



# Optimal design of groundwater remediation system using a probabilistic multi-objective fast harmony search algorithm under uncertainty



Qiankun Luo<sup>a</sup>, Jianfeng Wu<sup>b,\*</sup>, Yun Yang<sup>b,c</sup>, Jiazhong Qian<sup>a</sup>, Jichun Wu<sup>b</sup>

<sup>a</sup> School of Resources and Environmental Engineering, Hefei University of Technology, Hefei 230009, China

<sup>b</sup> Key Laboratory of Surficial Geochemistry, Ministry of Education, Department of Hydrosocieties, School of Earth Sciences and Engineering, Nanjing University, Nanjing 210023, China

<sup>c</sup> Huai River Water Resources Commission, Bengbu 233001, China

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## SUMMARY

This study develops a new probabilistic multi-objective fast harmony search algorithm (PMOFHS) for optimal design of groundwater remediation systems under uncertainty associated with the hydraulic conductivity ( $K$ ) of aquifers. The PMOFHS integrates the previously developed deterministic multi-objective optimization method, namely multi-objective fast harmony search algorithm (MOFHS) with a probabilistic sorting technique to search for Pareto-optimal solutions to multi-objective optimization problems in a noisy hydrogeological environment arising from insufficient  $K$  data. The PMOFHS is then coupled with the commonly used flow and transport codes, MODFLOW and MT3DMS, to identify the optimal design of groundwater remediation systems for a two-dimensional hypothetical test problem and a three-dimensional Indiana field application involving two objectives: (i) minimization of the total remediation cost through the engineering planning horizon, and (ii) minimization of the mass remaining in the aquifer at the end of the operational period, whereby the pump-and-treat (PAT) technology is used to clean up contaminated groundwater. Also, Monte Carlo (MC) analysis is employed to evaluate the effectiveness of the proposed methodology. Comprehensive analysis indicates that the proposed PMOFHS can find Pareto-optimal solutions with low variability and high reliability and is a potentially effective tool for optimizing multi-objective groundwater remediation problems under uncertainty.

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## 1. Introduction

Groundwater contamination, as one of the most important health-related environmental problems, has attracted more and more attention around the world. The NRC report (2012) pointed out that at least 126,000 contaminated sites required continued management throughout the United States, and the cost to cleanup these sites was estimated to exceed \$110–\$127 billion. Ehlers and Kavanaugh (2013) emphasized that both the number of contaminated sites and the remediation costs were underestimated in the NRC report (2012). Generally, groundwater remediation needs to undergo a relatively long time horizon of up to several decades due to inherent spatial variability of aquifer properties such as hydraulic conductivity and the uncertain fate of chemicals in the subsurface. Therefore, groundwater remediation has become one of the major technical and environmental challenges in the field of water resources.

Over the past three decades, the coupled simulation–optimization (S/O) models were often used for optimal design of groundwater remediation systems and have been successfully applied to a variety of groundwater management problems (Minsker and Shoemaker, 1998; Zheng and Wang, 1999a; Mayer et al., 2002; Cai et al., 2003; Wu et al., 2005, 2006; Kollat and Reed, 2006; Singh and Minsker, 2008; Singh and Chakrabarty, 2010; Chadalavada et al., 2011; Luo et al., 2012). However, there always exists a certain degree of uncertainty relating to aquifer simulation models. The uncertainty of an aquifer simulation model will inevitably lead to the uncertainty of the corresponding optimization model constrained by the simulation model. One of the most important parameters contributing to uncertainty is the hydraulic conductivity ( $K$ ). Especially the transport fate of contaminants in groundwater is mainly dominated by the spatial variation of  $K$  (Wu et al., 2006; Singh and Minsker, 2008; Singh and Chakrabarty, 2010). Thus, the optimal design of a groundwater remediation system has to be made under consideration of uncertainties in the aquifer simulation model, while maintaining its reliability and accuracy at a certain level of confidence.

\* Corresponding author.

E-mail addresses: [jfwu@nju.edu.cn](mailto:jfwu@nju.edu.cn), [jfwu.nju@gmail.com](mailto:jfwu.nju@gmail.com) (J. Wu).

The pump-and-treat (PAT) technology is a most commonly used groundwater remediation method in which the contaminated groundwater pumped from a number of wells at various locations is treated and then will either be reinjected into the aquifer or be used for agriculture, forestry and others (Mantoglou and Kourakos, 2007; Singh and Chakrabarty, 2010; Luo et al., 2012). Unfortunately, the ESTCP project found that the PAT method could only efficiently accomplish remediation to a certain level and, at the end of the PAT system it required inordinately large cost to clean up small amounts of residual contaminants in the aquifers (Minsker et al., 2003). From a practical perspective, such residual contamination should best be cleaned up using cheaper and more efficient remediation technologies (Singh and Minsker, 2008). Thus, it would be of value to decision makers to find the best compromise between the predicted cost and cleanup level for different PAT strategies (Erickson et al., 2002; Mantoglou and Kourakos, 2007; Singh and Minsker, 2008; Singh and Chakrabarty, 2010; Luo et al., 2012).

For real-world groundwater remediation problems, decision makers often need to simultaneously consider some competing objectives such as cleanup time, remediation cost, health risks and contaminant mass remaining in the aquifers. These multiple competing objectives will lead to a series of compromised solutions, known as non-dominated solutions or Pareto-optimal solutions, *i.e.*, solutions such that one objective cannot be improved without worsening at least one other objective (Deb, 2001; Deb et al., 2002). In traditional studies, it usually dealt with the multi-objective optimal design of groundwater remediation systems as a single-objective optimization problem by integrating all the objectives into a weighted sum, or optimizing only one objective while the rest constrained. However, these approach that based on reformulating the multi-objective problem as a single-objective problem only identify one combination of the objectives and thus needs to be run multiple times to identify the entire trade-off curve (Singh and Minsker, 2008). Recently, multi-objective evolutionary algorithms (MOEAs) have been used to solve groundwater remediation problems frequently because of their ability to obtain a set of Pareto optimal solutions with different target units of measurement in a single optimization run. The MOEAs use the speciation along with the theory of a spatially ordered search space (Goldberg, 1989) to search for the tradeoff curve (Pareto-optimal solutions) of multi-objective optimization problems. For instance, Reed et al. (2001) presented a nondominated sorted genetic algorithm (NSGA) to successfully find the Pareto optimal solutions to an existing groundwater monitoring network problem. Erickson et al. (2002) used a niched Pareto genetic algorithm (NPGA) to solve the multi-objective optimal design of groundwater remediation problem outperforming both the single genetic algorithm (SGA) and the random search (RS). Singh and Minsker (2008) developed a probabilistic multi-objective genetic algorithm (PMOGA) and applied it to a field-scale groundwater remediation problem at the Umatilla Chemical Depot site at Hermiston (Oregon, USA) under uncertainty. More recently, Singh and Chakrabarty (2010) coupled the non-dominated sorting genetic algorithm II (NSGAI) coded in C with FORTRAN programs (MODFLOW and MT3DMS) and used this methodology to successfully obtain a tradeoff between remediation cost and clean water extraction rate. Luo et al. (2012) developed a multi-objective fast harmony search algorithm (MOPHS) to search for optimal design of PAT systems, aiming at minimization of the remediation cost and the mass remaining in aquifers under general hydrogeological (deterministic) conditions.

However, most of the previous works in the field of multi-objective optimization of groundwater remediation systems were taken under general hydrogeological conditions. In this study, we develop a new probabilistic multi-objective fast harmony search

algorithm (PMOFHS) to search for Pareto-optimal solutions under considering uncertainty of both the simulation model and the optimization model caused by the uncertain  $K$ -field. The proposed PMOFHS is then coupled with the commonly used flow and transport codes, MODFLOW (Harbaugh and McDonald, 1996) and MT3DMS (Zheng and Wang, 1999b), under the framework of S/O model to find optimal design of groundwater remediation systems considering uncertainty for a two-dimensional hypothetical test problem and a three-dimensional field problem in Indiana (USA).

## 2. Methodology

In this study, the multi-objective S/O model for groundwater remediation system includes two main parts: a flow and transport simulation model and an evolutionary algorithm based optimization model for multi-objective optimal design of groundwater remediation systems under uncertainty of  $K$ -field distribution.

### 2.1. Flow and transport simulation model

A flow model based on the three-dimensional finite-difference groundwater flow simulator MODFLOW and a simulation model based on the three-dimensional contaminant fate and transport simulator MT3DMS were used in this study (Harbaugh and McDonald, 1996; Zheng and Wang, 1999b). Furthermore, under the S/O framework, the main program of the particular version of MODFLOW and MT3DMS were modified into modular subroutines so that they can be repeatedly called by the optimization program.

### 2.2. PMOFHS-based multi-objective optimization model of groundwater remediation system

#### 2.2.1. Multi-objective optimization model of groundwater remediation system

In this study, the purpose of groundwater remediation is to minimize the remediation cost and contaminant mass remaining in aquifer at the end of the remediation horizon, while satisfying some specific constraints and reliability requirements under uncertainty. Thus, there are two objectives to be minimized: (i) the remediation cost through the remediation horizon including capital cost associated with well installation, fixed cost associated with well drilling, operation cost associated with pumping and treatment over the full duration of the project, and (ii) the contaminant mass remaining in the aquifer measured by the percentage of mass remaining in the aquifer at the end of the remediation horizon.

The objectives can be mathematically expressed as follows (Zheng and Wang, 2003; Luo et al., 2012):

$$\text{Minimize } F_1 = \beta_1 \sum_{i=1}^{N_w} w_i + \beta_2 \sum_{i=1}^{N_w} w_i d_i + \beta_3 \sum_{i=1}^{N_w} \sum_{t=1}^{N_t} w_i |Q_i^t| (Z_i^{gro} - h_i^t) \Delta t_t + \beta_4 \sum_{i=1}^{N_w} \sum_{t=1}^{N_t} w_i M_i^t \quad (1)$$

$$\text{Minimize } F_2 = (\text{mass}_{\text{end}} / \text{mass}_0) \times 100\% \quad (2)$$

where  $F_1$  is the total remediation cost through the entire remediation horizon,  $N_w$  is the number of potential pumping wells to be optimized,  $w_i$  is a binary variable indicating whether well  $i$  is drilled (if  $w_i = 1$ , yes; if  $w_i = 0$ , no),  $d_i$  is the depth of well bore associated with well  $i$ ,  $Q_i^t$  is the pumping rate associated with well  $i$  during the  $t$ th management period,  $Z_i^{gro} - h_i^t$  is the pumping lift of well  $i$  during the  $t$ th management period,  $N_t$  is the total number of management periods,  $\Delta t_t$  is the duration of the  $t$ th management period,  $M_i^t$  is the amount of solute mass removed by well  $i$  during the  $t$ th

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