Journal of Hazardous Materials 333 (2017) 109–115

Contents lists available at ScienceDirect

Journal of Hazardous Materials

journal homepage: www.elsevier.com/locate/jhazmat

The impact of well-field configuration and permeability heterogeneity on contaminant mass removal and plume persistence

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HIGHLIGHTS

- Examined mass removal processes for very heterogeneous plume-scale systems.
- The relationship between reduction in CMD and MR (CMDR-MR) was used as a metric.
- Impact of well-field hydraulics was differentiated from the impact of heterogeneity.
- CMDR-MR profiles vary with system properties and are mediated by hydraulic conditions.

ARTICLE INFO

Article history:
Received 4 August 2016
Received in revised form 10 February 2017
Accepted 5 March 2017
Available online 8 March 2017

Keywords:
Plume
Back diffusion
Mass flux
Groundwater remediation
Pump and treat

ABSTRACT

The purpose of this study is to investigate the effects of well-field hydraulics and permeability heterogeneity on mass-removal efficiency for systems comprising large groundwater contaminant plumes. A three-dimensional (3D) numerical model was used to simulate the impact of different well-field configurations on pump-and-treat mass removal for heterogeneous domains. The relationship between reduction in contaminant mass discharge (CMDR) and mass removal (MR) was used as the metric to examine remediation efficiency. The impacts of well-field configuration on mass removal behavior are attributed to mass-transfer constraints related to regions of low flow associated with the well field, which can be muted by the influence of permeability heterogeneity. These impacts are reflected in the associated CMDR-MR profiles. Systems whose CDMR-MR profiles are below the 1:1 relationship line are associated with more efficient well-field configurations. The impact of domain heterogeneity on mass-removal effectiveness was investigated in terms of both variance and correlation scale of the random permeability distributions and indexed by the CMDR-MR relationship. Data collected from pump-and-treat operations conducted in a section of the Tucson International Airport Area (TIAA) federal Superfund site were used as a case study. The comparison between simulated and measured site data supports the general validity of the numerical model, and results from the case study are consistent with the conclusions of the theoretical study. These results illustrate that the CMDR-MR relationship can be an effective way to quantify the impacts of different factors on mass-removal efficiency.

1. Introduction

Contamination of groundwater resources by a variety of organic and inorganic substances continues to be a significant issue of import for human health and water-resources sustainability in many regions of the US and elsewhere. The remediation of groundwater-contamination sites is a costly, time-consuming endeavor that is constrained by the persistence of groundwater contaminant plumes [1]. Understanding and quantifying the factors that contribute to plume persistence is critical to effective site cleanup.

The results of prior investigations have clearly indicated that the presence of source zones containing organic liquids (NAPL sources) is typically a primary factor limiting the cleanup of groundwater contaminant plumes at many sites. However, research conducted at sites for which the source zone has been remediated or contained demonstrates that the contaminant plumes have continued

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http://dx.doi.org/10.1016/j.jhazmat.2017.03.012
0304-3894/

to persist [e.g.,1–8], indicating that additional factors contribute to persistence. The factors beyond uncontrolled source zones that contribute to plume persistence include dispersed reservoirs of dissolved and sorbed contaminant present in lower-permeability zones [e.g.,9–16] and hydraulic-related factors such as non-optimal remedial well-field performance [e.g.,9,17–20].

The results of several modeling- and field-based studies conducted over the past decade clearly illustrate the contribution of dispersed mass to plume persistence [e.g.,2–7,21–23]. The impact of this dispersed mass on plume persistence and its significance for constraining mass removal via for example pump and treat operations will depend on several factors, including the properties of the contaminant and associated transport and fate behavior, the magnitude of contaminant mass present, and physical properties of the domain (e.g., heterogeneity). Several studies have examined the impact of permeability heterogeneity on contaminant-mass removal [e.g.,13,18,24–26]. However, these studies employed domains with relatively small degrees of heterogeneity. For example, the variance of permeability ($\sigma^2_{\ln K}$) is often used as an index of the magnitude of permeability variability. In the prior studies cited, the $\sigma^2_{\ln K}$ values were small and spanned a relatively narrow range (0.5–3). However, recent field studies have shown that typical subsurface systems have significantly larger $\sigma^2_{\ln K}$ values, in the range of 5–15, and in some cases as high as 30 [e.g.,27,28]. Thus, studies need to be conducted with larger $\sigma^2_{\ln K}$ (>5) to more fully investigate mass-removal processes in heterogeneous systems.

As noted above, well-field hydraulics is another factor that can influence plume persistence. The impact of well-field hydraulics, such as well location and distribution, has been investigated by numerical modeling [e.g.,17,18] and in a field study [e.g.,20]. While the significance of well-field hydraulics for remediation effectiveness has long been recognized, there has to date been minimal investigation of the quantitative impacts on mass-removal efficiency or comparative analysis to other factors.

The objective of this research is to quantify the influence and significance of permeability heterogeneity and well-field hydraulics on mass-removal efficiency for domains with large degrees of heterogeneity. Numerical modeling is conducted for a wide range of permeability variabilities and several well-field configurations. The results are evaluated using a recently-developed metric that examines the relationship between reductions in contaminant mass discharge (CMDR) and reductions in contaminant mass (MR). This metric has been demonstrated to be an effective method to examine remediation efficiency [e.g.,4,6,29–35]. The previous research efforts that have applied the CMDR-MR metric were conducted for source-zone systems or for systems with combined sources and plumes. The work reported herein represents an initial application focused solely on mass removal for plume-scale systems in the absence of NAPL sources.

2. Methods

The flow model used in this work was the finite-difference numerical model MODFLOW developed by the U.S. Geological Survey [36,37]. The solute transport model MT3DMS [38] was used to simulate solute transport. Groundwater Vista (GV) [39] and Groundwater Modeling System (GMS) [40] were used as graphical user interfaces. The model study area was 400,000 square meters. The domain was divided into a regular orthogonal grid consisting of 40 rows and 100 columns with grid space 10-m × 10-m. Specified head boundaries were used along the four borders of the domain, with a 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 provided in the Supplementary materials.

Several sets of simulations were conducted to examine the impact of permeability heterogeneity on mass removal. A fully heterogeneous domain was developed using the standard stochastic approach. The application and potential limitations of this approach are discussed in Section 1 of Supplementary Materials. A random field generator [41] was used to derive realizations of K for the aquifer unit of the domain (5 m thickness), which was divided into 20 layers with thickness of 0.25 m for each layer. The permeability was treated as a stationary, lognormally distributed stochastic property, with a mean $\langle \ln K \rangle$ and variance σ^2_Y. The random fields were generated with an arithmetic mean value of K equal to 20 m/d and correlation scales of 50-m (longitudinal) × 20-m (transverse) × 0.25-m (vertical). R_λ was used to represent the ratio of domain length to correlation length,

$$R_\lambda = L/\lambda,$$

where L[L] is the domain length, and λ[L] is the correlation length. Scenarios with or without adjoining clay units present above and below the aquifer unit were simulated (Table SM-2). The total thickness of the domain with adjoining clay units is 15 m (60 layers). Simulations were also conducted to investigate the impact of well-field hydraulics. This was done by testing four different well-field configurations (Fig. SM-1). Details of the model configurations and simulations are provided in Supplementary Materials (SM-1.1 and SM-1.2). Additional simulations were conducted for a contaminated site that is part of the Tucson International Airport Area (TIAA) federal Superfund site in southern Arizona. Details are presented in SM-1.4. Simulation results were analyzed by evaluating CMDR-MR profiles (see details in Supplementary materials).

3. Results and discussion

3.1. Impact of well-field configuration

The impact of well-field configuration on mass removal is presented in Fig. 1. The simulated elution curves for four different well-field configurations are presented in Fig. 1A. The elution curve for the natural-gradient scenario shows the most ideal behavior in which the concentration decreased rapidly to lower values. In contrast, for scenarios with pumping wells, the elution curves express earlier concentration decreases and asymptotic approach to low concentrations (tailing). 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 varying degrees of non-ideal behavior for simulations produced for all three well-field systems compared to the natural-gradient control is due to mass-transfer constraints associated with stagnation zones that are caused by well-field hydraulics.

The contaminant mass distributions at selected time periods for each simulation are presented in Fig. SM-7. Fig. SM-7A shows the mass distribution at 160 days of the natural gradient simulation when CMD started to decrease with approximately 25% of mass removed. Apparent preferential flow is observed and lower concentration zones start to appear in downgradient regions much earlier compared to the expected time frame for a homogeneous domain, which is due to preferential flow associated with the higher K regions. 90% of the initial mass was removed by day 920 (1.6 PV). Fig. SM-7B and D present the mass distributions after 180 days of pumping for the simulations with Longitudinal and Distributed well-field configurations, respectively. With more wells, the Distributed well-field configuration was less influenced by preferential flow compared to the Longitudinal well-field con-