational increase of RRT in warm seasons.

Seasonal variations in RRT (Fig. 8) show quantity and intrusion location of MTBE in warm seasons to have a negligible effect on RRT values in the case of evaporation-based and evapo-release-based rules, whereas their effect was quite apparent for release-based rules. The relation between the RRT values and MTBE intrusion location and quantity became more highly significant in the colder seasons for all specified operation rules. Analogously, analysis of the released MTBE (Fig. 9a) shows that in fall and winter, considering both the lower air temperatures and the characteristics of release-based rules, the possibility of removing pollution by volatilization was reduced, and a majority of the injected MTBE reached the reservoir outlets. Moreover, as the MTBE intrusion location approached the reservoir outlets, the reservoir’s role in removing MTBE was diminished, thereby increasing the amount of discharged pollution. Hence, the level of impact of MTBE quantity and intrusion location on the effectiveness of operation rules is highly dependent on pollution season (thermal conditions) and the operation rule selected.

Considering RRT values, evaporation-based rules were satisfactory in specified operation rules. Analogously, analysis of the released MTBE (Fig. 9a) shows that in fall and winter, considering both the lower air temperatures and the characteristics of release-based rules, the possibility of removing pollution by volatilization was reduced, and a majority of the injected MTBE reached the reservoir outlets. Moreover, as the MTBE intrusion location approached the reservoir outlets, the reservoir’s role in removing MTBE was diminished, thereby increasing the amount of discharged pollution. Hence, the level of impact of MTBE quantity and intrusion location on the effectiveness of operation rules is highly dependent on pollution season (thermal conditions) and the operation rule selected.

### Table 1: Options for the conflicts between the Ministries of the Environment, Agriculture, and Energy over reservoir pollution control.

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<tr>
<td>Energy</td>
<td>Reach a minimum RRT with no reduction in power generation (RRT up to 1 week) (Non-stop)</td>
</tr>
<tr>
<td></td>
<td>Stop power generation (RRT of 40 to 70 days) (Shutdown)</td>
</tr>
<tr>
<td>Environment</td>
<td>Insist on pollution control inside the reservoir with no release (No-release)</td>
</tr>
<tr>
<td></td>
<td>Limit the amount of released MTBE to a maximum of (3 \times 10^5) g (Restricted release)</td>
</tr>
<tr>
<td></td>
<td>Limit the amount of released MTBE to a maximum of (1.5 \times 10^7) g (Controlled release)</td>
</tr>
<tr>
<td></td>
<td>Warn the water consumers about the water pollution (the released MTBE exceeds (1.5 \times 10^7) g) (Warn-only)</td>
</tr>
<tr>
<td>Agriculture</td>
<td>Meet all water demand (more than 80%) (Fully-satisfied)</td>
</tr>
<tr>
<td></td>
<td>Meet more than 45% of the water demand (Partially-satisfied)</td>
</tr>
<tr>
<td></td>
<td>Meet the water demand up to 45% (Poorly-satisfied)</td>
</tr>
<tr>
<td></td>
<td>Meet less than 25% of the agricultural water demand (Not-satisfied)</td>
</tr>
</tbody>
</table>

\(^1\) As an example, the RRT of the evaporation-based rule was equal to the average of RRT values related to the Pareto-front solutions number 7 and 9 to 12.
...objections against their selection for such an application. Meeting water demands, especially in hot seasons, which may raise ministry conflict over reservoir pollution control.

...were modeled. Table 1 shows the viable options for the multi-ministry conflict between the ministries using the GMCR decision support system. First, the decision-makers’ options and preferences were modeled. Table 1 shows the viable options for the multi-ministry conflict over reservoir pollution control.

...the goals of the Energy and Agriculture ministries is an arguable point with regard to the release of polluted water from reservoir outlets. Despite such overlaps, the inherent conflicts of existing goals and desires needed to be investigated, especially when the purpose was to obtain a compatible solution through game-theory-based GMCR modelling. The combination of these two goals as a single objective may accordingly disturb the developed model’s robustness and eliminate the bargaining possibility between the authorities selected. This is clearly illustrated in Fig. 10, where considering solution #3 during the warmer seasons (spring and summer), would fully satisfy the Ministry of Energy’s desires, while the Ministry of Agriculture would find the conditions less desirable, but acceptable.

Based on seasonal compromise solutions for the spring (Fig. 11), the Ministry of Energy could choose between the “Non-stop” and “Stand-by” options; the Ministry of Environment could select between “Non-release” and “Restricted release,” while the Ministry of Agriculture could choose from “Partially-satisfied,” “Poorly-satisfied,” or “Not-satisfied” options. To facilitate conflict resolution, solution 3, corresponding to stable state 7, was adopted (Table 2 and Fig. 10). The same pattern was followed in...
other seasons, with solution 3 adopted in summer and solution 12 in fall and winter. It is noteworthy that in fall and winter, the Ministry of Energy had no choice but to shut down the power generators in agreement with states 2, 4, and 6. Hence, in these seasons, state 1 was the stable state considering the GMCR unilateral moves (Fig. S3, Supplementary Material, Section S.5).

The RRT, released MTBE, and satisfied water demand of solution 3 (release-based rule) and solution 12 (evaporation-based rule) under different pollution scenarios (Fig. 12) showed that solution 12 could control the MTBE pollution in a shorter time (Fig. 12a) with less environmentally destructive effects (Fig. 12b) than solution 3. However, the satisfied water demand of 22.5% vs. 46.0% (spring) and 23.2% vs. 46.8% (summer) (Fig. 12c), for solutions 12 and 3, respectively, finally led to an agreement on solution 3.

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**Fig. 10.** Sorting and categorizing the values of affecting parameters by the available options. Note: the outcomes are sorted top-to-bottom for each season according to the available options; the seasonal ideal scenario is provided in Fig. 11.
Fortunately, higher temperatures in warmer seasons accelerated the process of pollution control inside the reservoir, and the amount of released polluted water in both solutions remained within an acceptable range (Fig. 12b). In fall and winter, the results given by solutions 3 and 12 were similar. Solution 12 remained more environmentally friendly in these seasons, but required a longer RRT and provided less water demand satisfaction than solution 3, which made a choice difficult. With the developed GMCR model (Fig. 11), the decision-makers chose solution 12, considering the slight differences in RRT and acceptable values of unsatisfied water demand for both solutions. It was apparent that the compromise operational rules developed in this study were in direct contradiction with those chosen by strictly comparing RRT values. This contrast indicated the importance of including regional conditions in determining reliable reservoir operational rules after sudden reservoir pollution.

The MTBE concentrations at the reservoir outlets for solutions 3 and 12 for different pollution scenarios (Fig. 13 and Fig. S4, respectively) show that the maximum daily MTBE release from the reservoir outlets in the cold seasons (fall and winter) was considerably greater than in the spring and summer (Fig. 13). Moreover, the time required for the daily released MTBE to reach its maximum was much shorter in the cold seasons, confirming the direct effect and importance of reservoir thermal conditions in controlling the amount of MTBE released downstream.

5. 1. Analysis of solution reliability

As inadequate calibration of the developed CE-QUAL-W2 model and implementation of the surrogate model can lead to errors in the optimization process, one must evaluate the reliability of the operational rules obtained. A post-audit concept was employed in this study to investigate the robustness of the CE-QUAL-W2 and PCA-MLP models employed to estimate the reservoir responses under different pollutant intrusion scenarios. The post-audit concept requires the introduction of meaningful changes to the model to see whether expected shifts occur in the results considering the model’s expected behavior. As a reasonable straightforward test, post-audit evaluates the simulation model’s capacities by assessing the occurrence of anticipated changes (Wells, 2019). Variations in RRT, released MTBE, and satisfied water demand values for three operational rule categories and for 36 pollution scenarios were investigated (Figs. 8 and 9). The different operational policies, i.e., “Evaporation-based Rule,” “Evapo-release-based Rule,” and “Release-based Rule” led to responses from the reservoir that were acceptable based on the existing understanding of the processes.
modeled, as well as knowledge of the system being simulated. Accordingly, based on the post-audit, errors due to the calibration and implementation of a surrogate were deemed negligible.

6. Summary and conclusions

As large dam reservoirs are often exposed to intentional or accidental pollution, an appropriate operational response when sudden reservoir pollution occurs is key to avoiding harmful health effects. The model developed in this study imposed optimal operational rules by simultaneously minimizing the unsatisfied water demand, the risk of frequency-magnitude violations of water quality standards, and the risk of modified reservoir recovery time (RRT). It considered 36 different pollution scenarios (a combination of location, quantity, and time of pollution intrusion). The gasoline additive MTBE was considered as the injected pollutant. A direct effect of thermal conditions on the relative performance of different operational rules used to control MTBE pollution was noted. The evaporation-based rules performed satisfactorily in spring and summer due to the higher temperatures, whereas release-based rules provided a superior alternative in the colder seasons. Accordingly, reliable operational rules can only be determined when the pollution intrusion time uncertainties are included.

Similarly, the significant difference between the objective values related to the pollution scenarios in each season indicated that the uncertainties related to the location and quantity of MTBE input should also be taken into account to reduce the risk of operational rules’ inadequacy in the worst possible pollution cases. Due to the optimization model’s conflicting objectives, a compromise solution was chosen through a GMCR model. The compromise solutions were actually in direct contrast with the preliminary judgments, with a release-based rule selected for warmer seasons. At the same time, the decision-makers agreed on an evaporation-based rule for fall and winter. The significant impact of environmental conditions, priorities of the decision-makers, and local rules on selecting appropriate operational rules indicate the importance of implementing conflict-resolution models in managing water allocation from reservoirs. In ongoing work, the proposed framework is being combined with a pollutant detection framework, such as that introduced by Pourshahabi et al. (2018), to examine the possibility of real-time reservoir operation under accidental pollution.

CRediT authorship contribution statement

Sadegh Vanda: Investigation, Methodology, Software, Formal analysis, Visualization, Validation, Writing – review & editing. Mohammad Reza Nikoo: Supervision, Conceptualization, Resources, Methodology, Software, Validation, Writing – review & editing. Parnian Hashempour Bakhtiari: Writing – original draft, Writing – review
Fig. 13. MTBE concentrations at the reservoir outlets for solution 3 for different pollution scenarios.


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