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The Impact of Well-Field Configuration on Contaminant Mass Removal and Plume Persistence for Homogeneous versus Layered Systems

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Abstract

A three-dimensional numerical model was used to simulate the impact of different well-field configurations on pump-and-treat mass removal efficiency for large groundwater contaminant plumes residing in homogeneous and layered domains. Four well-field configurations were tested, Longitudinal, Distributed, Downgradient, and natural gradient (with no extraction wells). The reductions in contaminant mass discharge (CMDR) as a function of mass removal (MR) were characterized to assess remediation efficiency. Systems whose CMDR-MR profiles are below the 1:1 relationship curve are associated with more efficient well-field configurations. For simulations conducted with the homogeneous domain, the CMDR-MR curves shift leftward, from convex-downward profiles for natural gradient and Longitudinal to first-order behaviour for Distributed, and further leftward to a sigmoidal profile for the Downgradient well-field configuration. These results reveal the maximum potential impacts of well-field configuration on mass-removal behaviour, which is attributed to mass-transfer constraints associated with regions of low flow. In contrast, for the simulations conducted with the layered domain, the CMDR-MR relationships for the different well-field configurations exhibit convex-upward profiles. The nonideal mass-removal behaviour in this case is influenced by both well-field configuration and back diffusion associated with low-permeability units.

Keywords

Groundwater contaminant plume; back diffusion; mass flux; pump and treat; plume persistence

1. Introduction

Pump and treat continues to be used at many sites to contain and treat groundwater contamination. A recent National Research Council report concludes that it is unlikely that remediation of these complex sites will be achieved in a time frame of 50–100 years under

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current methods and standards (NRC, 2013). Multiple factors, including the presence of source zones containing organic liquids, dispersed reservoirs of dissolved contaminant present in lower-permeability zones, sorbed contaminant, and hydraulic-related factors such as non-optimal remedial well-field performance, have long been identified as contributing to plume persistence and limited effectiveness of pump and treat (e.g., Chapman and Parker, 2005; Parker et al., 2008; Brusseau et al., 2007, 2011; Rasa et al., 2011; Brusseau and Guo, 2014; Matthieu et al., 2014; Keely, 1989; Johnson and Pankow, 1992; Mutch et al., 1993; Wilson et al., 1993; Rabideau and Miller, 1994; Keely, 1989; Goltz and Oxley, 1991; Brusseau, 1993; Rabideau and Miller, 1994; Berglund and Cvetkovic, 1995). One set of factors that have received relatively minimal attention are those related to well-field hydraulics, such as the number and location of pumping wells and the associated pumping schemes (e.g., Satkin and Bedient, 1988; Keely, 1989; Schafer and Kinzelbach, 1992; Cohen et al., 1997; Rivett et al., 2006; Guo and Brusseau, 2017). In particular, few of these studies have investigated the quantitative impacts of well-field hydraulics on mass-removal efficiency or provided a comparative analysis to other factors.

Guo and Brusseau, 2017 evaluated the impact of well-field configuration for very heterogeneous systems that were generated using the standard stochastic approach based on the Gaussian method and described by Gutjahr, 1989. However, they did not investigate the particular case of sites with areally extensive low-permeability layers adjacent to regional-scale aquifer systems, which are prevalent at many hazardous waste sites. Previous studies have demonstrated the importance of diffusive mass transfer into, within, and out of low-permeability (minimal flow) zones for solute transport (e.g. Gillham et al., 1984; Feenstra et al., 1984; Haggerty and Gorelick, 1995; Labolle and Fogg, 2001) and specifically for plume persistence and removal (e.g., Labolle and Fogg, 2001; Chapman and Parker, 2005; Brusseau and Guo, 2014; Matthieu et al., 2014). However, there has been minimal prior investigation of the relative contributions of diffusive mass transfer (back diffusion) and well-field hydraulics to contaminant mass removal and plume persistence.

The objective of this research is to quantify the influence and significance of well-field hydraulics on mass-removal efficiency. A 3D mathematical model is used to simulate solute transport and removal for three model well-field configurations, and in addition for natural-gradient conditions as a control. Simulations are generated for homogeneous systems to focus exclusively on the impact of well-field configuration, and for layered systems to allow comparative assessment of the impacts for systems with extensively continuous low permeability layers. Mass-removal efficiency is assessed by characterizing reductions in contaminant mass discharge (CMDR) as a function of reductions in contaminant mass (MR). Prior investigations of remediation efficiency have used this metric successfully (e.g., Jawitz et al., 2005; Brusseau et al., 2008; Kaye et al., 2008; DiFilippo et al., 2010; Brusseau et al., 2013; Brusseau and Guo, 2014). The previous research efforts that have applied the CMDR-MR metric were conducted primarily for source-zone systems or for systems with combined sources and plumes. The work reported herein represents an application focused solely on mass removal for plume-scale systems.

2. Materials and Methods

2.1. Numerical Model

The flow model used in this work was the 3D finite-difference numerical model MODFLOW developed by the U.S. Geological Survey (McDonald and Harbaugh, 1988). The 3D solute transport model MT3DMS (Zheng and Wang, 1999) was used to simulate solute transport. Groundwater Vista (GV) (Rumbaugh and Rumbaugh, 2007) was used as the graphical user interface. For layered systems, accurate simulation of diffusion processes is important to obtain robust results. Therefore, a random-walk based method, RWet, which was developed to solve transport problems without causing numerical dispersion (Labolle, 2006), was used for select simulations to evaluate the accuracy of MT3DMS in representing diffusion processes.

The 3D movement of ground water is described by the partial-differential equation (McDonald and Harbaugh, 1988):

$$\frac{\partial}{\partial x} \left(K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial h}{\partial z} \right) + W = S_s \frac{\partial h}{\partial t} \quad (1)$$

where K_{xx} , K_{yy} , and K_{zz} (L/T) are values of hydraulic conductivity along the x, y, and z coordinate axes; h (L) is the potentiometric head; W (T^{-1}) is a volumetric flux per unit volume representing sources ($W > 0$) and/or sinks ($W < 0$) of water. S_s (L^{-1}) is the specific storage of the porous material and t is time (T).

The 3D solute transport in transient groundwater flow systems can be described by the partial differential equation (Zheng and Wang, 1999):

$$\frac{\partial(\theta c)}{\partial t} = \frac{\partial}{\partial x_i} \left(\theta D_{ij} \frac{\partial c}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (\theta v_i c) + q_s c_s + \sum r_n \quad (2)$$

where θ (dimensionless) is the porosity of the subsurface medium; c (M/L^3) is the dissolved concentration; $x_{i,j}$ (L) is the distance along the respective Cartesian coordinate axis; D (L^2/T) is the hydrodynamic dispersion coefficient tensor; v_i (L/T) is the seepage or linear pore water velocity; q_s (T^{-1}) is the volumetric flow rate per unit volume of aquifer representing fluid sources (positive)/ sinks (negative); c_s (M/L^3) is the aqueous solute concentration of the source or sink flux, $\sum r_n$ ($M/L^3/T$) is the chemical reaction term.

RWet adds an additional term to manage the discontinuities of the standard advection–dispersion equation, which is written as (LaBolle et al., 1996; Labolle, 2006):

$$\begin{aligned} \frac{\partial}{\partial t}[\theta(\mathbf{x}, t)c(\mathbf{x}, t)] = & - \sum_i \frac{\partial}{\partial x_i} [v_i(\mathbf{x}, t)\theta(\mathbf{x}, t)c(\mathbf{x}, t)] + \sum_{i,j} \frac{\partial}{\partial x_i} \left[\theta(\mathbf{x}, t)D_{ij}(\mathbf{x}, t) \frac{\partial c(\mathbf{x}, t)}{\partial x_j} \right] \\ & + \sum_k Q_k(\mathbf{x}, t)c_k(\mathbf{x}, t)\delta_k(\mathbf{x} - \mathbf{x}_k) + \sum_n R_n - s_{dd} \end{aligned} \quad (3)$$

where c_k [M/L³] is the aqueous phase concentration in the flux Q_k [L³/T] of water at $\mathbf{x}_k$, δ is a Dirac function; s_{dd} represents the rate of loss or gain of aqueous mass to and from a second domain in a dual domain (mobile-immobile) regime, such as would occur through matrix diffusion to and from the matrix domain in a fracture-matrix regime. The concentration of an aqueous solute is represented by a finite system of N_p particles of mass $m_p(t)$ via (Tompson, 1987; LaBolle et al., 1996):

$$R\Theta(\mathbf{x})c^s(\mathbf{x}, t) = \sum_{p \in N_p} m_p(t)\xi(\mathbf{x} - \mathbf{X}_p(t)) \quad (4)$$

where R is the retardation factor; $\mathbf{X}_p(t)$ is the location of particle p at time t ; ξ is an interpolation, or projection function (Bagtzoglou et al., 1992) to “smooth” the spatial distribution of concentration.

The model study area was 400,000 square meters. The domain was divided into a regular orthogonal grid consisting of 20 rows and 50 columns with grid space 20-m $\times$ 20-m. Specified head boundaries were used along the four borders of the domain, with natural gradient (0.001) inducing groundwater flow under confined conditions from the west to east. Details of the model domain and associated input parameters are given in Table SM-1. Parameters used in the model were determined according to information generated from geologic borehole-logs, pumping tests, and historic data collected for the Tucson International Airport Area Superfund site (Zhang and Brusseau, 1999). First order sorption kinetics was used with a retardation factor of 1.43, a distribution coefficient of 0.04 cm³/g, and sorption rate coefficient of 15 d⁻¹. Initial solute concentration was set as 1 g/m³ in the whole domain, representing a mature site that has been formed over decades. No additional contaminants were introduced into the system.

Simulations were conducted for both homogeneous and layered domains. For the majority of simulations, the domain was 15 m in total thickness split into fifteen layers of equal, uniform thickness. For the homogenous system, characteristics such as hydraulic conductivity (K) and porosity were identical for each layer. For the layered system, the upper and lower five layers were set as low hydraulic conductivity representing clay units, while the center five layers was set as high permeability representing a sand unit. The pumping wells were screened through the middle (sand) layers.

2.2. Simulations

All simulations were conducted with MT3DMS with exception to those additional simulations conducted with RWheT. Four major variables, well-field configuration, pumping

rate, permeability, and aquifer thickness were investigated in this study. The simulations were organized into three groups (Table 1). Domain thickness and pumping rates were varied within reasonable ranges.

Group 1 was designed to investigate the impact of well-field configuration. Three simplified representative well-field configurations were tested (Fig. 1). The Distributed configuration comprises 9 wells distributed uniformly within the plume and the pumping rate for each well was $100 \text{ m}^3/\text{d}$. The Downgradient configuration comprises 3 wells located at the downgradient edge of the plume, oriented normal to the mean flow direction. The Longitudinal configuration comprises 3 wells placed along the centerline of the plume, oriented parallel to the mean flow direction. The pumping rate for each well was $300 \text{ m}^3/\text{d}$ for simulations with the Downgradient and Longitudinal configurations. In addition, a “natural-gradient” configuration (with no extraction wells) was used as a control. Solute mass removal was monitored at the downgradient edge of the domain for this simulation, and the magnitude of the natural hydraulic gradient was increased from 0.001 to 0.0075 to match the total extraction-well discharge ($900 \text{ m}^3/\text{d}$) for the other scenarios. The impact of back diffusion was also examined by comparing the simulations conducted for the homogeneous and layered domains with different well-field configurations.

One additional simulation was performed for the Longitudinal well-field scenario to investigate the impact of well-field modification during operations. Specifically, the total time was split into 3 periods. In period 1, the original well-pumping locations were used; in period 2, the well-pumping locations were moved to regions wherein concentrations remained relatively high because of stagnation zones caused by pumping in period 1; in period 3, the well-pumping locations were relocated to their original locations.

Group 2 was set up to test the impact of pumping rate on mass-removal efficiency. The simulations were conducted using the Distributed well-field configuration that was used in the Group 1 simulations for the homogeneous and layered domains (Table 1). Three different pumping rates (Q), 300, 100, $50 \text{ m}^3/\text{d}$ for each well, were tested, with pumping continuous and constant throughout the simulation period. An additional simulation was conducted to test the impact of changes in Q during operation. For this simulation, the total simulation time was divided into three periods. For the 1st and 3rd periods, pumping was constant at $100 \text{ m}^3/\text{d}$. For the 2nd period, the pumping rates of individual wells were adjusted (Table SM-2). The Damkohler number (ω), which represents the ratio of the hydraulic residence time to the characteristic time of mass transfer, was used to identify conditions wherein mass transfer was constrained and thus limiting to mass removal. The definition of ω is provided in the Supplemental Materials.

Group 3 was developed to examine the impact of domain thickness on mass removal. The simulations were conducted for homogeneous and layered domains with two thicknesses using the Longitudinal and the natural-gradient configurations. The total thickness was 1.5 m for the first set of simulations and 15 m for the second simulation set (5 m sand and 10 m clay). The 1.5 m domain was split into 3 layers with 0.5 m thickness for each layer (0.5 m sand and 1 m clay). The total pumping rates were 900 and $90 \text{ m}^3/\text{d}$ for the 15-m and 1.5-m simulations.

2.3. Data analysis

Elution curves were plotted and compared for different scenarios. Simulations with more significant mass-transfer constraints are anticipated to produce more non-ideal behavior, including earlier reductions in concentrations and more extensive tailing. The simulated time-continuous profile of CMD was determined as the product of the pumping rate and the simulated concentration. The cumulative mass removed was calculated from the CMD-time function. The CMDR-MR profile was constructed using the CMD and mass removal data.

Generally, the relationship between reductions in contaminant mass discharge and mass removal exhibits one of three types of behavior (Fig. SM-1). One is the 1 to 1 relationship, which represents for example the special case of first-order mass removal. The second is a curvilinear convex-upward profile residing above the 1 to 1 reference line, which shows significant initial reduction in CMD with minimal mass removed, followed in later stages by smaller rates of CMD reduction. This behavior is often associated with the impacts of mass-transfer constraints related to contaminant mass present in hydraulically poorly accessible zones. The third relationship is the convex-downward profile residing below the reference line, which shows relatively ideal mass removal behavior wherein there is minimal reduction in CMD until a large proportion of mass has been removed. In this study, for scenarios wherein mass was lost due to boundary outflow, the CMDR-MR relationship curves were corrected using the final total removed mass to force the mass removal fraction to reach 1. Analysis of both temporal concentration data and the CMDR-MR profiles make the assessment of contaminant removal dynamics more robust.

3. Results and discussion

3.1. Homogeneous domain

The simulated elution curves with four different well-field configurations for the homogeneous domain are presented in Fig. 2A. The elution curve for the natural-gradient scenario shows the most ideal behavior in which the concentration decreased rapidly after approximately 1 pore volume (PV) of water was displaced. In contrast, for scenarios with pumping wells, the elution curves exhibit earlier decreases in concentration as well as asymptotic approaches to low concentrations (tailing). The simulation for the Distributed well-field configuration shows first-order mass removal behavior. Notably, the simulation for the Downgradient well-field configuration shows multi-step behavior, with an initial sharp decrease followed by a steady state period, and then a rapid decline to low concentration.

The results presented above show that varying degrees of non-ideal behavior were observed for the simulations produced for all three well-field systems compared to the natural-gradient control. Given that the simulations were conducted for a homogenous domain with uniform initial concentration, the non-ideal mass removal behavior must be caused by mass-transfer constraints associated with well-field hydraulics. The formation of stagnation zones wherein contaminant removal is delayed due to low groundwater velocities is an obvious source of such constraints.

The contaminant mass distributions at selected time periods for each simulation are presented in Fig. SM-2. Fig. SM-2A shows the mass distribution at 1000 days of the natural

gradient simulation, which produced a near-ideal elution curve. The mass was completely removed by day 4040 (2.4 PV). This is consistent with the absence of stagnation zones. Fig. SM-2B and E present the mass distributions after 1000 days (0.6 PV) of pumping for the simulations with Longitudinal and Distributed well-field configurations, respectively. It is apparent that more mass remained for the Distributed well field, which is a result of more inter-well stagnation zones formed for the Distributed well field.

For the Downgradient well-field simulation, the concentration started to decrease 15 days after pumping started, and stabilized after 860 days (0.5 PV). The steady state period lasted until 6520 days (3.9 PV), after which concentration began to decrease again until the remaining mass was removed. Fig. SM-2F presents the mass distribution after 500 days (0.3 PV) of pumping for the Downgradient well-field simulation. The concentration decreased quickly because of the rapid mass removal and strong dilution occurring in the vicinity of the wells. Fig. SM-2G displays the mass distribution after 4000 days (2.4 PV). This is during the steady state period for contaminant removal, which is mediated by slow advective transport of the upgradient mass via natural-gradient flow. Fig. SM-2H shows the concentration distribution at 8000 days (4.8 PV). By this time, all of the remaining contaminant mass had migrated into the zone of influence of the extraction wells, allowing for more rapid removal and attendant reduction in concentration. This spatially and temporally non-uniform mass-removal behavior resulted in the multi-step elution curve.

The differences in the proportion of mass remaining in the domain for the different simulations indicate that the Longitudinal well-field developed the least amount of stagnation area among the three systems with pumping wells. The scenario with the Downgradient well-field configuration, which presented multi-step mass removal behavior, had the greatest proportion of regions with low flow that included the downgradient stagnation zones and the upgradient low flow area where no wells were present.

The CMDR-MR profiles are presented in Figure 2B. The CMDR-MR relationship for the natural gradient simulation exhibits a curvilinear convex-downward profile residing below the one-to-one reference line. The CMD did not start to decrease until 60% of the initial mass was removed, indicating ideal mass-removal conditions. This result is expected given that the simulation employed a homogeneous domain with no pumping wells (and associated stagnation zones), and therefore no non-accessible mass, nor associated mass-transfer limitation, was present. The CMDR-MR curve for the Longitudinal well-field scenario also exhibits a convex-downward profile residing below the reference line. However, it is shifted leftward such that CMD started to decrease after approximately 15% mass removal, reflecting the presence of mass-transfer constraints associated with stagnations zones.

The Distributed well-field simulation expresses an approximately one-to-one profile, consistent with the pseudo first-order concentration reduction exhibited by the elution curve. The Downgradient simulation shows a multi-step CMDR-MR profile wherein CMD started to decrease after minimal mass removal, and attained ~80% reduction by 30% mass removal. After this point there was minimal further reduction in CMD until approximately 80% mass removal, after which the profile exhibited approximate one-to-one behavior.

Rivett et al. (2006) conducted a small field experiment at the Borden (ON) research site to examine plume removal behavior after isolation of the source zone. The experiment was conducted in a sandy aquifer with mild heterogeneity. A permeable reactive barrier and an extraction well were used to contain the source zone. Two extraction wells located along the centerline of the plume were used for mass removal. This configuration is similar to the Longitudinal well-field configuration used herein. The rate of contaminant removal was observed to be slower than expected for ideal conditions, and the elution curves exhibited concentration tailing. The authors concluded that permeability heterogeneity and sorption processes had minimal impact on plume persistence because the experiment was conducted in a mildly heterogeneous sandy aquifer and the plume was freshly formed. Hence, the mass-removal limitation was attributed to inter-well stagnation zones associated with the well field. The raw concentration-time data reported in Rivett et al. were used herein to determine CMDR and mass removal values, which were then used to create the CMDR-MR profile presented in Fig. 2B. The measured profile for the Borden study is similar to the simulated profile obtained for the Longitudinal well-field configuration, which supports the validity of the simulation results.

3.2. Layered domain

The elution curves for simulations conducted with MT3DMS and RWheT for natural gradient and Longitudinal well-field configurations in the layered domain are presented in Fig. SM-3 and Fig. SM-4, respectively. For both configurations, significant differences are observed between the higher-resolution (1-m thick layers) and lower-resolution (5-m thick layers) MT3DMS simulations. Comparison to the RWheT results shows that the higher-resolution MT3DMS results match very well, demonstrating that diffusion processes were accurately represented for that case. These results illustrate that finer grids are necessary to simulate diffusion processes accurately, as indicated by previous studies (Chapman et al., 2012; Rasa et al., 2011; Carey et al., 2015).

The elution curves obtained for the layered domain, with a sand unit sandwiched between two clay units, are presented in Fig. 3A. For the natural gradient simulation, the concentration decreased asymptotically after an initial sharp decrease. The initial decrease represents removal of mass from the sand unit, while the tailing represents the impact of back diffusion from the clay units. Similar results were observed for the Longitudinal and Distributed well-field configuration scenarios. Conversely, the simulation results for the Downgradient well-field configuration shows multi-step behavior, as discussed for the homogeneous domain, followed by low-concentration tailing. For all of the layered-domain simulations, essentially all contaminant mass was removed from the sand unit before the start of the asymptotic stage. After mass was removed from the sand unit, the concentration tailing for all scenarios merged into the same line, which indicates the strong mass-transfer constraints attributed to the clay units. The impact from well-field configuration is minimal at this stage. The mass distributions in the sand unit were very similar to those obtained for their corresponding homogeneous-domain simulations (data not shown).

The CMDR-MR profiles for the layered-domain simulations are presented in Fig. 3B. The profile for the natural gradient simulation is strongly sigmoidal, with an initial steady-state

period, during which the mass discharge reduction was minimal. After approximately 20% of the mass was removed, the mass discharge decreased significantly ($>95\%$) with a small reduction in mass ($<20\%$). Finally, the remaining mass discharge reduction occurred asymptotically. For the Longitudinal and Distributed well-field configurations, the mass discharge decreased significantly ($\sim 95\%$) after a very small fraction of mass was removed, and thereafter exhibited asymptotic behavior. The distribution of remaining mass for the simulation with the Longitudinal well-field in the layered domain is presented in Fig. SM-5. After 0.8 PV of water was extracted, almost all of the mass in the sand unit had been removed and the remaining mass was in the clay units. As expected, the concentration started to decrease asymptotically after this point (Fig. 3A). The simulation results of the Downgradient well-field configuration display a multi-step profile as observed for the homogeneous domain.

The CMDR-MR profiles for mass removal from the middle (sand) unit are presented in Fig. 3C. The profiles are observed to be very similar to the corresponding profiles obtained for the homogeneous-domain simulations. The different mass removal behaviors during this period are the result of different well-field configurations as discussed above. The CMD reduction reached asymptotic condition immediately after the contaminant mass in the sand unit was removed for all the layered-domain simulations (Fig. 3B), which indicates that the persistence of CMD in the latter period was due to mass-transfer constraints associated with back diffusion of the contaminants present in the upper and lower clay units.

The results of two simulations with Longitudinal well-field configuration for the layered domain with K of the clay units equal to 0.1 m/d and 0.00001 m/d are also presented in Fig. 3 as “Longitudinal_clay_0.1” and “Longitudinal_clay_0.00001”. The boundary conditions were changed to constant head boundaries for the west and east borders for these two simulations to prevent mass loss from the north and south boundaries, which will impact the CMDR-MR relationship. As expected, minimal differences are observed for the elution curves and CMDR-MR profiles. After mass was removed from sand unit, the concentrations for the simulation with K of clay unit equal to 0.1 m/d is higher than the concentrations for other simulations as the larger vertical flow from clay to sand (10^4 times larger than simulations with K of clay units equal to 0.00001 m/d). The mass in clay transported to sand through advection and diffusion, and the higher concentration in later period resulted in more mass removal reflected in the CMDR-MR profile with rightward shift after approximately 25% mass was removed. The difference between curves of “Longitudinal” and “Longitudinal_clay_0.00001” is caused by the impact of boundary condition, which is discussed in Supplementary Materials. The comparison between simulations conducted for the layered domain with thicknesses of 15 m and 1.5 m is presented in Fig. 4. As expected, the elution curves and CMDR-MR profiles for simulations conducted for the domain with 15 m thickness are less ideal compared to the corresponding curves for the domain with 1.5 m thickness. Because the thicker clay layers mean longer mass transfer time compared to the residence time of the aquifer, resulting in relatively non-ideal mass transfer behavior.

3.3. Impact of well-pumping location and pumping rate

As discussed above, low flow regions are introduced as a result of well-field operations. Under these circumstances, initiating pumping in these stagnation zones can remove the trapped mass more effectively. The impact of changing well-pumping location was investigated for the Longitudinal well-field configuration, with the first adjustment implemented after 1500 days (0.9 PV) in the homogeneous domain. Inspection of the elution curve in Fig. 2A shows that the concentration increases after the change of locations of the pumping wells, as would be expected. The contaminant distribution after 1700 days of operation for the original (no change in pumping locations) and the modified scenarios are presented in Fig. SM-2C and Fig. SM-2D, respectively. It is apparent that the mass remaining after operation of 1700 days (~1 PV) is much less for the modified scenario. After adjustment, it took 2040 days (1.2 PV) to remove 90% of the mass instead of 2120 days (1.3 PV). The CMDR-MR profile shifts rightward after the adjustment for the simulation with adjusted locations of extraction, reflecting the reduced mass-transfer constraint (Fig. 2B). The similar shapes of the profiles for original and modified scenarios indicate that repositioning the well-pumping locations did not have a significant impact on the general shape of the CMDR-MR profile for this specific scenario.

The impact of pumping rate on mass removal efficiency in the homogeneous and layered domains was examined for the Distributed well-field configuration. Three rates were used, 50, 100 (value used for all prior simulations), and 300 m³/d, and the results are presented in Fig. 5 for the homogeneous system. Similar CMDR-MR profiles are observed for the 100 and 300 m³/d pumping rates, indicating that mass removal is insensitive to pumping rates for these conditions. Plume capture was incomplete for the lower pumping rate of 50 m³, and thus a portion of mass was not recovered with the extraction wells. The CMDR-MR curve was generated in this case using the mass remaining in the model domain at each time step, resulting in the profile shifting rightward of the other two (Fig. 5).

For simulations conducted with the layered domain, similar mass-removal behavior was observed for all three pumping rates both before and after mass was completely removed from the sand (Fig. SM-6). Asymptotic conditions were attained in the later stage of mass removal for all three pumping rates because of mass-transfer constraints associated with the clay units (Fig. SM-6A). The ω values are 0.028, 0.014, and 0.005, respectively, for the pumping rates of 50, 100, and 300 m³/d. As illustrated in Fig. SM-7, mass removal is not sensitive to the change in pumping rates over the tested range, which is also reflected in the similar CMDR-MR profiles (Fig. SM-6). The very low ω values (close to or less than 0.01) reflect the condition wherein mass transfer is very slow compared to the hydraulic residence time. Hence, the observed insensitivity of mass removal to Q is to be expected.

The small ω values, which is inversely correlated to the thickness of the low-permeability unit, are likely typical for sites with continuous, thick low-permeability units. Conversely, the ω values would likely be larger for systems with thin, discontinuous clay units for all other factors being the same. This latter scenario was investigated with additional simulations, using pumping rates for each well of 5, 10, and 30 m³/d and thinner clay units (thickness = 0.5 m each). The corresponding ω values are 2.7, 1.3, and 0.4, respectively, for these conditions. Mass removal is observed to be sensitive to the pumping rates (Fig. SM-7)

for the ω values used in these simulations. Hence, the CMDR-MR curves in Figure SM-8 show clear differences for the different pumping rates. Comparison of the profiles presented in Figure SM-6A and SM-8 shows that larger pumping rates lead to leftward shifts of the profiles to a point at which the profile becomes insensitive to Q .

The CMDR-MR profile for the simulation for which pumping rates were adjusted 1000 days after the operation started is also presented in Fig. 5 and Fig. SM-6. The adjusted pumping rates for each well are listed in Table SM-2. The CMDR-MR curve for the simulation with adjusted pumping rates shifts to the right of the curve obtained for the system with constant pumping rates. After the pumping rates were adjusted, the contaminant that was trapped in the inter-well stagnation zones was pumped out along the changed flow paths, removing more mass with higher CMD. It took 2750 days for the system with changed pumping rates to remove 90% of mass instead of 3760 days for the system with constant pumping rates.

For the simulations conducted for the layered domain, this effect was reflected in the process when removing mass from the sand (Fig. SM-6B). After all contaminant was removed from the sand, mass removal was dominated by back diffusion from the clay units, therefore, the impact of pumping rate was not significant. The system with constant pumping rates took 2430 days to remove all mass from the sand layer, whereas the system with adjustment of pumping rates only took 2020 days, shortening the period by approximately one year. Fig. SM-6 presents mass distribution maps for the simulations conducted for the layered domain after 1500 days of pumping for both the constant- Q (Fig. SM-9A) and non-constant- Q (Fig. SM-9B) systems. The mass remaining after 1500 days of pumping in the domain was much less for the simulation with pumping rates changed. Therefore, adjustment of the pumping rates during the operation period can change the flow patterns, reduce and even remove the stagnation zones formed by previous well-field hydraulics, and therefore, increase mass-removal efficiency.

4. Conclusion

For the homogenous-domain simulations, the CMDR-MR relationships exhibit convex-downward profiles residing below the 1:1 reference line for natural gradient flow. With the advent of low-flow zones formed for different well-field configurations, the CMDR-MR curves shift leftward, from convex-downward profiles for natural gradient and Longitudinal to first-order behavior for Distributed, and further leftward to a sigmoidal profile for the Downgradient well-field configuration. The homogeneous-domain results reveal the maximum potential impact of well-field configuration, for which the observed non-ideal behavior is attributed solely to mass-transfer constraint caused by formation of low flow regions (i.e., well hydraulics). The formation of these stagnation zones reduces the effectiveness of pump and treat. This illustrates the need for dynamic system operations, wherein the system is routinely monitored and operational conditions are modified to maintain peak performance.

In contrast to the homogeneous system, the simulations conducted for the layered domain exhibit convex-upward CMDR-MR profiles for the different well-field configurations. Differential mass-removal behaviors are observed during the initial stage of mass-removal

from the middle (sand) unit (during which well-field configuration is controlling) and the latter, asymptotic stage wherein mass removal is mediated by diffusive mass transfer from the clay units. The results of this study illustrate that well-field configuration can have a significant impact on mass-removal and plume-persistence behavior for plume-scale systems.

The natural-gradient configuration exhibited the most ideal behavior due to the absence of stagnation zones. While this produces the most effective mass-removal operation in terms of lowest volume of groundwater extracted, it typically is not the optimal approach in general. First, the remediation time frames would typically be longer for natural-gradient systems, which may be an issue for some sites. Second, the natural-gradient condition provides no plume control, which is critical for many sites.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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Contaminant Treatment Zone

Figure 1.

Schematic presenting the three tested well-field configurations. The fourth configuration tested was a natural-gradient system with no wells.

A

B

Figure 2. Impact of well-field configuration on mass removal behavior in homogeneous domain: A. Elution curves; B. CMDR-MR relationships, results from Rivett et al. (2006) also included in the figure.

A

B

C

Figure 3.

Impact of well-field configuration on mass removal behavior in layered domain: A. Elution curves; B. CMDR-MR relationships. C. CMDR-MR for mass removal process in sand layer. “Longitudinal_clay_0.1” and “Longitudinal_clay_0.00001” represent the results of simulations conducted with Longitudinal well-field configuration in layered domains with K of the clay layers equal to 0.1 m/d and 0.00001 m/d. The boundary conditions were changed to constant head boundaries in west and east borders for these two simulations.

A

B

Figure 4. Impact of aquifer thickness on mass removal behavior for the Longitudinal well-field and natural gradient simulations in layered domain: A. Elution curves; B. CMDR-MR relationships.

Figure 5. Impact of total pumping rate, Q (m³/d), on mass removal for Distributed well-field configuration in homogeneous domain. Damkohler numbers are close or less than 0.01.

Table 1

Simulation summary

Group ID	Parameters	Scenarios	Well-field Configuration	Permeability Distribution	Notes
G1	Well-field configuration and Permeability	1	Natural Gradient	Homo/Layered	Simulations with well-pumping location adjustment were conducted.
		2	Longitudinal		
		3	Distributed		
		4	Downgradient		
G2	Pumping rate	1	Distributed	Homo/Layered	Q=300m ³ /d/well
		2			Q=100m ³ /d/well
		3			Q=50m ³ /d/well
		4			Adjusting pumping rate in period 2, after 1000d
G3	Thickness	1	Natural Gradient	Homo/Layered	Domain thickness, 1.5 m and 15 m.
		2	Longitudinal		
		3	Distributed		
		4	Downgradient		