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Effect of Hydraulic Conductivity Uncertainty on In Situ Bioremediation of Groundwater Contaminated with Dissolved Petroleum Hydrocarbons

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Abstract: The hydraulic conductivity of soils varies over several orders of magnitude, and its measurement is affected by experimental and field conditions. This paper applies Monte Carlo simulation (MCS) to ascertain the impact of hydraulic conductivity's uncertainty on the bioremediation of groundwater contaminated with dissolved petroleum hydrocarbons. The model *BIO PLUME II* is implemented for simulating the bioremediation treatment. The effect of hydraulic conductivity uncertainty on bioremediation is assessed by means of MCS. This paper's results indicate that the uncertainty in prediction of the residual contaminant concentration produced by bioremediation is higher at the center of mass of the contaminant plume than at its periphery. The results also show that the effect of hydraulic conductivity uncertainty on residual contaminant concentration is larger at intermediate times since the start of bioremediation than at early or late times of the treatment phase. DOI: 10.1061/(ASCE)IR.1943-4774.0001252. © 2017 American Society of Civil Engineers.

Author keywords: Groundwater; Hydraulic conductivity; Uncertainty; Bioremediation; Monte Carlo simulation.

Introduction

In situ bioremediation has been shown to remove dissolved petroleum hydrocarbons such as benzene, toluene, ethyl-benzene, and xylene (BTEX) from groundwater. In situ bioremediation relies on microorganisms to transform hazardous hydrocarbons into harmless or low-risk byproducts mediated by oxygen, electron acceptors (nitrate and sulphate), nutrients, and other compounds. Minsker and Shoemaker (1998a, b) reported optimization methods for the design of in situ bioremediation. Yoon and Shoemaker (1999) compared the performance of different optimization methods for the cost-effective design of in situ bioremediation systems in contaminated groundwater. Liu and Minsker (2004) developed a full multiscale approach to optimize the constrained problem of in situ bioremediation design. Shieh and Peralta (2005) developed a simulation and optimization (S-O) model for design of an in situ bioremediation system that combined optimization algorithms and *BIO PLUME II* as the simulation model. Prasad and Mathur (2008) introduced a neural network to determine the optimal locations of monitoring wells. Mategaonkar and Eldho (2012) developed a S-O model for optimal design of a pump-and-treat (PAT) remediation system with the particle swarm optimization (PSO) algorithm. Yang et al. (2013) presented a niched Pareto tabu search (NPTS)

for designing an optimal PAT remediation system. Kazemzadeh-Parsi et al. (2014) developed a S-O model based on the firefly algorithm (FA) coupled with finite-element modeling (FEM) to optimize a PAT groundwater remediation system design. Akbarnejad-Nesheli et al. (2015) developed a S-O model for designing a groundwater bioremediation system at a petroleum-contaminated site. *BIO PLUME II* was implemented for simulating a bioremediation process combined with the nondominated sorting genetic algorithm II (NSGA II).

The uncertainty of specifying parameters affects the quality of modeling results and the analysis of groundwater processes. A case in point is the modeling of the bioremediation of contaminated groundwater, in which knowledge of hydraulic conductivity is essential for accurate modeling results. Hilton and Beckford (2001) developed a GA-based model for assessing the uncertainty of hydraulic conductivity in the optimal design of a PAT remediation strategy. Smalley and Minsker (2000) presented a management model for the prediction of risk in a cost-effective groundwater remediation system and proposed options for reducing risk under uncertainty in the management model. The noisy genetic algorithm (NGA) was combined with a transport model, numerical fate, and risk assessment for model building. Mantoglou and Kourakos (2007) developed a methodology for optimizing design of a PAT remediation system under hydraulic conductivity uncertainty. Monte Carlo simulation (MCS) was implemented for considering the uncertainty of hydraulic conductivity in the optimization process. He et al. (2008) developed a simulation-based fuzzy chance constrained programming (SFCCP) model for designing an optimal groundwater remediation system under uncertainty based on possibility theory. He et al. (2009) presented a S-O model for optimizing a remediation system of petroleum-contaminated groundwater under uncertainty. Yan and Minsker (2010) applied dynamic surrogate models with noisy genetic algorithms to optimize groundwater remediation designs. Luo and Lu (2014) developed a probabilistic multiobjective fast-harmony search (PMOFHS) algorithm for optimizing a PAT remediation design under hydraulic conductivity uncertainty.

Several previous studies have stressed the importance of taking into account the uncertainty of hydraulic conductivity in the design

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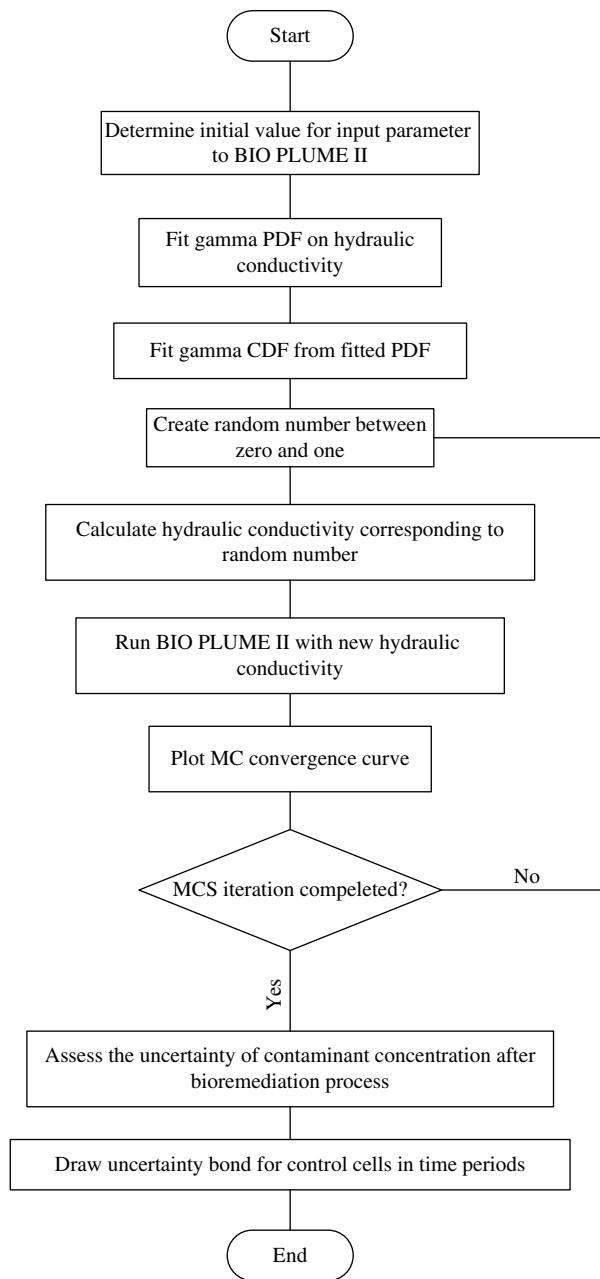


Fig. 1. Flowchart of MCS

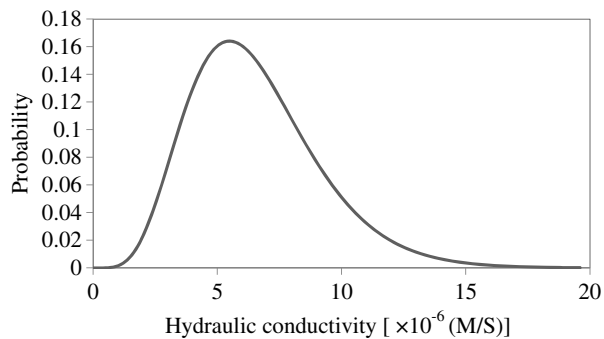


Fig. 2. Fit of the gamma PDF to hydraulic conductivity

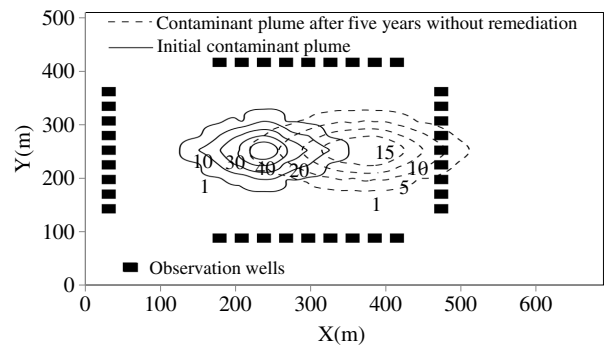


Fig. 3. Site map of the case study showing the contaminant plume without treatment five years after initiation of contamination

Table 1. Input Parameters for *BIO PLUME II*

Input parameter	Value	Unit
Grid size	30 × 30	—
Cell size	19 × 25	m × m
Aquifer thickness	15	M
Hydraulic gradient	0.004	—
Longitudinal dispersivity	10	M
Transverse dispersivity	2	M
Effective porosity	0.3	—
Retardation factor	1	—
Anisotropy factor	1	—
Injected concentration of oxygen	8	mg/L
Initial concentration of oxygen	5	mg/L
Remediation time	3	Years

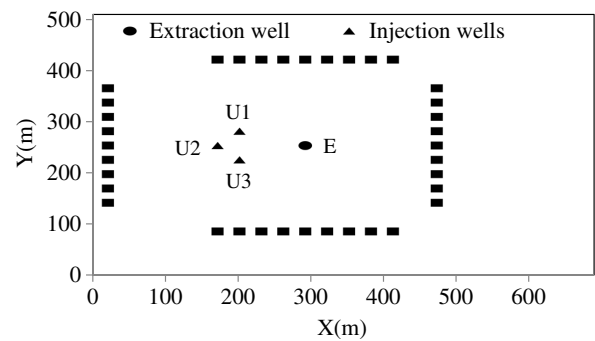


Fig. 4. Site map of the injection wells (U) and the extraction well (E)

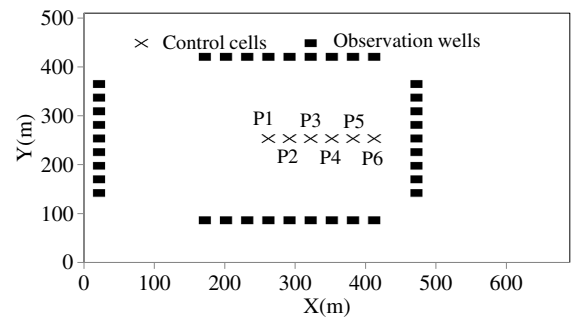


Fig. 5. Selected control cells (P) and observation well cells

Table 2. Symbols Showing Coordinates of Control Cells (P) and Time Periods (T) in *BIO PLUME II* Runs

Control cell	Coordinates		Time period (months)					
	X	Y	T1 0–6	T2 6–12	T3 12–18	T4 18–24	T5 24–30	T6 30–36
P1	10	11	P1T1	P1T2	P1T3	P1T4	P1T5	P1T6
P2	11	11	P2T1	P2T2	P2T3	P2T4	P2T5	P2T6
P3	12	11	P3T1	P3T2	P3T3	P3T4	P3T5	P3T6
P4	13	11	P4T1	P4T2	P4T3	P4T4	P4T5	P4T6
P5	14	11	P5T1	P5T2	P5T3	P5T4	P5T5	P5T6
P6	15	P6T1	P6T2	P6T3	P6T4	P6T5	P6T6	

of groundwater remediation systems, a topic that has been overlooked in many studies (Bozorg-Haddad et al. 2013). This paper assesses the impact that uncertainty in the specification of hydraulic conductivity has on residual contaminant concentrations produced

by bioremediation treatment of groundwater contaminated with dissolved petroleum hydrocarbons. The assessment relies on Monte Carlo simulation.

Methods

Simulation of In Situ Bioremediation

There are numerous papers on the modeling of groundwater biodegradation and bioremediation (e.g., Angelakis and Rolston 1985; Baehr and Corapcioglu 1985; Kosson et al. 1985; Borden and Bedient 1986; Molz et al. 1986). In this paper the model *BIO PLUME II* is applied for simulating the groundwater bioremediation process. Borden et al. (1986) presented the mathematical formulas applied in *BIO PLUME II*. This model simulates dissolved hydrocarbon transport affected by restriction of oxygen in a two dimensional (2D) domain. It solves the solution transport equations

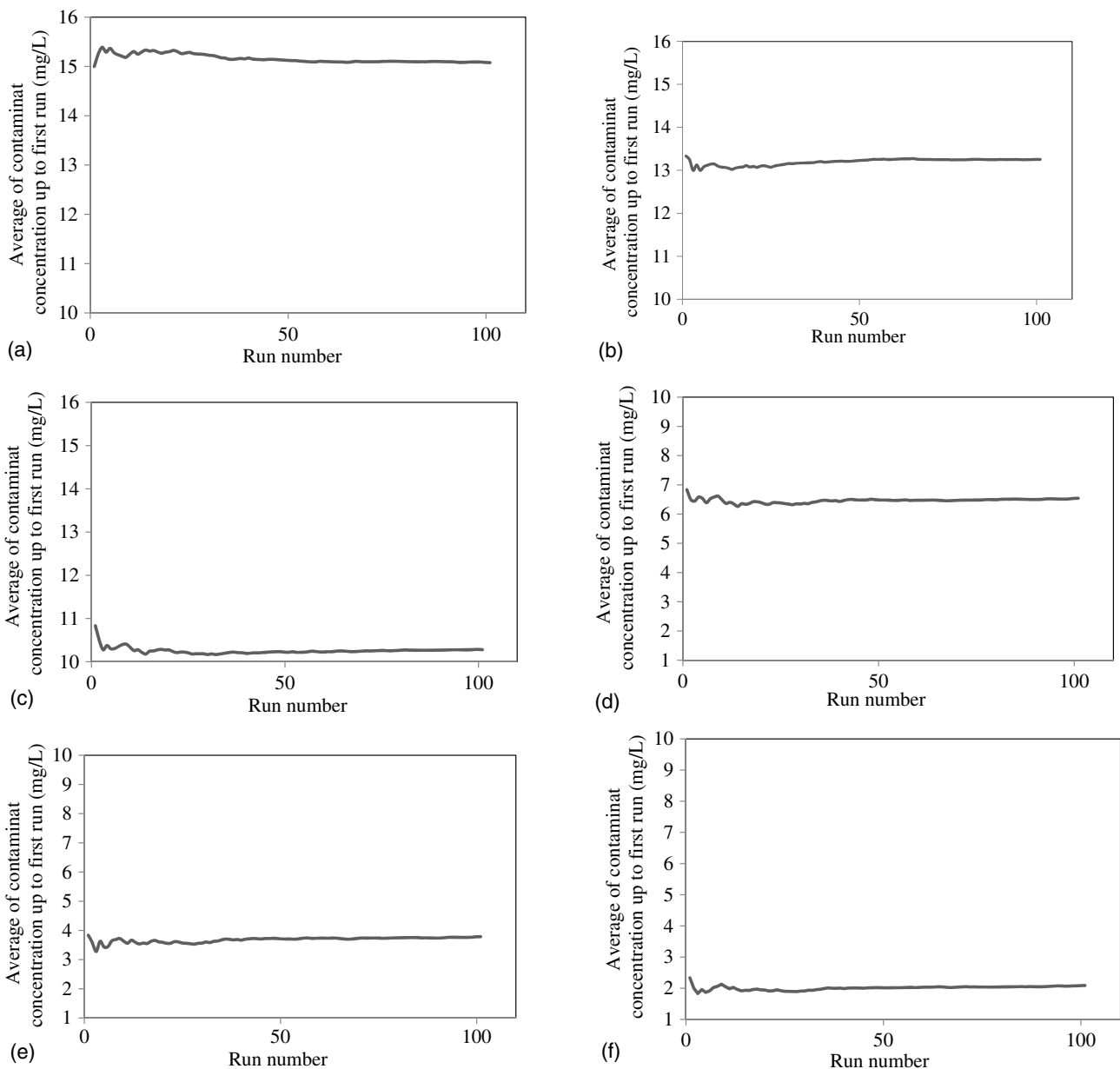


Fig. 6. MCS convergence curve for time periods: (a) T1; (b) T2; (c) T3; (d) T4; (e) T5; (f) T6

for hydrocarbons and for oxygen. Subsurface microorganism growth and removal of oxygen and hydrocarbon are simulated by a modified Monod function

$$\frac{dH_C}{dt} = -M_{C_T} \cdot K \cdot \frac{H_C}{R_H + H_C} \cdot \frac{O_C}{R_O + O_C} \quad (1)$$

$$\frac{dO_C}{dt} = -M_{C_T} \cdot K \cdot I \cdot \frac{H_C}{R_H + H_C} \cdot \frac{O_C}{R_O + O_C} \quad (2)$$

$$dM_{C_T} \cdot K \cdot M_Y \cdot \frac{H_C}{R_C + H_C} \cdot \frac{O_C}{R_O + O_C} + R_{OC} \cdot M_Y \cdot N_{CC} - M_{dr} \cdot M_{C_T} \quad (3)$$

where H_C = concentration of hydrocarbon (ML^{-3}); O_C = concentration of oxygen (ML^{-3}); M_{C_T} = total concentration of microbes (ML^{-3}); K = maximum hydrocarbon consumption (utilization) rate per unit mass of microorganisms; t = time (s); R_H = half-saturated hydrocarbon constant; R_O = half-saturated oxygen

constant; I = stoichiometry coefficient of hydrocarbon to oxygen; M_Y = coefficient of microbial efficiency (yield); R_{OC} = rate of first-order decay of natural organic carbon; N_{CC} = concentration of natural organic carbon (ML^{-3}); and M_{dr} = rate of microbial rate.

Bear (1979) combined Eqs. (1) and (2) with the advection-dispersion equation for a solute undergoing linear instantaneous adsorption, resulting in Eqs. (4) and (5)

$$\frac{\partial H_C}{\partial t} = \nabla(D_{hc} \cdot \nabla H_C - V_D \cdot H_C) - \frac{M_{C_T} \cdot K}{R_F} \cdot \frac{H_C}{R_H + H_C} \cdot \frac{O_C}{R_O + O_C} \quad (4)$$

$$\frac{\partial O_C}{\partial t} = \nabla(D_{hc} \cdot \nabla O_C - V_D \cdot O_C) - M_{C_T} \cdot K \cdot I \cdot \frac{H_C}{R_H + H_C} \cdot \frac{O_C}{R_O + O_C} \quad (5)$$

where D_{hc} = dispersion tensor coefficient (L^2T^{-1}); V_D = Darcy velocity for groundwater movement (L^2T^{-1}); and R_F = hydrocarbon retardation factor.

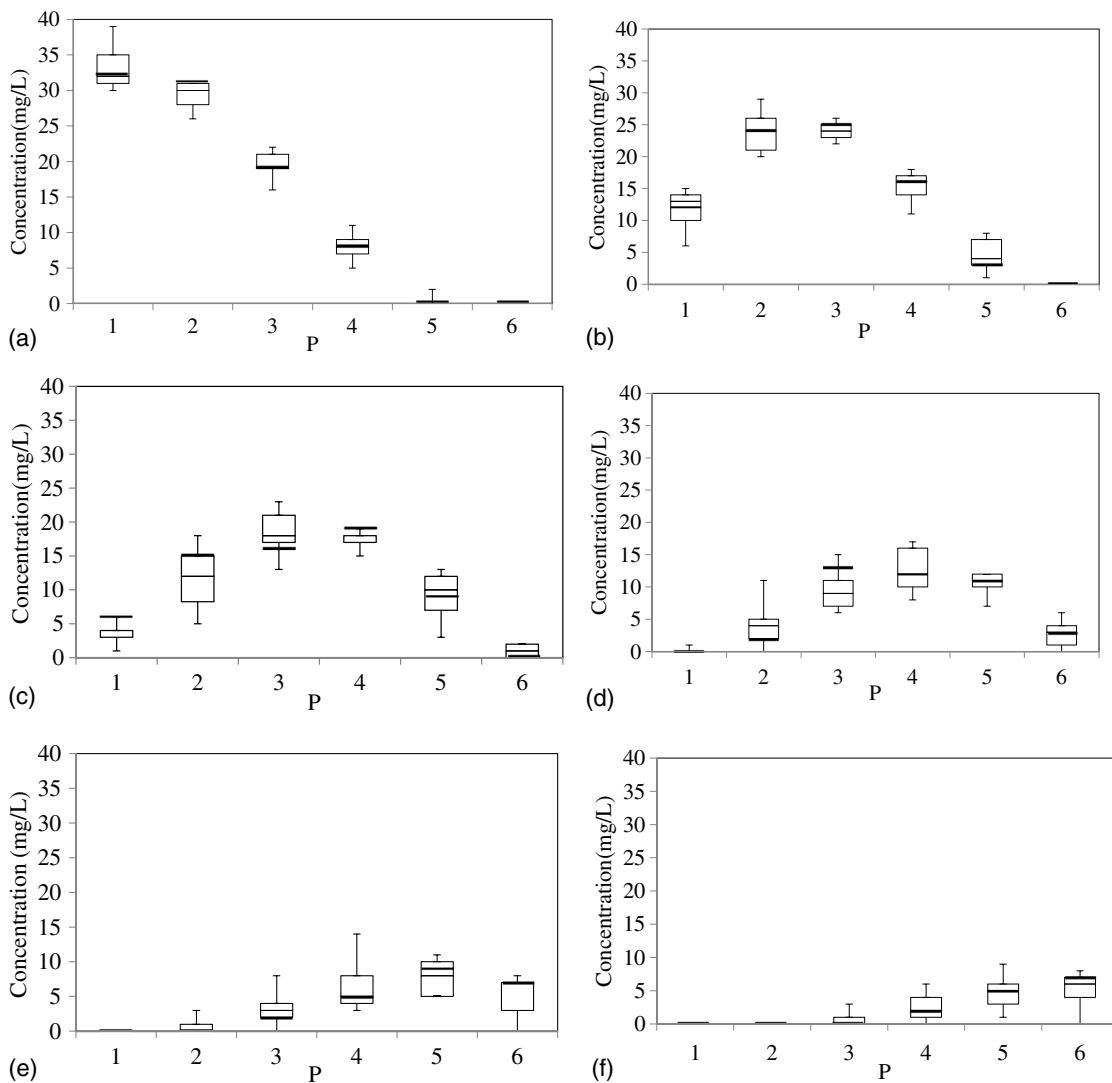


Fig. 7. Uncertainty box plot for residual contaminant concentration after bioremediation at the control cells (P) in different time periods: (a) T1; (b) T2; (c) T3; (d) T4; (e) T5; (f) T6

The exchange of microorganisms between the free solution and the soil surface is assumed to be rapid and to follow a linear relation to total concentration. *BIO PLUME II* simulates the movement of microorganisms by the simple retardation factor method (Freeze and Cherry 1979) as written in Eqs. (6)–(8)

$$\frac{\partial M_{C_s}}{\partial t} = \frac{\nabla(D_{hc} \cdot \nabla C_{M_s} - V_D \cdot C_{M_s})}{M_{R_f}} + C_{M_s} \cdot K \cdot M_Y \cdot \frac{H_C}{R_H + H_C} \cdot \frac{O_C}{R_O + O_C} + \frac{R_{OC} \cdot M_Y \cdot N_{CC}}{M_{R_f}} - M_{dr} \cdot C_{M_s} \quad (6)$$

$$M_{C_A} = R_M \cdot M_{C_s} \quad (7)$$

$$M_{C_T} = M_{C_s} + M_{C_A} = (1 + R_M) \cdot M_{C_s} = M_{R_f} \cdot M_{C_s} \quad (8)$$

where M_{C_s} = microbial concentration in solution (ML^{-3}); M_{C_A} = concentration of microbes attached to soils (ML^{-3}); R_M = ratio of adsorbed microbes per microbes in solution; and M_{R_f} = microbial retardation factor.

Assessment of Uncertainty by MCS

This paper applies MCS coupled with runs of the model *BIO PLUME II* to assess the effect of hydraulic conductivity uncertainty on bioremediation. Fig. 1 shows the flowchart of the MCS applied in this study.

Fitting the Gamma Probability Density Function to Hydraulic Conductivity

The gamma probability density function (PDF) is a continuous distribution on positive probability variables. It is widely used to represent skewed data (Loaiciga 2015) and features shape (α) and scale (β) parameters

$$f(x|\alpha, \beta) = \frac{\beta^\alpha}{\Gamma(\alpha)} (\beta x)^{\alpha-1} \exp(-\beta x) \quad (9)$$

where $\Gamma(\alpha)$ = gamma function. Fig. 2 shows the gamma distribution fitted to hydraulic conductivity which is indicative of the hydraulic conductivity range.

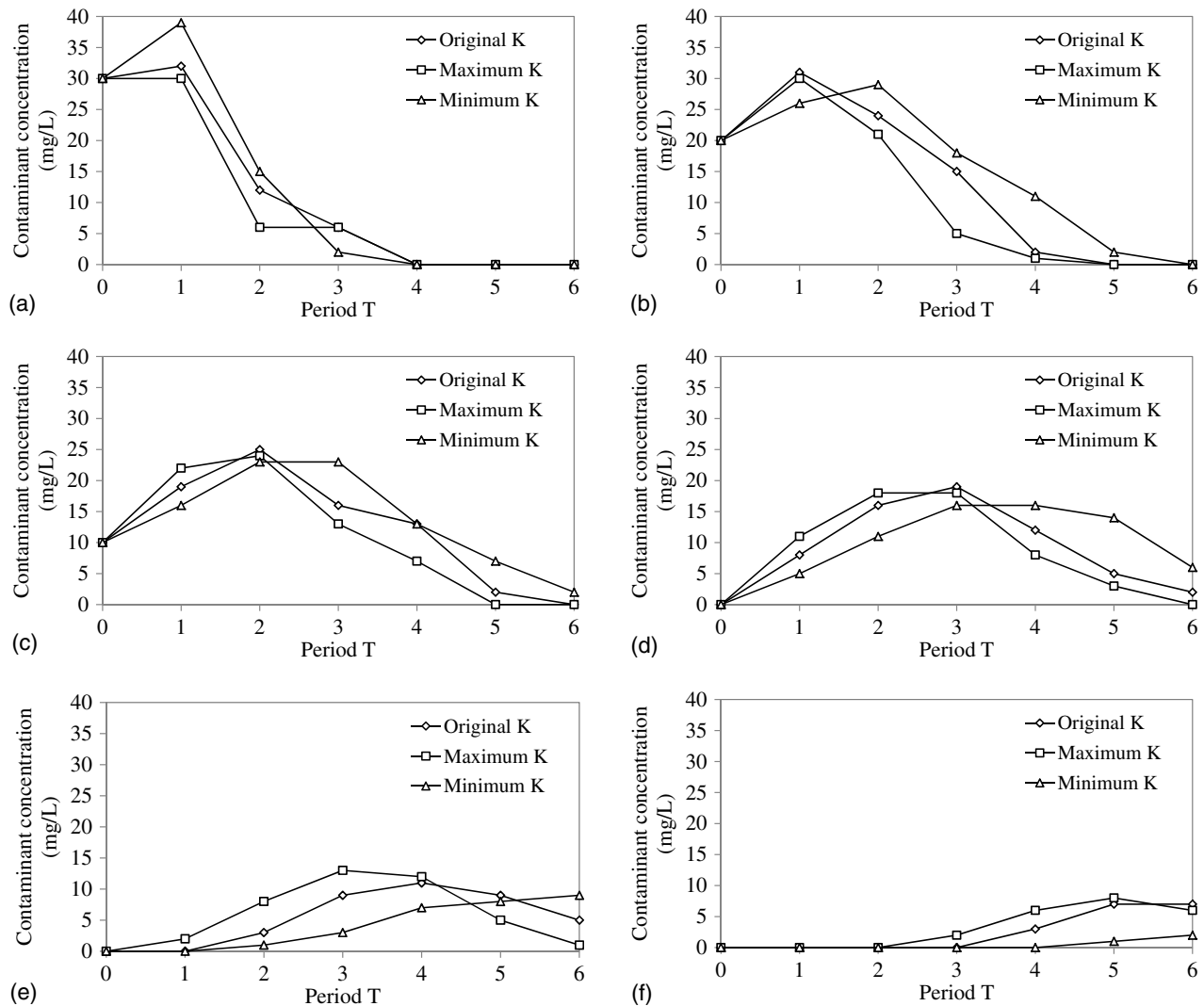


Fig. 8. Breakthrough curves corresponding to minimum, original, and maximum hydraulic conductivity (K) chosen for the case study in MCS at control cells: (a) P1; (b) P2; (c) P3; (d) P4; (e) P5; (f) P6

Monte Carlo Simulation

Monte Carlo simulation is a commonly used stochastic method for assessing the impact of input parameters' uncertainty on output parameters by repeated simulation of a process. This method repeatedly generates random values of the input parameters drawn from a probability distribution function, and each generated value is input to simulate the process of interest by means of a model, which in this case is *BIOPLUME II* for bioremediation. This paper treats hydraulic conductivity as the uncertain input parameter to *BIO PLUME II*; the residual contaminant concentration produced by bioremediation is treated as the output variable.

Case Study

A case study introduced by Shieh and Peralta (2005) is adopted in this paper for assessing the impact of hydraulic conductivity uncertainty on residual contaminant concentration after the bioremediation process. Fig. 3 is a site map of the case study showing the contaminant plume without treatment five years after the initiation of contamination. Table 1 lists the input parameters to *BIO PLUME II*. The dimensions of this case study are 690×510 m. The aquifer is homogenous, with a thickness equal to 15 m. The hydraulic head ranges between 27.7 m in the eastern boundary and 35.5 m in the

western boundary. There is no groundwater flow in the north-to-south direction. The groundwater flow direction is from west to east, and the hydraulic gradient is 0.004. Fig. 4 plots the location of the injection wells (U) and the extraction well (E) selected for this study. The locations of these wells and their pumping rates [U1: 1.03; U2: 0.45; U3: 1.22; and E: 1.24 (L/s)] were retrieved from the results of Shieh and Peralta (2005), who achieved remediation at minimal cost. Three injection wells were used for injecting oxygen with 8-mg/L concentration into the contaminated groundwater; they are denoted U; one extraction well, denoted E, withdraws contaminated water to the surface. Observation or monitoring wells surround the remediation system site. These wells are not part of the bioremediation system.

Selecting the Control Cells

Six cells were selected for assessing the impact of hydraulic conductivity uncertainty on the residual contaminant concentration produced by the bioremediation process. Fig. 5 shows the locations of the selected control cells in the case study.

BIO PLUME II was run with the original hydraulic conductivity for this case study (6×10^{-5} m/s) specified by Shieh and Peralta (2005) in six time periods—Months 0–6, 6–12, 12–18, 18–24, 24–30, 30–36—since the initiation of bioremediation. The cells

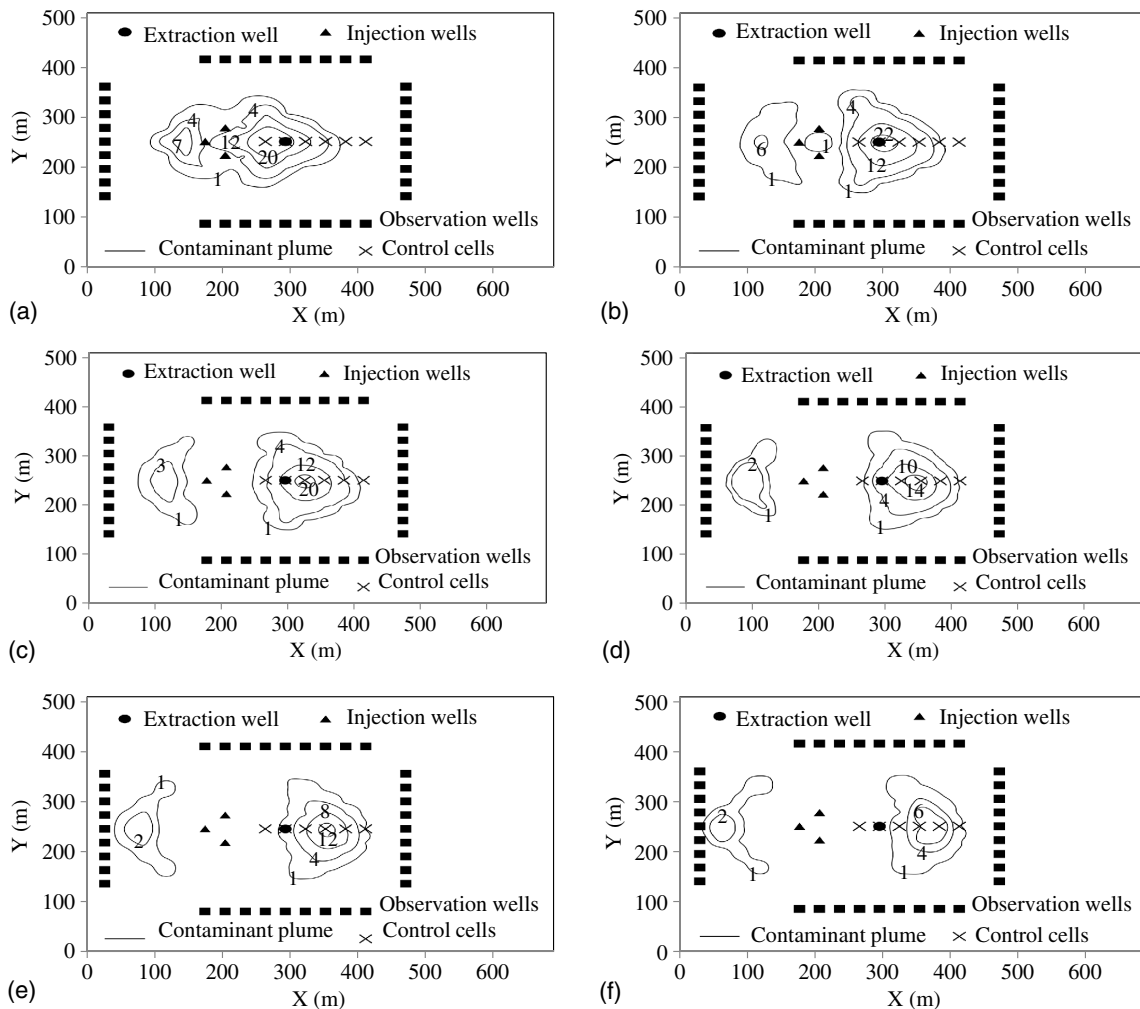


Fig. 9. Contour line of residual contaminant concentration (mg/L) in the aquifer produced by bioremediation when minimum hydraulic conductivity is selected in MCS: (a) T1; (b) T2; (c) T3; (d) T4; (e) T5; (f) T6

with the maximum contaminant concentration in each run and time period were selected as the control cells for assessing the impact of hydraulic conductivity uncertainty on the residual concentration of contaminant produced by bioremediation. The control cells' coordinates and simulation periods are listed in Table 2.

Adequacy of the Number of Data in the MCS

Fig. 6 graphs the MCS convergence curve for the six time periods after 100 simulations.

Results and Discussion

The results from 100 runs of *BIOPLUME II* with different hydraulic conductivity values in the six time periods yielded a box plot for the aquifer's residual contaminant concentration produced by bioremediation. Fig. 7 shows the box plots of the residual contaminant for the six control cells in the six time periods. The thick black line in Fig. 7 shows the contaminant concentration (OCC) corresponding to the original hydraulic

conductivity produced by bioremediation. *BIO PLUME II* ran with the original hydraulic conductivity of this case study specified by Shieh and Peralta (2005). In this study, the contaminant uncertainty interval (IB) was chosen for assessing the impact of hydraulic conductivity uncertainty on the residual contaminant concentration produced by the bioremediation process. In Period T1, the maximum IB was in Cell P1 at the center of the contaminant plume (the largest contaminant concentration). The concentration of the contaminant plume decreased toward the periphery of the study site where the magnitude of the IB at Cell P6 reached zero in Period T1. In Period T2, the IB at Cells P1, P3, and P6 was identical to that of Period T1, and at cells P2, P4, and P5 the magnitude of IB increased relative to Period T1 because of the contaminant plume's movement in the direction of groundwater flow, and because the center of the contaminant plume was located near these cells. In Period T2 the maximum uncertainty was at P2, the center of the plume, and decreased with increasing distance from it. Other patterns of uncertainty in the contaminant concentration produced by bioremediation at the control cells and in simulation periods corresponding to the various values of hydraulic conductivity are shown in Fig. 7, where it is also seen that at Cells P1 and P2 in Period T6 the contaminant concentration was zero for any

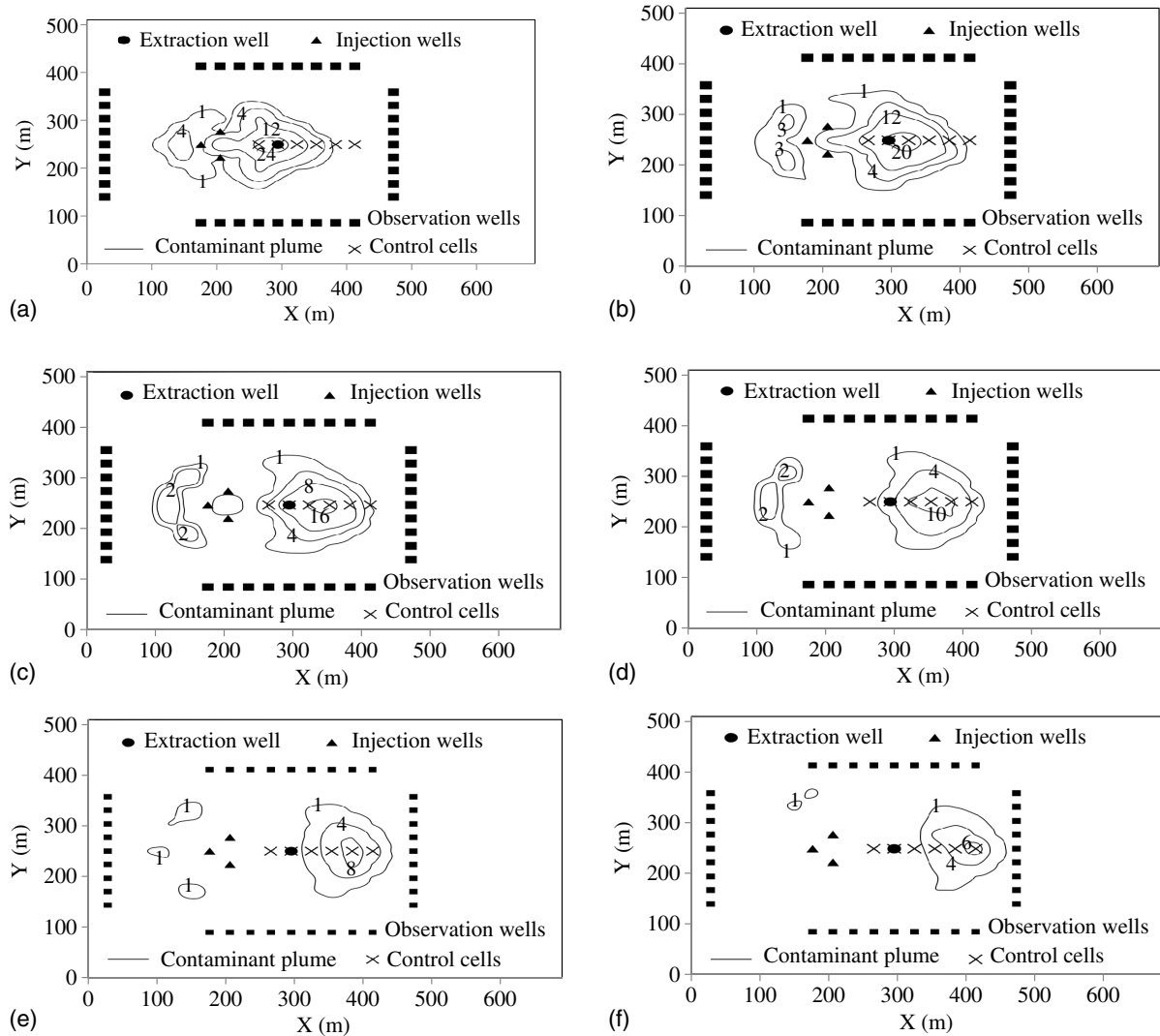


Fig. 10. Contour line of residual contaminant concentration (mg/L) in the aquifer produced by bioremediation when the original hydraulic conductivity is selected in MCS: (a) T1; (b) T2; (c) T3; (d) T4; (e) T5; (f) T6

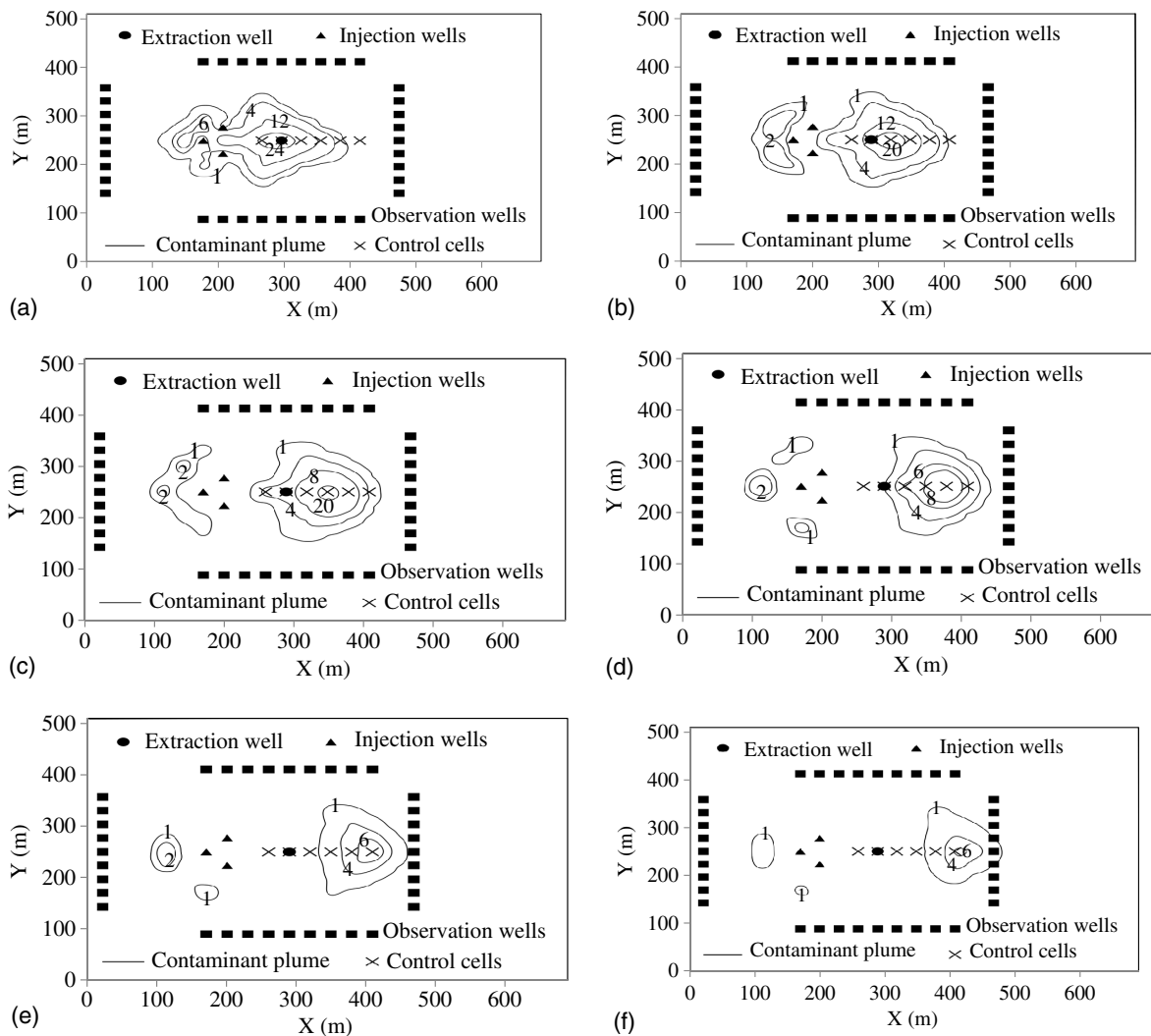


Fig. 11. Contour line of residual contaminant concentration (mg/L) in the aquifer produced by bioremediation when the maximum hydraulic conductivity is selected in MCS: (a) T1; (b) T2; (c) T3; (d) T4; (e) T5; (f) T6

value of hydraulic conductivity. It is therefore inferred from Fig. 7 that the uncertainty of the contaminant plume was greater at its center than at its periphery. It is also inferred from Fig. 7 that the uncertainty in the middle time periods was higher than in the first and the last time periods. This is because the time of remediation in Period T1 was relatively short and there was minimal movement of groundwater. In Period T6, the time of remediation was long, which reduced the impact of hydraulic conductivity uncertainty on the residual contaminant uncertainty. In Periods T2, T3, T4, and T5, the time of remediation was intermediate and the transport process was more influenced by hydraulic conductivity uncertainty insofar as the residual contaminant concentration is concerned.

Fig. 8 shows the breakthrough curves at the control cells corresponding to the minimum, original, and maximum hydraulic conductivity chosen for the MCS. It is apparent that increasing the hydraulic conductivity caused the contaminant plume to move faster and biodegrade more quickly than it would otherwise.

The contour lines of the residual contaminant concentrations corresponding to the minimum, original, and maximum hydraulic conductivities in the six time periods are graphed in Figs. 9–11, respectively. It is clear from Figs. 9–11 that the downgradient

Table 3. Performance of Bioremediation System after Three Years for Several Hydraulic Conductivity Values

Number	Hydraulic conductivity $\times 10^{-5}$ (m/s)	Number of contaminated cells	Maximum value of contaminant concentration (mg/l)	Biodegraded mass (%)
1	2.2	30	8	75
2	4.6	28	8	79.2
3	6	32	7	79.4
4	7.3	27	7	84
5	8.46	25	6	84.1

movement of the contaminant plume was fastest (slowest) and the extent of the contaminant area was smallest (largest) for the maximum (minimum) hydraulic conductivity.

Table 3 summarizes the performance of the bioremediation system for several values of hydraulic conductivity. It is evident that increasing hydraulic conductivity decreased both the number of contaminated cells and the maximum value of contaminant concentration in the plume. This confirms that biodegradation increases as hydraulic conductivity increases.

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