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Modified Well-Field Configurations for Improved Performance of Contaminant Elution and Tracer Tests

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Abstract

Contaminant elution and tracer (CET) tests are one method for characterizing the impact of mass transfer, transformation, and other attenuation processes on contaminant transport and mass removal for subsurface systems. The purpose of the work reported herein is to explore specific well-field configurations for improving CET tests by reducing the influence of preferential flow and surrounding-plume effects. Three injection-extraction well configurations were tested for different domain conditions using a three-dimensional numerical model. The three configurations were the traditional configuration with a single pair of injection-extraction wells, modified configuration I with one extraction well located between two injection wells, and modified configuration II with two pairs of injection-extraction couplets (one nested within the other). Elution curves for resident contaminant and breakthrough curves from simulated tracer tests were examined for specific landmarks such as the presence and extent of steady-state (relatively high concentrations) and asymptotic (asymptotic decrease to low concentrations) phases, as well as distinct changes in slope. Temporal-moment analysis of the breakthrough curves was conducted to evaluate mass recovery. Effective diffusion coefficients were obtained by fitting selected functions to the elution curves. Based on simulation results for a homogeneous domain, full isolation of the inner extraction well from the surrounding plume was obtained for the modified configuration II, whereas the extraction wells are impacted by the surrounding plume for the other two configurations. Therefore, configuration II was used for additional simulations conducted with layered and heterogeneous domains. Tracer-test simulations for homogeneous and layered domains indicate 100% mass recovery for the inner extraction well. For the heterogeneous domain, decreasing the distance between the inner injection-extraction well couplet and adjusting the pumping-rate distribution between the two extraction wells increased the mass recovery from 69% to 99%.

Keywords

contaminant plume; site characterization; attenuation; mass transfer

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1. Introduction

Groundwater contamination continues to pose significant threats to human health in many locales. A recent National Research Council report stated that most sites with large groundwater contaminant plumes will require many decades or longer to achieve cleanup under current methods and standards (NRC, 2013). This realization has resulted in the search for more cost-effective alternatives to pump and treat, the standard method for treatment of groundwater contaminant plumes.

Monitored natural attenuation (MNA) and enhanced attenuation (EA) have been examined as alternatives to pump and treat for sustainable management of large, complex plumes because of their potentially lower cost. Evaluating the feasibility of MNA/EA necessitates access to information that is not typically collected with standard site characterization methods. Advanced methods are required to characterize sites for the occurrence of specific attenuation processes and to determine their associated rates. Matrix diffusion, sorption, and transformation are critical attenuation processes that can impact remediation effectiveness. Understanding the contributions of these processes to overall attenuation at a given site can enhance guidance for long-term management (NRC, 2013; SERDP, 2013). Moreover, improved predictive modeling that can account for the various attenuation and transport processes is needed for cost-effective site management (e.g., EPA, 2009). This in turn requires better determination of the relevant model input parameters.

Several methods, such as plume-scale spatial concentration transects, mass-flux fences, and measuring sediment-phase concentrations, have been used for evaluating attenuation processes and the feasibility of MNA/EA (e.g., Johnson et al., 1989; Ball et al., 1997; Borden et al., 1997; King et al., 1999; Bockelmann et al., 2001; Newell et al., 2002; Parker et al., 2004; Chapman and Parker, 2005; Basu et al., 2006). These methods provide measures of aggregate attenuation and can have significant uncertainties because of preferential-flow phenomena and other factors, which can limit their usefulness to evaluate and quantify specific attenuation processes (e.g., Brusseau, 1998; Chapelle et al., 2007).

Induced-gradient contaminant elution tests, also referred to as contaminant mass discharge tests, are another option for characterization of mass-transfer and attenuation processes and associated parameters (Bahr, 1989; Brogan and Gailey, 1995; Thorbjarnarson and Mackay, 1997; Blue et al., 1998; Brusseau et al., 1999a, 2007a, 2011a, 2013; Johnston et al., 2013). Conservative tracers can be employed as part of these tests to enhance evaluation of mass-transfer processes (Bahr, 1989; Thorbjarnarson and Mackay, 1997; Blue et al., 1998; Brusseau, 1993; Brusseau et al., 1999a, 1999b, 2007; Nelson et al., 2003). And, non-conservative tracers, such as biotracers, can be used to assess attenuation (Brusseau et al., 1999c; Sandrin et al., 2004).

The standard well-field configuration used for most contaminant elution and tracer (CET) tests is the injection-extraction dipole. For this configuration, the extraction well remains influenced by the surrounding plume, which can be a significant limitation in attempting to delineate and quantify mass-transfer or attenuation processes. This is particularly true for mass-transfer or transformation processes with slower characteristic rates. Isolation of the

test zone from the plume ensures that contaminant elution behavior observed during a CET test is influenced solely by mass-transfer and attenuation processes occurring within the test zone. Hence, there is interest in investigating alternative well-field configurations that may enhance the implementation and analysis of CET tests.

A number of studies have been conducted to evaluate effective well-field configurations for various hydrologic applications. For example, the influence of well-field configuration on the effectiveness of contaminant mass removal has been investigated for pump-and-treat systems (e.g., Satkin and Bedient, 1988; Keely, 1989; Schafer and Kinzelbach, 1992; Cohen et al., 1997; Rivett et al., 2006). In addition, two-well recirculation systems have been investigated for in-situ bioremediation of groundwater (Gandhi et al., 2002; Luo and Kitanidis, 2004; Luo et al., 2006). Gandhi et al. (2002) examined the performance of the recirculation system with a single injection-extraction well pair. Luo and Kitanidis (2004) and Luo et al. (2006) tested the performance of the standard injection-extraction dipole configuration compared to that of a four-well system comprising two sets of nested dipoles. Field tracer tests were conducted to evaluate capture and recovery effectiveness and residence times for the nested system (Luo et al., 2007). Burberry and Wang (2010) demonstrated that aquifer heterogeneity and pumping rates strongly impact the solute mass recovery for tracer tests conducted with two-well recirculation. Minimal research has been conducted to investigate optimal well-field configurations for CET tests specifically (e.g., Burberry and Wang, 2010; Burberry et al., 2013), particularly for heterogeneous systems with non-uniform flow fields or for applications focused on characterizing natural-attenuation processes.

The purpose of this research is to investigate the ability of two modified well-field configurations to isolate the extraction well in comparison to the standard injection-extraction well couplet in domains with significant heterogeneity, with a specific focus on characterizing natural-attenuation processes. Numerical modeling was used to generate synthetic CET test data, namely elution curves for resident contaminants and breakthrough curves (comprising both arrival and elution waves) for tracers. The data were used to determine mass recoveries and dilution factors to evaluate performance. The utility of obtaining process-parameter values from the results of CET tests was illustrated by determining effective diffusion coefficients via fitting analytical solutions of selected functions to the simulated breakthrough curve data.

2. Methodology

2.1 Numerical Model

The flow model used in this work was MODFLOW, the three-dimensional (3D) finite-difference numerical model developed by the U.S. Geological Survey (McDonald and Harbaugh, 1988; Harbaugh et al., 2000). The 3D solute transport model MT3D with TVD solver (Zheng, 1990) was used to simulate solute transport. Groundwater Vista (GV) version 6.85 (Rumbaugh and Rumbaugh, 2007) and Groundwater Modeling System (GMS) version 7.1 (EMRL, 2005) were used as graphical user interfaces, depending upon the features needed. Both programs provided robust results according to the test simulations (results not show).

The model domain was 247,500 square meters to ensure sufficient domain size for a typical CET test configuration. Thus, the CET well field exerted minimal impact on the domain boundaries. The domain was divided into a regular orthogonal grid consisting of 45 rows and 50 columns with grid space ranging from 0.625 m to 73 m. The grid size was set to ensure numerical accuracy for the given simulation conditions. Finer grid spacing was used for the test zone to account for the larger hydraulic and concentration gradients. The test zone where the injection-extraction well systems were set up was 10x5 m with 0.625x0.625 m for each grid cell. Vertical discretization was set differently for homogeneous and heterogeneous domains to ensure simulation accuracy for the heterogeneous simulations, which are described in section 2.2.

Specified head boundaries were used along the four horizontal borders of the domain, with a natural gradient of 0.001 under confined conditions to establish groundwater flow from the left to right side. No flow boundaries were set for the top and bottom of the model. Select parameters used in the modeling were determined according to information generated from geologic borehole-logs, pumping tests, and historic data from the Tucson International Airport Area (TIAA) Superfund site (Zhang and Brusseau, 1999). Hydraulic conductivity (K) of 10 m/d and porosity of 0.2 were used for sand units, whereas K of 10^{-4} m/d and porosity of 0.3 were used for clay units. The K in the vertical direction is 1000 times lower than K in horizontal direction. Longitudinal dispersivity was set to 0.5 m, and transverse, and vertical dispersivities were set to 0.05, and 0.005 m, respectively. The aqueous diffusion coefficient was 7.6×10^{-5} m²/d, representing TCE (Zhang and Brusseau, 1999).

2.2. Approach

The simulation experiments were designed to represent implementation of a set of CET tests conducted at a site with existing contamination. The zone influenced by the CET tests will be referred to as the test zone. The test zone is assumed to be surrounded by a uniform groundwater contaminant plume, wherein groundwater flow occurs under the regional (site-wide) hydraulic gradient.

Three specific well-field configurations were evaluated. The first one is the traditional configuration with a single pair of injection-extraction wells (Fig.1A), which was used as a baseline. The second one is modified configuration I, with one extraction well located between two injection wells (Fig. 1B). The third one is modified configuration II, with two pairs of injection-extraction couplets wherein one is nested within the other (Fig. 1C). The flowlines shown in Figure 1 represent conceptualized flow within the capture zones of the extraction wells and are for illustrative purposes only.

Four types of domains were simulated, homogeneous (baseline), layered, 2D heterogeneous, and fully 3D heterogeneous. For the homogeneous simulation, the domain was set as sand with a thickness of 3 m. For the layered simulation, the domain was split into three units, with the upper and lower units as clay of 1 m thickness for each and the middle unit as sand with 3 m thickness. Each unit comprises 10 model layers, each 0.1 m thick. For the fully 3D heterogeneous system, a random field generator (Gutjahr, 1989) was used to derive realizations of K for the sand unit of the domain. It was assumed that the permeability of the

sand was lognormally distributed with mean $\langle \ln K \rangle$ and variance σ_Y^2 . The random fields were generated with an arithmetic mean value of K equal to 10 m/d, σ_Y^2 as 10, and correlation scales of 2-m (longitudinal) $\times$ 1-m (transverse) $\times$ 0.1-m (vertical). Note that the variance and correlation lengths are not meant to represent the TIAA site specifically. For the 2D heterogeneous system, the domain was generated randomly similarly to the fully heterogeneous domain in the horizontal direction, but with uniform K in the vertical direction. For the 2D and 3D heterogeneous systems, 30 model layers were used with 0.1 m for each layer.

Four scenarios were simulated for the homogeneous domain (Table 1) to evaluate the performance of the well configurations as assessed with the selected metrics detailed below. The purpose of scenario 1 is to investigate the isolation of the extraction well from the surrounding plume. In scenario 1, the test zone was clean, and the surrounding plume was present. For the standard (baseline) configuration, clean water was injected and extracted at a rate of 3 m³/d. For modified configuration I, water was injected into both injection wells with the injection rate of 1.5 m³/d for each and was extracted from the middle well with rate of 3 m³/d. For configuration II, the injection rates for In1 and In2 were 1 and 2 m³/d, respectively, and the extraction rate was 1.5 m³/d for each extraction well. The combined injection rate is approximately 1/50 of total inflow from the boundary and thus has minimal impact on overall hydrodynamics of the model domain. The distance between outer injection-extraction well couplet (In2-Ex2) is 9.375 m for all scenarios.

Scenarios 2, 3, and 4 were simulated only for configuration II (two pairs of injection-extraction couplets wherein one is nested within the other). Table 1 lists a summary of simulations conducted with configuration II for various conditions. For scenario 2, the time needed to remove resident contaminant from the test zone was examined. In this scenario, the entire domain was contaminated, and clean water was injected via both injection wells with rates of 1 m³/d for In1 and 2 m³/d for In2. Scenario 3 was simulated to test the magnitude of mass recovery for the inner extraction well Ex1. The initial contaminant concentration was zero for the entire domain for this scenario, clean water was injected via In2 with an injection rate of 2 m³/d, and tracers were injected via In1 continuously during the simulation period with an injection rate of 1 m³/d. The extraction rates were 1.5 m³/d for each extraction well for all three scenarios, and the simulated time periods were 500 days.

Scenario 4 was simulated as a tracer test with a pulse injection of a conservative tracer to examine the performance of a CET test using well configuration II. The concentration for Ex1 was monitored for much longer than the injection time to ensure capture of the elution curve. Breakthrough curve data were analyzed and used to determine the relevant mass-transfer parameter. In scenario 4, clean water was injected via In2 with an injection rate of 2 m³/d, and tracer was injected via In1 with a rate of 1 m³/d continuously for 10 days followed by clean water injection for 100 days. No background plume was present. In scenario 4, the distance between inner injection-extraction well couplet (In1-Ex1) for configuration II was 3.125 m, whereas for the other three scenarios, the distance was 4.375 m. Breakthrough curves of data collected from the extraction wells were plotted to analyze the performance of each configuration.

The same scenario setup used above was used for the layered simulations, with modifications to address the presence of the clay units. In scenario 1a, the clay units within the test zone were contaminated whereas the sand unit within the test zone was clean, and the plume was present. In scenario 1b, the entire test zone was clean and the plume was present. In scenario 1c, the upper and lower units were contaminated and K values for the upper and lower units were changed such that all three units were set as sand (homogeneous). For Scenarios 2, 3, and 4, the plume is present in the sand and clay units. Simulations for all scenarios were repeated for the 2D heterogeneous domain. Additional CET tests with different extraction rate distributions and distance between the inner injection-extraction well couplet were simulated for the 2D heterogeneous system. Simulations for scenarios 1, 2 and 4 were conducted for the 3D heterogeneous domain. In all scenarios, the injection and extraction wells were screened only in the vertically central 3 m of the domain.

2.3 Estimation of effective diffusion coefficients

The relevant CET-test simulations described above produced breakthrough curves for the injected tracer for Ex1. These data were analyzed with two mathematical functions to determine the effective diffusion coefficient (D_e), where $D_e = \phi D_0 / \tau$, D_0 is the aqueous diffusion coefficient [L^2/T], ϕ is porosity [-], and τ is tortuosity [-]. The values so determined were then compared to the model input value to evaluate representativeness. In typical field applications, the D_e values obtained from analysis of tracer-test data would be used for example as input for a modeling effort. The values could be used directly, or they could be used to characterize ϕ and/or τ . Both functions are based on the assumption that for systems with a sand unit abutted above and below by clay units, advective flux is typically dominant for the sand whereas mass removal for the clay occurs essentially exclusively via diffusive flux.

Method 1 is based on the matrix diffusion model that was developed by Parker et al. (1994) with the configuration of two clay units on top and bottom, and a sand unit in the middle. The mass discharge rate and the total mass loaded into clay units during a tracer-injection period can be described as (Parker et al. 1994; AFCEE, 2007; Mcdade et.al, 2013):

$$J_a(t \leq t') = \phi_{clay} C_p A \sqrt{\frac{R_{clay} D_e}{\pi t}} \quad (1)$$

$$M(t \leq t') = 2\phi_{clay} C_p A \sqrt{\frac{R_{clay} D_e t'}{\pi}} \quad (2)$$

where J_a [M/T] is the mass discharge rate from the sand to clay units, M [M] is the total mass loaded into the clay units, t' is the time when injection stopped. ϕ_{clay} is the porosity of the clay units, C_p [M/L³] is the average concentration in the study area (assumed equal to the injection concentration for a continuous injection), A [L²] is the area that is influenced by

extraction well, and R_{clay} (equal to 1 in this study) is the retardation factor for sorption by the clay units.

The model was developed with the major assumption that the solute mass in the sand unit is immediately removed after the loading period stops at time t' . Then solute starts to diffuse back to the sand unit. Here we considered as the residence time, t_R [T] that is calculated by moment analysis with M_0 , M_1 are zeroth and first moment, respectively:

$$t_R = \frac{M_1}{M_0} - \frac{t'}{2} \quad (3)$$

The mass discharge rate and the estimated mass that remains in the clay units during the back diffusion period are (AFCEE, 2007; Mcdade et.al, 2013):

$$J_a(t \geq t') = \phi_{clay} C_p A \left[\sqrt{\frac{R_{clay} D_e}{\pi(t-t')}} - \sqrt{\frac{R_{clay} D_e}{\pi t}} \right] \quad (4)$$

$$M(t \geq t') = 2\phi_{clay} C_p A \sqrt{\frac{R_{clay} D_e}{\pi}} (\sqrt{t} - \sqrt{t-t'}) \quad (5)$$

Based on total mass that was loaded in the clay units and the remaining mass, corrected by residence time, the mass that diffused out from the clay units can be calculated by:

$$M_{out}(t > t') = 2\phi_{clay} C_p A \sqrt{\frac{R_{clay} D_e}{\pi}} \left(\sqrt{t-t' - \frac{t_R}{2}} - \sqrt{t} + \sqrt{t' + \frac{t_R}{2}} \right) \quad (6)$$

Results calculated by the analytical solution (6) will be matched to the simulated cumulative solute mass removed from Ex1 during the time period from $t' + \frac{t_R}{2}$ to t , optimizing for D_e .

Here it is assumed that all of the mass that diffused back to the sand unit was recovered by Ex1, which is true according to the simulated results.

Method 2 is based on fitting a selected function to breakthrough curves (Cunningham et al., 1997; Haggerty et al., 2000). Based on the modeling setup, the total simulation time (t) and the mean residence time in the immobile domain (clay units) are much longer than the mean residence time (t_{ad}) in the advective domain. Therefore, the mass balance equation can be written as (Haggerty et al., 2000):

$$-\frac{v}{R_a} \frac{\partial C}{\partial x} = \Gamma(x, t), \quad (7)$$

where v [L/T] is pore fluid velocity, R_a is the retardation factor in mobile zone, C [M/L³] is the solute concentration, and $\Gamma(x, t)$ [M/L³/T] is the source-sink term based on mass exchange with immobile domain and sorption. We can solve the equation (7) by integration:

$$C(x = L, t) = - \int_0^L \frac{R_a(x)}{v(x)} \Gamma(x, t) dx \quad (8)$$

It can be further simplified as:

$$C(x = L, t) = - t_{ad} \Gamma(t) \quad (9)$$

For the linear mass transfer problem with uniform initial conditions, it can be expressed as:

$$\Gamma(t) \cong M_0 \frac{\partial g}{\partial t} - C_0 g, \quad (10)$$

where M_0 is the zeroth temporal moment of injection, $g(\tau)$ is a “memory function” to be defined [T⁻¹] and in this problem using finite layer model, the corresponding function is:

$$g(t) = \sum_{j=1}^{\infty} 2\beta_{tot} \frac{D_a}{a^2} \exp \left[- \frac{(2j-1)^2 \pi^2 D_a}{4 a^2} t \right] \quad (11)$$

where β_{tot} is the capacity coefficient that represents the ratio of mass in the immobile domains (clay units) to mass in the mobile domain (sand units), which can be expressed as:

$$\beta_{tot} = \frac{R_{im} \theta_{im}}{R_m \theta_m} \quad (12)$$

R_m and R_{im} represent retardation factors in mobile and immobile domains. D_a [L²/T] is the apparent diffusion coefficient, equal to:

$$D_a = \frac{D_e}{R_{im}} \quad (13)$$

a [L] is the distance from the center to the edge of immobile zone, and j is the index of N distinct immobile phases, C_0 [M/L³] is the initial concentration. Employing (9) and (10), we obtain the solution for concentration:

$$C = t_{ad}(C_0g(t) - M_0 \frac{\partial g(t)}{\partial t}) \quad (14)$$

The diffusion coefficient was determined by fitting the late-time tailing of breakthrough curves plotted using the analytical solution (14) to the simulated curves obtained from the numerical modeling.

3. Results and Discussion

3.1. Isolation of the extraction well

Three well-field configurations were tested to determine the extent to which the extraction well is isolated from the surrounding plume. Breakthrough curves for scenario 1, the homogeneous domain with no contaminant initially present in the test zone, are shown in Fig. 2. A small concentration increase occurs at the beginning of the test for configuration II, after which the concentration decreases to and remains at zero for the remainder of the test period. The small initial concentration increase is due to capture of the surrounding plume by the inner extraction well (Ex1). However, the concentration decreased to zero after water injected via In2 was captured by Ex2, resulting in isolation of Ex1 from the regional plume. Conversely, concentrations for both the traditional configuration and configuration I reach asymptotic conditions in later periods because the regional flow remains captured by the extraction well. The results indicate that configuration II provided full isolation of Ex1 from the plume. Therefore, this configuration was the focus of additional investigation.

Breakthrough curves for scenario 1b, the layered domain with clay units inside the test zone not initially contaminated, with configuration II are presented in Fig. 3A. Concentrations stabilize at certain values in the later period because mass residing in the clay units located outside of the test zone slowly diffuses to the clay units within the test zone and thereafter diffuses to the sand unit. The concentration stabilizes at a higher value for the layered simulation in which the clay units both inside and outside the test zone are initially contaminated (scenario 1a), as would be anticipated. These results are in contrast to those obtained for the simulations for the homogeneous domain, wherein the concentrations decrease to 0, and illustrate the impact of back diffusion from the clay units.

Breakthrough curves for scenario 1 for the 2D heterogeneous domain with clay units present and absent are presented in Fig. 3B. An asymptotic elution curve is observed for the simulation where clay units were absent. Conversely, as noted above, no tailing was observed for the homogeneous simulations. These results suggest that Ex1 is still influenced by the surrounding plume for the 2D heterogeneous simulation, which can be attributed to the preferential flow caused by the permeability heterogeneity. The breakthrough curve for the simulation with clay units present shows greater tailing than the curve for the corresponding simulation with no clay units, exhibiting the additional impact of back diffusion. A simulation was conducted with an adjusted distance between the inner well couplet, In1 and Ex1, from 4.375 m to 3.125 m. The results show that the concentration stabilizes at a very low C/C_0 value (Fig. 3B). This indicates that reducing the inner-well

distance achieved full isolation of Ex1 soon after test initiation, with only a very small concentration blip observed initially. The isolation status of Ex1 was examined for the 3D heterogeneous domain, and the results show breakthrough at a higher concentration and longer tailing than for the 2D heterogeneous domain (Fig. 3B). Clearly, Ex1 was influenced by the surrounding plume. Adjustment of the well separation distance and flow-rate distribution may improve isolation, as was observed for the 2D simulation.

A contaminant plume is typically present at sites of interest, which may influence results obtained for CET tests. Therefore, the time required to remove resident dissolved contaminant from the advective portion of the test zone was simulated. Forty three days (2.2PV) were required to sweep the test zone for the homogeneous simulation, whereas 90 days (4.5PV) were required for the layered simulation (Fig. SM-1). The late-time tailing of the breakthrough curve for this scenario and the curves for scenario 1 in which the sand unit within the test zone was clean are essentially identical, which indicates that after the test zone was swept, Ex1 was fully isolated from the plume and the tailing is caused by back diffusion. For the 2D simulation, approximately 150 days (7.7 PV) was required to sweep the test zone. For the 3D simulation, because of preferential flow, Ex1 remained impacted by the surrounding plume. The extent of this continued impact is further investigated below in section 3.2.

3.2. Magnitude of mass recovery

The magnitude of mass recovery was investigated in scenario 3 with modified configuration II for which the entire domain was clean and tracer solution was injected via In1. Concentration data were collected from Ex1 for the analysis. Concentrations were also monitored for the outer extraction well to evaluate capture effects, particularly for the heterogeneous simulations. Cumulative tracer mass extracted from each well was calculated. The magnitude of mass recovery for Ex1 was defined as the ratio of mass extracted from Ex1 to the total mass extracted from both wells. Results are presented in Fig. SM-2 and Table 2. Mass balance was checked by comparing the total mass extracted from wells and mass remaining in the domain to the total tracer mass injected. Mass balance was conserved for all simulations with errors within $\pm 5\%$.

100% mass was recovered by Ex1 for the homogeneous and layered simulations (Table 2). As seen in Fig. SM-2, the concentration for Ex1 for both homogeneous and layered simulations reached steady state and the concentration for Ex2 stabilized at 0 during the entire simulation period. According to the results of scenario 1 discussed in section 3.1 in simulations with modified configuration II, Ex1 was completely isolated from the surrounding plume, therefore, the dilution for Ex1 was caused only by water injected via In2. All mass removed from the domain was attributed to extraction from Ex1.

The mass recovery proportions for Ex1 were also calculated for scenario 4 wherein the tracer was injected for 10 days, followed by clean water injection for the conditions listed in Table 2. Low mass recovery for Ex1 was observed for both 2D and 3D heterogeneous simulations due to preferential flow phenomena. As discussed above for results of scenario 1, in simulations with modified configuration II, Ex1 was still impacted by the surrounding plume, therefore, significant dilution caused by the regional flow occurred in this scenario.

Additional simulations wherein the distance between injection and extraction wells and flow rates were changed were simulated for the 2D heterogeneous domain to investigate the impact of these two factors on mass recovery and dilution. These simulations and the corresponding mass recovery proportions are listed in Table SM-1. With the distance between inner wells reduced from 4.375 m to 3.125 m, and a larger pumping rate for Ex1, the mass recovery increased to 99%. Moreover, according to the results for scenario 1, full isolation from the surrounding plume was established for Ex1 with adjustment of distance between inner wells. These results indicate that appropriate configuration of the system can increase the mass-recovery proportion and significantly decrease the dilution impact from regional flow for Ex1 in a highly heterogeneous field.

3.3 Parameter estimation for tracer tests with pulse injection

Breakthrough curves produced for scenario 4 are presented in Fig. 4. The breakthrough curve for the homogeneous simulation shows the most ideal behavior wherein after breakthrough, the concentration drops continuously to 0. Conversely, the breakthrough curves exhibit different degrees of tailing for the layered and heterogeneous simulations. The asymptotic condition is attained at a much lower concentration value for the 2D heterogeneous simulation than the layered simulation. This occurred because the mass was trapped in the region north of Ex1 in the sand (Fig. SM-3) wherein the permeability was relatively low compared to surrounding regions. Fig. SM-4 and Fig. SM-5 show the concentration contour maps for the clay layer adjoining with sand in the 2D heterogeneous domain and the layered domain. After tracer injection stopped, the concentration in the clay units in the regions above and below the sand wherein Ex1 was screened was lower than the concentration in the regions surrounding Ex1 within the sand unit (Fig. SM-4), leading to a lower persistent concentration.

Effective diffusion coefficients were estimated for the layered and heterogeneous simulations using two selected functions. Results are shown in Table 3. The values estimated by both methods are lower than the input value used for the numerical model. The calculated errors of the estimations compared to the input value are approximately 20% for method 1 and 60%~80% for method 2. According to the results in Table 3, method 1 provided reasonable estimations in three different conditions, which indicates that the heterogeneity of the field did not have a significant impact on parameter estimation.

Method 1 was based on a matrix diffusion model. The configuration that was used to develop the model was based on uniformly distributed concentration in the high-permeability unit during the loading period and a key assumption was made that the plume was removed immediately at time t' when the loading process stopped (Mcdade et.al., 2013). Conversely, for this study, the tracer was injected via the injection well, transported along with groundwater flow, and captured by the extraction well screened in the high permeable units within the test zone. Therefore, the concentration was not uniformly distributed and a certain amount of time was needed until the contaminant was removed from the transmissive unit. The differences in system conditions contributed to the lower estimation of the effective diffusion coefficient.

The breakthrough curves for numerical simulations and associated analytical solutions for method 2 are presented in Fig. SM-6. The analytical solutions match the late-time tailing behavior of the simulated breakthrough curves for the three different conditions, but the calculated errors of the estimation compared to the input value are as high as 79%. This is because the analytical solution was developed to characterize the coefficient from a single-well injection-withdrawal tracer test. For the coupled injection-extraction system in this study, the flow field around Ex1 is impacted by the pumping of Ex2, which is another reason for the resulting smaller estimated results.

4. Summary

Two modified well-field configurations were studied in homogeneous, layered, and heterogeneous domains using 3D numerical modeling. Different scenarios were simulated to investigate the isolation status of and mass recovery for the extraction well, and the time frame to remove resident contaminant from the test zone. Results demonstrate that the inner extraction well (Ex1) can be fully isolated from the plume with configuration II. The impact of dilution from regional flow on concentration for Ex1 can be eliminated with appropriate well-couplet distance and flow rate distributions. The time period to remove resident contaminant from the test zone depends on the size of the test zone and well-field configuration including pumping rates and well locations. The results of this research indicate that the performance of contaminant elution and tracer tests can be improved by use of well-field configuration II employed in this work.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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Fig. 1. CET tests well-field configuration with schematic flow patterns. A. Traditional single injection-extraction dipole configuration. B. Modified coupled injection-extraction configuration I. C. Modified coupled injection-extraction configuration II.

Fig. 2. Breakthrough curves for scenario 1 with three different well configurations simulated in homogeneous domain. For the simulation with modified configuration II, data were collected from Ex1.

A

B

Fig. 3.

Breakthrough curves for scenario 1 with modified well configurations II. A. Layered domain. B. 2D and 3D heterogeneous domain. In figure 3A, “diff IC” represents the results for scenario 1a in which the clay units within the test zone were contaminated initially while the sand unit within the test zone was clean, and “same IC” represents the results for scenario 1b in which the initial concentration within the test zone is uniform as 0. In figure 3B, ‘No clay’ represents the results for simulations conducted in 2D heterogeneous domain with clay units absent. ‘4.375m’ and ‘3.125m’ represents the distance between inner wells.

A

B

Fig. 4. CET tests for scenario 4 with modified configuration II under different conditions. A. Arithmetic scale. B. Logarithmic scale.

Table 1

Summary of simulations conducted with configuration II in various conditions

Cases	Simulation ID	Well-field	Aquifer	Initial condition
S1	1	Traditional ECET	Homo ²	Test zone was clean, background was contaminated. Clean water was injected via injection well.
	2	MWC I ¹	Homo	
	3	MWC II	Homo	
	4	MWC II	Layered ³	S1a The clay units were all contaminated.
				S1b The regions in clay units above and below the test zone were clean.
				S1c The upper and lower units were contaminated, and all three units were set as sand.
	5	MWC II	2D Heter ⁴	Note: Distance of inner well couplets was 4.375 m
S2	6	MWC II	2D Heter	Note: Distance of inner well couplets was 3.125 m
	7	MWC II	3D Heter ⁵	
	1	MWC II	Homo	The entire domain was contaminated. Clean water was injected via both injection wells.
	2		Layered	
	3		2D Heter	
	4		3D Heter	
S3	1	MWC II	Homo	The entire domain was clean. In2 injected clean water, In1 injected contaminants with constant concentration 1g/m ³ . Mass recovery for Ex1 was determined.
	2		Layered	
	3		2D Heter	
S4	1	MWC II	Homo	The entire domain was clean. In2 injected clean water, In1 injected tracer for 10 days followed by clean water injection.
	2		Layered	
	3		2D Heter	
	4		3D Heter	

¹ Modified well configuration

² Homogeneous domain

³ Layered domain with clay unit, sand unit, clay unit

^{4,5} 2D and 3D heterogeneous domains generated randomly

Table 2

Magnitude of mass recovery for Ex 1

	Mass in (g)	Mass out (g)		Remaining mass (g)	Mass balance error ³	Mass recovery ⁴
	injected	extracted by Ex1	extracted by Ex2			
Homo ¹	500.00	498.9	0.003	8.67	-1.5%	100%
Layered ¹	500.00	473.9	0.002	8.57	3.5%	100%
Homo ²	10.00	9.9	0.14	0.00	-0.4%	99%
Layered ²	10.00	9.6	0.07	0.29	0.1%	99%
2D Heter ²	10.00	7.7	1.9	0.29	0.3%	77%
3D Heter ²	10.00	4.7	3.9	1.24	1.3%	55%

¹For scenario 3, mass was injected constantly via In1 through the entire simulation period.²For scenario 4, mass was injected via In1 for 10 days followed by clean water injection for 100 days.³The mass balance error represents the difference between the sum of extracted mass + remaining mass and the total injected mass.⁴Mass recovery is calculated as mass extracted by EX1 divided by the total mass extracted from both extraction wells.

Table 3

Estimated diffusion coefficient (cm²/d) using two selected functions in different conditions

Domains	Method 1 estimation (Error) ¹	Method 2 estimation (Error) ¹	Model input
Layered	60 (54-65) ² (-21%) ¹	31 (29-33) ² (-59%) ¹	76
2D heterogeneous	56 (50-61) ² (-26%) ¹	16 (14-18) ² (-79%) ¹	
3D heterogeneous	60 (54-66) ² (-21%) ¹	25 (23-27) ² (-67%) ¹	

¹The calculated difference between mean estimation and model input.

²Values reported in the parentheses represent the range of estimates with 95% confidence level (Table SM-2).