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Research Article

A Fuzzy Simulation-Based Optimization Approach for Groundwater Remediation Design at Contaminated Aquifers

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A fuzzy simulation-based optimization approach (FSOA) is developed for identifying optimal design of a benzene-contaminated groundwater remediation system under uncertainty. FSOA integrates remediation processes (i.e., biodegradation and pump-and-treat), fuzzy simulation, and fuzzy-mean-value-based optimization technique into a general management framework. This approach offers the advantages of (1) considering an integrated remediation alternative, (2) handling simulation and optimization problems under uncertainty, and (3) providing a direct linkage between remediation strategies and remediation performance through proxy models. The results demonstrate that optimal remediation alternatives can be obtained to mitigate benzene concentration to satisfy environmental standards with a minimum system cost.

1. Introduction

Contaminated groundwater due to the spill and leakage of petroleum hydrocarbons may pose significant threats to local environment and human health. This provides an adequate reason for a great effort to remediate such contamination. Previously, many remediation methods (i.e., pump and treat, bioremediation, surfactant-enhanced aquifer remediation, etc.) were applied to mitigate groundwater contamination. However, many process variables in a groundwater remediation system, such as well location, pumping rate, oxygen-addition rate, and additive-addition rate, have significant impacts on the performance of remediation systems. The deficiency in understanding processes controlling the fate of contaminants may lead to a large inflation of expenses [1]. Simulation and optimization models were therefore developed in order to improve remediation efficiency [2].

Previously, many simulation and optimization methods were undertaken to identify effective groundwater remediation strategies [3–5]. Ahmad et al. [6] applied a response surface approach to a palm oil mill effluent treatment system for mitigating membrane fouling problems. Huang et al. [7] proposed an integrated numerical and physical modeling system to tackle natural attenuation and biodegradation processes for site remediation. He et al. [8] provided a coupled simulation-optimization approach for optimal design pumping rates of a pump-and-treat (PAT) system. However, most of previous simulation and optimization methods tended to focus on one fixed remediation technique, leading to relatively low efficiencies or high costs. For example, bioremediation via anaerobic dechlorination would not be an instantaneous process, which required time to develop the appropriate environmental conditions and to grow a microbial population (i.e., the capable degradation time may be several months to years) [9]; PAT might require significant costs for continuous pumping and extraction, as well as system maintenance; in detail, the operation cost of PAT would be 3 times higher than bioremediation [10]. Therefore, it is essential to develop simulation and optimization system for integrated remediation alternatives to enhance the remediation efficiency and reduce system cost.

Due to the difficulties in incorporating the complicated numerical simulation model within an optimization framework [11], a series of effective surrogates were applied to replace complex simulation equations [12–14]. Moreover, uncertainties may extensively exist in process forecasting (i.e., measurement and/or estimation errors related to hydrogeological and physicochemical parameters), which may significantly increase the complexity related to remediation design [15]. In the past decades, many stochastic theories were applied to optimal groundwater remediation design under uncertainty [16–19]. However, high computational cost and amounts of data requirement in stochastic analysis may constrict its application to some practical groundwater remediation problems. Consequently, fuzzy set theory has been used as an supplementary tool for many groundwater remediation optimization problems [20]. Guan and Aral [21] used fuzzy sets and optimization algorithms to optimize design of a PAT system under uncertainty. Nasiri et al. [22] developed a decision support system for the prioritization of remediation options based on the estimated compatibility index. The system combined fuzzy sets theory, environmental risk assessment with compatibility analysis procedure, which can be used to find a better remediation technology. Kerachian et al. [23] proposed a fuzzy game theoretic approach for groundwater resources management, which combined groundwater simulation models with the optimization model. Nonetheless, there are few considerations for identifying integrated groundwater remediation strategies (such as using PAT and bioremediation simultaneously) under uncertainty.

In this paper, a fuzzy simulation-based optimization approach (FSOA) is developed for identifying optimal remedial strategies for a petroleum-contaminated site. The objective entails the following tasks: (i) providing a fuzzy simulation model for biodegradation and PAT remediation processes, (ii) carrying out the model for generating a number of statistical samples, (iii) developing a fuzzy-mean-value-based optimization technique, and (iv) applying the proposed method to a petroleum-contaminated site for demonstration.

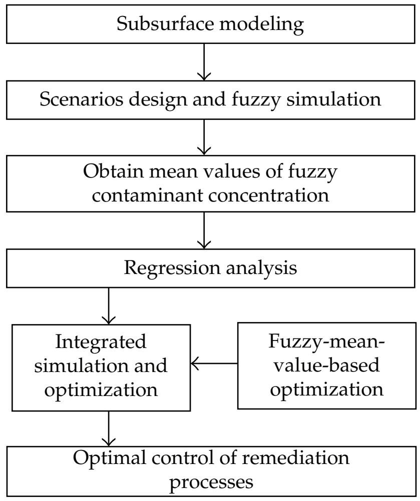

Figure 1: Integrated simulation and optimization framework for remediation-process control.

2. Methodology

FSOA consists of two major components: (2.1) fuzzy simulation and (2.2) fuzzy-mean-value-based optimization. The framework of FSOA is shown in Figure 1. The fuzzy simulation component is used to predict contaminant transport under various remediation scenarios. The obtained contaminant concentrations are presented as fuzzy sets. Then the mean values of these fuzzy contaminant concentrations are obtained and applied to establish a set of surrogates for providing a bridge between remediation strategies (pumping rates at the wells) and contaminant concentrations. Finally a nonlinear optimization method is advanced by incorporating the surrogates into an optimization framework to identify optimal remediation strategies. The detailed procedures are described in the following sections.

2.1. Stimulation Model

2.1.1. Stimulation of Contaminant Transport Process

In this study, BIOPLUME III is used to simulate organic contaminants transport processes in groundwater, which has been used in many studies [10, 24, 25]. The mass transport equations are solved to calculate the spatial variation of the contaminant concentration [26]. In biodegradation processes, the aerobic biodegradation using oxygen as electron acceptors is simulated as an instantaneous reaction. The general equations are as follows [27]:

$$\frac{\partial(bH)}{\partial t} = \frac{1}{R_h}\left[\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial H}{\partial x_j}\right) - \frac{\partial(bHV_i)}{\partial x_i}\right] - \frac{H'W}{n} - \frac{Q}{n}\delta\left(x - x^{(r)}\right)H,$$

$$\frac{\partial Pb}{\partial t} = \left[\frac{\partial}{\partial x_i}\left(bD_{ij}\frac{\partial P}{\partial x_j}\right) - \frac{\partial(bPV_i)}{\partial x_i}\right] - \frac{P'W}{n},$$

$$\Delta H_{so} = \frac{P}{F_O}, \quad P = 0 \quad \text{if } H > \frac{P}{F_O},$$
$$\Delta P_{os} = HF_O, \quad H = 0 \quad \text{if } P > HF_O,$$
$$H(x,y,t)\big|_{t=0} = H_0(x,y), \quad (x,y) \in \Omega,\ t = 0,$$
$$H(x,y,t)\big|_{t=\Gamma 1} = H_1(x,y,t), \quad (x,y) \in \Gamma_1,\ t \geq 0, \tag{2.1}$$

where P is the concentration of oxygen [M/L^3]; P' is the concentration of oxygen in source or sink fluid [M/L^3]; Q is the pumping rate [L^3/T]; $x^{(r)}$ is the coordinates of the well; $\Delta H_{\mathbf{SO}}$ is the loss of the contaminant concentration due to aerobic biodegradation; ΔP_{OS} is the concentration loss of the electron acceptor; F_O is the stoichiometric ratio for oxygen; Ω is the study domain; Γ_1 is the first boundary condition.

2.1.2. Fuzzy Simulation

In the past decades, the increasing awareness for uncertainties of porous media led to an improved understanding of contaminant transport in subsurface [14]. Fuzzy set theory is widely used for addressing uncertainties derived from vagueness in input parameters of subsurface models [28, 29]. The primary procedures of fuzzy simulation are as follows [24]: (1) discretize the range of membership grade [0, 1] into a number of α-cut levels; (2) select an alpha-cut level for fuzzy inputs and generate 2^m combinatorial arrays for the input vector through fuzzy vertex analysis, where m is the number of fuzzy parameters; (3) use the 2^m new vectors as inputs for the simulation model and generate 2^m outputs; (4) assign the smallest and largest values of outputs to the lower and upper limits, respectively; and (5) return to process 2 to assign other α-cut levels and repeat processes 3 and 4. The fuzzy sets of the predicted items are finally approximated based on the obtained lower and upper boundaries of simulation outputs under various α-cut levels.

2.2. Optimization Model

2.2.1. Fuzzy Regression Analysis

In this subsection, regression analysis is used for studying the relationships between the response (y) (i.e., contaminants concentrations) and a number of input variables (x_i) (i.e., pump and injection rates). Considering the uncertainty of the outputs from the simulation model, a fuzzy regression analysis method is proposed to build relationships between contaminants concentrations and control variables. Then these relationships are used as constraints in the optimization framework.

Fuzzy regression analysis method consists of four stages, including (i) generating solutions through fuzzy simulation model, (ii) obtaining the mean values of the outputs, based on the method proposed by Fortemps and Roubens [30], (iii) fitting the inputs and outputs through a general polynomial regression analysis, and (iv) testing the predicting performance of the surrogates. If the surrogates have satisfactory performances, they can be used for substituting the numerical simulation model in further optimization framework.

2.2.2. Fuzzy-Mean-Value-Based Optimization

In a groundwater remediation system, the installation cost can be generally neglected since it would be significantly less than well operation cost [31]. In addition, most costs for a remediation system are mainly functions of well pumping rates. Therefore, in this paper, the total pumping rate is used as decision variables of the optimization model, which will be minimized subject to environmental and economical constraints in order to obtain a minimum cost for the groundwater remediation system. The constraints of the optimization model include (i) contaminant concentrations at some locations, which should be less than or equal to a regulated environmental standard; (ii) the injection and extraction rates, which would be limited within a desired range; and (iii) water balance constraint, meaning that the sum of pumping rates at all extraction wells should be equal to the sum of injection rates at all injection wells. So, the optimization model can be formulated as follows [8]:

$$\begin{aligned}
&\text{Minimize } f = A \times \sum_{i=1}^{I} Q_i^{\text{In}} + B \times \sum_{j=1}^{J} Q_j^{\text{Ex}} \\
&\text{subject to } C_k\left(Q_i^{\text{In}}, Q_j^{\text{Ex}}\right) \le C_{\max}, \quad k = 1, 2, \ldots, K, \\
&\sum_{i=1}^{I} Q_i^{\text{In}} = \sum_{j=1}^{J} Q_j^{\text{Ex}}, \\
&0 \le Q_i^{\text{In}} \le Q_{i,\max}^{\text{In}}, \qquad i = 1, 2, \ldots, I, \\
&0 \le Q_j^{\text{Ex}} \le Q_{j,\max}^{\text{Ex}}, \qquad j = 1, 2, \ldots, J,
\end{aligned} \tag{2.2}$$

where f is the total pumping/extraction cost; A and B are the unit injection and extraction cost, respectively; Q_i^{In} and $Q_j^{\text{Ex}}$are the pumping rates for the ith injection well and jth extraction well, respectively; $Q_{i,\max}^{\text{In}}$ and $Q_{j,\max}^{\text{Ex}}$ are the maximum pumping rates for the ith injection well and jth extraction well; $C_{\max}$ is the maximum acceptable contaminant concentration; C_k is the expected contaminant concentration of kth monitoring well after remediation. C_k can be regarded as a polynomial function of injection/extraction rates $(Q1, Q2, \ldots, Qn)$. The surrogate can be formulated as follows:

$$C_k = \beta_{0,k} + \sum_{i=1}^{n} \beta_{i,k} Q_i + \sum_{i=1}^{n} \sum_{j=1}^{n} \beta_{ij,k} Q_i Q_j \quad (i \ne j), \tag{2.3}$$

where $\beta_{0,k}$ is an intercept term of surrogate k; $\sum_{i=1}^{n} \beta_{i,k} Q_i$ are linear terms of surrogate k; $\sum_{i=1}^{n} \sum_{j=1}^{n} \beta_{ij,k} Q_i Q_j$ $(i \ne j)$ are interaction terms of surrogate k; n is the number of explanatory variables.

Table 1: Parameters of the simulation model.

Input parameter	Values
Grid size	20×20
Cell size	100×100 ft
Hydraulic conductivity	6.56×10^{-4} ft/sec
Hydraulic gradient	0.005
Retardation factor	1.0
Anisotropy factor	1.0
Background concentration of oxygen	1 ppm
Storage coefficient	0.2
Longitudinal dispersivity	Support = (11, 19), Core = 15
Transverse dispersivity	Support = (1.1, 1.9), Core = 1.5
Effective porosity	Support = (0.2, 0.4), Core = 0.3

3. Case Study

3.1. Overview of the Study Site

The developed FSOA model is applied to a hypothetical petroleum-contaminated aquifer (see Figure 2). The contaminated plume is assumed to be produced by a leaking underground storage tank (UST). The aquifer system of the site is unconfined, homogeneous, and anisotropy. The stratigraphy consists of sand with the depth varied within 13 and 20 ft from the surface. The base of the aquifer ranges in elevation from about −3 to −7 ft, and the groundwater flow direction is northeastwards with a gradient of approximate 0.005. The horizontal hydraulic conductivity across the entire grid is 6.56×10^{-4} ft/sec, and the storage coefficient is about 0.2. Table 1 shows parts of parameters. The previous UST was at the up gradient location of the site where the benzene concentration (approximate 16 mg/L) in groundwater is higher than the regulated environmental guideline (0.005 mg/L) [32]. Thus, this site may pose impacts on surrounding communities and environment; remediation actions are desired for cleaning up contaminated groundwater.

The integration of PAT and biodegradation for remediating contaminated groundwater can be more efficient and cost-effective in comparison to simple PAT or biodegradation (as stated before). So, 2 injection (biodegradation), 4 (pump and treat) extraction, and 3 monitoring wells are constructed to inject nutrients for microorganism, install a PAT system, and monitor benzene concentrations, respectively. It is suggested that effective number of wells and their behaviors can improve remediation efficiency [33]. A simulation–optimization model is therefore an attractive tool for identifying optimal alternatives on these design components. However, since fuzzy uncertainty (as stated before) may exist in groundwater remediation design, fuzzy simulation-based optimization approach (FSOA) is desired for generating effective solution to address this issue.

3.2. Results Analysis

The simulation model is firstly run m times to generate m samples for further surrogates construction. In this study, 6 explanatory variables (pumping rates of the injection and extraction wells) and 3 response variables (expected contaminant concentrations at the monitoring wells M1 to M3) are interpreted by the surrogates. Within the range of pumping

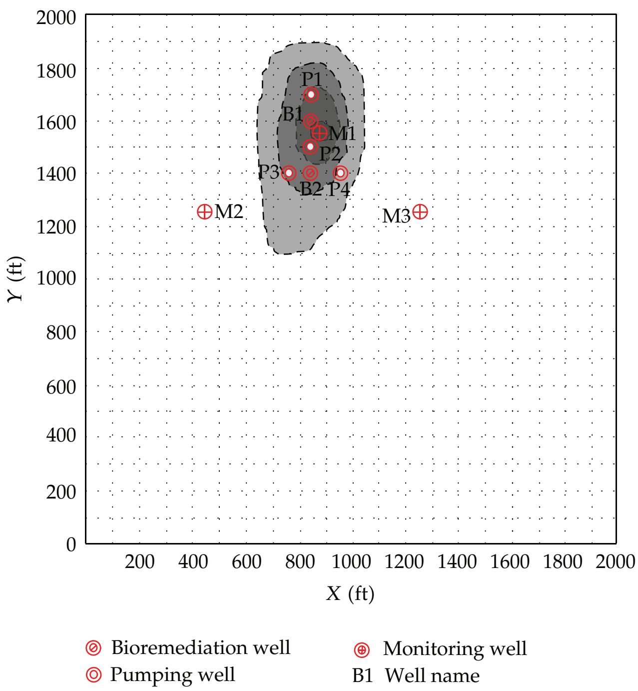

Figure 2: Simulation domain and well location.

rate between 0.0 and 0.08 ft^3/sec, 51 scenarios of operation conditions (b1, b2, p1, p2, p3, and p4) are randomly generated (as listed in Table 2). Since some parameters of the system (e.g., porosity, dispersivity) are presented as fuzzy sets, a fuzzy simulation model is applied to deal with these uncertain parameters and generate contaminant concentrations under various operation scenarios. The outputs of the fuzzy simulation model are also presented as fuzzy sets. Therefore, a fuzzy regression method is applied to establish the surrogates between contaminant concentrations and operation variables.

Biodegradation injection rates (b1 and b2) in injection wells B1 and B2 and extraction rates (p1, p2, p3, and p4) in extraction wells P1, P2, P3, and P4 are selected as control variables to produce a series of operation scenarios. The benzene concentrations in monitoring wells are simulated during a 2-year remediation period under each operation condition. Figure 3 shows the results of expected benzene concentrations of wells M1, M2, and M3. It appears that different results are generated under different scenarios. Thus, it is worthwhile to identify the interactive relations between system operation patterns and contaminant concentrations, such that the trade-off between system cost and remediation efficiency can be analyzed.

Figure 4 presents the comparison of the results from fuzzy regression analysis and the mean value of benzene concentrations from numerical simulation. It is indicated that the fuzzy regression models can generally reflect the variation of benzene concentration under different operation scenarios. The peak values in three monitoring wells can be well caught. The RSME values of three models are 0.03114, 0.102, and 0.0532, respectively. These results demonstrate that the established surrogates have satisfactory prediction accuracy.

A nonlinear optimization model is then developed to identify the optimal operating conditions. When the maximum concentration standard is set as 0.001 mg/L, the injection rates in wells b1 and b2 are 0.0 and 0.0499 ft^3/s, respectively; the extraction rates are

Table 2: Scenarios of flow rates in injection and extraction wells (ft^3/sec).

Scenario	p1	b1	p2	b2	p3	p4
1	0.01	0.020	0.01	0.02	0.01	0.010
2	0.015	0.030	0.015	0.03	0.015	0.015
3	0.012	0.025	0.014	0.025	0.008	0.016
4	0.009	0.010	0.021	0.058	0.018	0.020
5	0.013	0.037	0.006	0.01	0.02	0.008
6	0.02	0.049	0.018	0.036	0.029	0.018
7	0.03	0.052	0.025	0.04	0.025	0.012
8	0.006	0.044	0.028	0.016	0.021	0.005
9	0.025	0.032	0.008	0.033	0.006	0.026
10	0.029	0.042	0.017	0.045	0.032	0.009
11	0.005	0.029	0.009	0.028	0.012	0.031
12	0.007	0.035	0.013	0.038	0.021	0.032
13	0.018	0.002	0.012	0.048	0.009	0.011
14	0.026	0.057	0.018	0.018	0.011	0.020
15	0.016	0.040	0.026	0.022	0.013	0.007
16	0.021	0.042	0.019	0.029	0.017	0.014
17	0.014	0.026	0.011	0.012	0.005	0.008
18	0.019	0.034	0.007	0.019	0.014	0.013
19	0.022	0.038	0.02	0.024	0.016	0.004
20	0.024	0.008	0.005	0.032	0.007	0.004
21	0.005	0.038	0.033	0	0	0.000
22	0.033	0.031	0	0.021	0.019	0.000
23	0.023	0.087	0.022	0	0.023	0.019
24	0	0.008	0.016	0.06	0.035	0.017
25	0.008	0.059	0.029	0.006	0.022	0.006
26	0.004	0.003	0.021	0.08	0.03	0.028
27	0.012	0.029	0.023	0.029	0.013	0.010
28	0.02	0.041	0.016	0.031	0.021	0.015
29	0.017	0.033	0.006	0.02	0.019	0.011
30	0.008	0.026	0.011	0.025	0.011	0.021
31	0.011	0.028	0.007	0.015	0.024	0.001
32	0.016	0.055	0.021	0.032	0.038	0.012
33	0.020	0.074	0.016	0.006	0.012	0.033
34	0.029	0.072	0.028	0.060	0.036	0.039
35	0.012	0.000	0.022	0.039	0.004	0.001
36	0.004	0.024	0.007	0.022	0.003	0.033
37	0.018	0.039	0.013	0.026	0.009	0.025
38	0.019	0.023	0.005	0.061	0.037	0.022
39	0.001	0.016	0.029	0.026	0.003	0.010
40	0.027	0.076	0.011	0.005	0.011	0.033
41	0.029	0.074	0.001	0.014	0.040	0.018
42	0.011	0.072	0.023	0.003	0.008	0.033
43	0.010	0.047	0.027	0.040	0.020	0.030
44	0.028	0.056	0.009	0.009	0.012	0.016
45	0.031	0.057	0.008	0.037	0.027	0.028
46	0.022	0.038	0.028	0.078	0.038	0.028
47	0.019	0.029	0.004	0.054	0.031	0.030
48	0.036	0.080	0.028	0.026	0.027	0.016
49	0.018	0.016	0.021	0.058	0.005	0.029
50	0.032	0.033	0.025	0.043	0.004	0.015
51	0.000	0.014	0.000	0.000	0.000	0.000

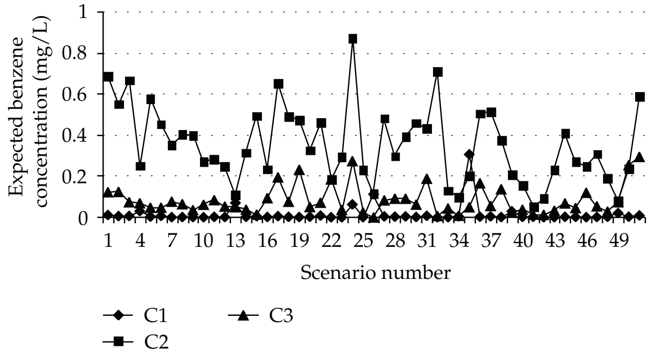

Figure 3: Expected benzene concentrations under 51 operation scenarios (on day 730).

p1 = 0.027 ft^3/s, p2 = 0.0 ft^3/s, p3 = 0.0065 ft^3/s, and p4 = 0.0164 ft^3/s. Under this standard, wells B2 and P1 would play more important role while wells P3 and P4 would have less contributions to contaminant reduction. When the maximum concentration standard is set as 0.004 mg/L, the injection rates are b1 = 0.0 ft^3/s and b2 = 0.0492 ft^3/s; the extraction rates are p1 = 0.0267 ft^3/s, p2 = 0.0 ft^3/s, p3 = 0.0072 ft^3/s, and p4 = 0.0153 ft^3/s. Comparing results between these two scenarios, the system is sensitive to variations of the maximum concentration standard. Under stricter standard, the remediation system should conduct larger pumping rates, which would enhance the remediation efficiency but accordingly cause the growth of remediation cost. Conversely, looser standard would lead to less pumping rates, which corresponds to low remediation cost and efficiency. Therefore, the developed method can help decision maker make a trade-off for the operation condition between system cost and efficiency under uncertainty.

3.3. Discussions

In this study, we consider parameters of soil porosity, longitudinal dispersivity, and transverse dispersivity as fuzzy sets due to insufficient data for specifying related probability density functions. Actually, fuzzy simulation can handle more fuzzy parameters. One should know that the uncertainty in output concentration increases as the number of uncertain parameters increases [24]. In addition to the performance of fuzzy simulation, the accuracy of optimization results also depends upon the surrogates used to represent the relationships between expected concentrations and pumping rates. A major concern is that approximation errors of surrogates may lead to large deviations of solutions. On one hand, this concern can be mitigated by using higher-order regression analysis based on large volumes of testing samples. On the other hand, the approximation accuracy may benefit from improvement of pretreatment method for uncertain outputs such as fuzzy expected value models [34, 35].

For comparison, if uncertain parameters are defuzzified to generate related representative deterministic values before conducting simulation, the procedures of defuzzified simulation-based optimization approach (DSOA) can be obtained and generalized as follows: step 1, defuzzify parameters; step 2, generate a number of remediation scenarios; step 3, compute the contaminant concentrations under the defuzzified parameters through the simulator; step 4, establish a set of surrogates for providing bridges between remediation strategies and contaminant concentrations; step 5, incorporate the surrogates into the optimization framework; and step 6, solve the optimization model.

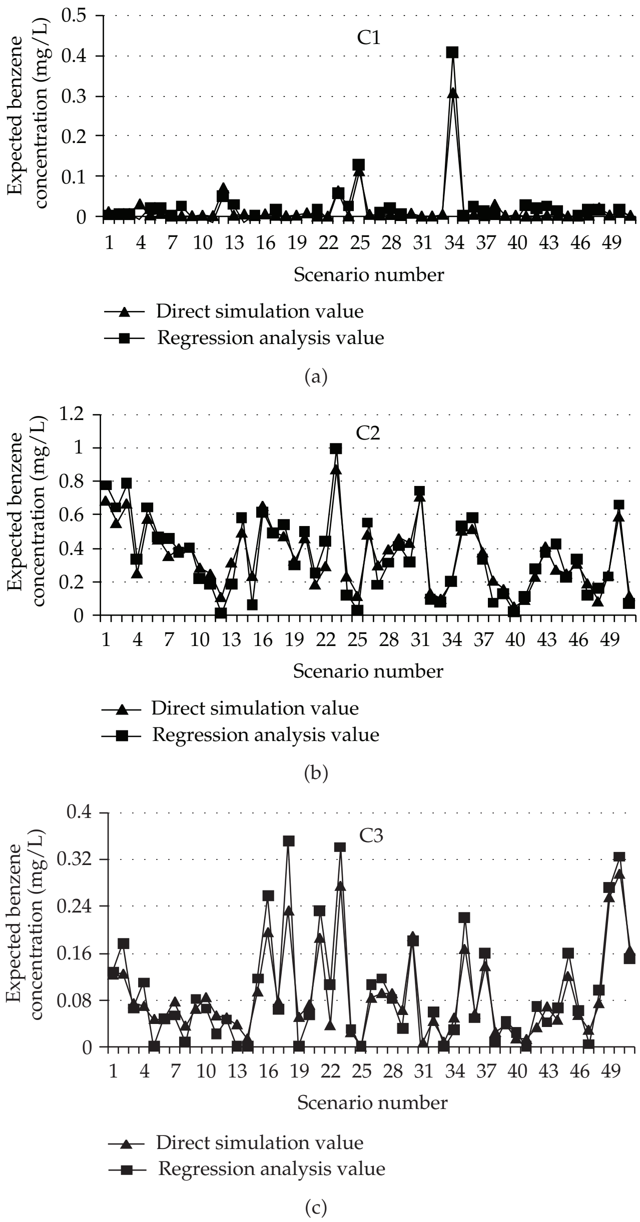

Figure 4: Regression analysis versus direct simulation in benzene concentrations.

Figure 5 presents mean values of benzene concentration obtained from FSOA versus DSOA at different monitoring wells. Both methods used triangular possibility distributions to present uncertainty. The results from DSOA and FSOA are similar with each other. However, to some extent, DSOA may take an obvious role in reduction of peak value. For example, the mean values of benzene concentrations obtained by DSOA may be 0.254, 0.456, and 0.138 mg/L at wells M1, M2, and M3, respectively (shown as red remarked). These values are lower than those obtained by FSOA (0.3072, 0.7115, 0.2329). This indicates that DSOA may

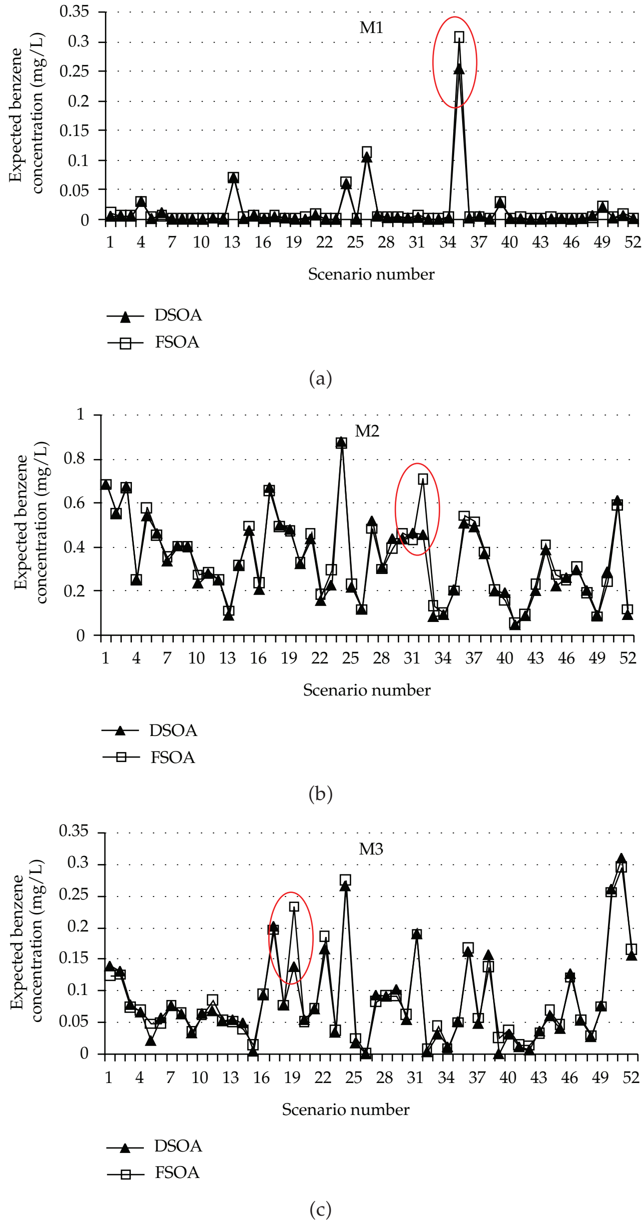

Figure 5: Simulation results by DSOA versus FSOA in benzene concentrations.

not well represent system uncertainty and may be too idealistic for the effect of remediation. In addition, defuzzification before simulation cannot well reflect the impact of uncertainty to the simulation model system.

4. Conclusion

In this paper, a fuzzy simulation-based optimization approach (FSOA) has been developed for supporting process control of remediation at petroleum-contaminated sites. FSOA integrated fuzzy simulation and fuzzy regression analysis method into a nonlinear optimization framework for generating desired operation conditions. The developed method was applied to a hypothetical petroleum-contaminated case study. FSOA can address the uncertainty of modeling parameters in simulating flow and transport of contaminants in groundwater and then generate optimal remediation strategies. The results can provide bases for guiding remediation performances. They are also useful for decision makers to analyze trade-offs between system cost and treatment efficiency.

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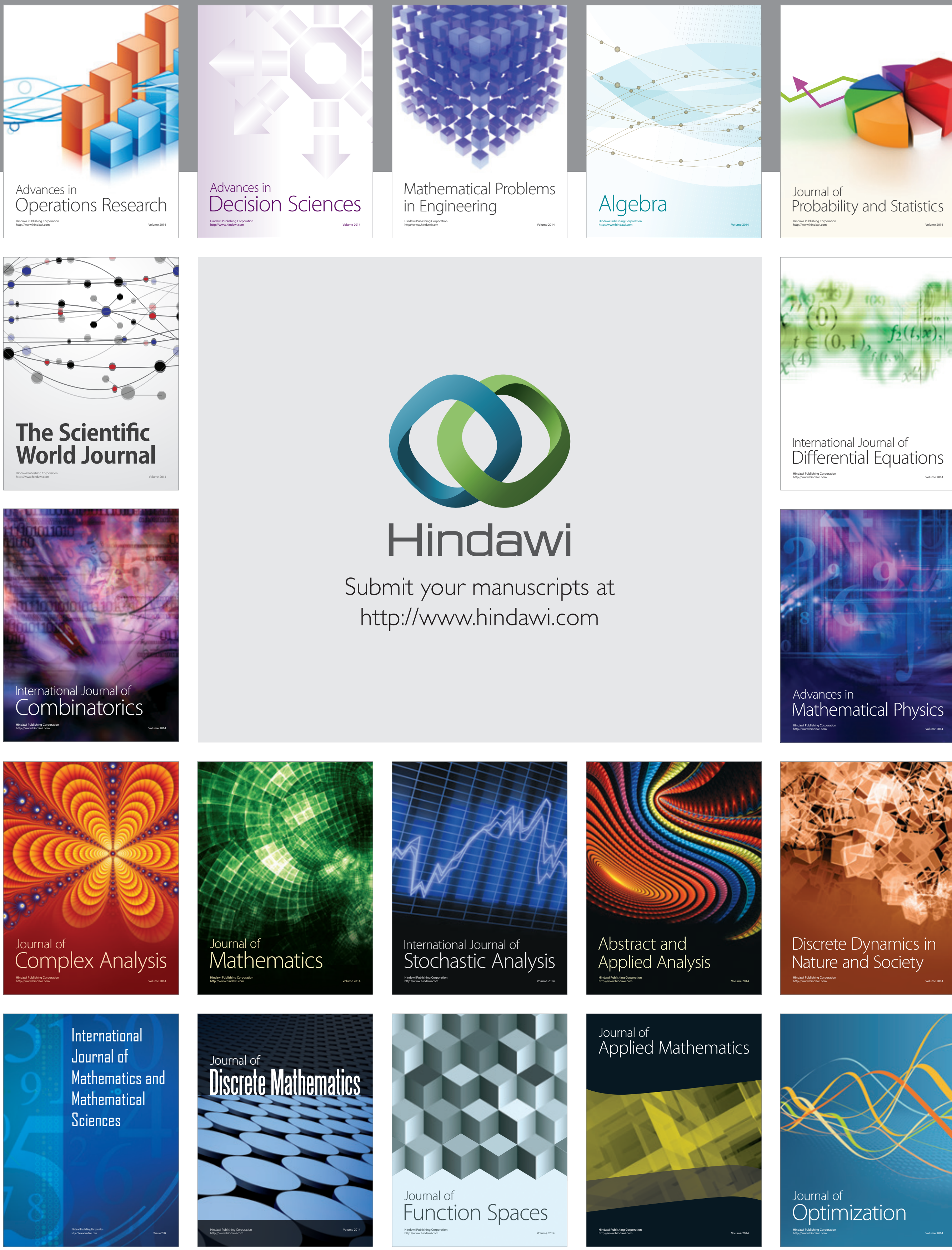
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