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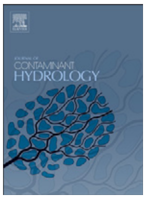

Optimal design of active spreading systems to remediate sorbing groundwater contaminants in situ

Amy N. Piscopo *, Roseanna M. Neupauer, Joseph R. Kasprzyk

University of Colorado Boulder, 1111 Engineering Drive, Boulder, CO 80309, USA

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ABSTRACT

The effectiveness of in situ remediation to treat contaminated aquifers is limited by the degree of contact between the injected treatment chemical and the groundwater contaminant. In this study, candidate designs that actively spread the treatment chemical into the contaminant are generated using a multi-objective evolutionary algorithm. Design parameters pertaining to the amount of treatment chemical and the duration and rate of its injection are optimized according to objectives established for the remediation – maximizing contaminant degradation while minimizing energy and material requirements. Because groundwater contaminants have different reaction and sorption properties that influence their ability to be degraded with in situ remediation, optimization was conducted for six different combinations of reaction rate coefficients and sorption rates constants to represent remediation of the common groundwater contaminants, trichloroethene, tetrachloroethene, and toluene, using the treatment chemical, permanganate. Results indicate that active spreading for contaminants with low reaction rate coefficients should be conducted by using greater amounts of treatment chemical mass and longer injection durations relative to contaminants with high reaction rate coefficients. For contaminants with slow sorption or contaminants in heterogeneous aquifers, two different design strategies are acceptable — one that injects high concentrations of treatment chemical mass over a short duration or one that injects lower concentrations of treatment chemical mass over a long duration. Thus, decision-makers can select a strategy according to their preference for material or energy use. Finally, for scenarios with high ambient groundwater velocities, the injection rate used for active spreading should be high enough for the groundwater divide to encompass the entire contaminant plume.

1. Introduction

Sorbing contaminants in groundwater pose many challenges to remediation methods. Because some portion of the sorbing contaminant remains attached to the soil matrix, remediation methods that remove only the aqueous-phase contaminant, such as pump-and-treat, have proven unsuccessful at remediating sorbing contaminants (Kavanaugh et al., 2003). With in situ remediation, a treatment chemical is injected into the contaminated aquifer to react with and degrade the aqueous-phase contaminant. As the aqueous-phase contaminant is degraded, the sorbed-phase contaminant partitions into the aqueous-phase, allowing the degradation process to continue. The effectiveness of in situ remediation depends on the degree of contact between the injected treatment chemical and the contaminant (Siegrist et al., 2012); therefore, a key challenge in the design of in situ remediation systems is to ensure that the treatment chemical is adequately delivered throughout the contaminant plume.

Some recent advances to address this challenge involve modifying treatment chemical properties or modifying the subsurface flow conditions. Since viscosity is one property that affects the mobility of the treatment chemical in the subsurface, studies have investigated the use of amendments to increase

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* Corresponding author at: UCB 428, Boulder, CO 80309-0428, USA.
E-mail addresses: amy.piscopo@colorado.edu, amy.piscopo@gmail.com (A.N. Piscopo).

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viscosity of the treatment chemical. For instance, McCray et al. (2010) demonstrated in lab experiments with tanks layered with sands of different grain sizes that the proportion of the tank contacted by the treatment chemical could be increased significantly by amending the treatment chemical with xanthan gum to increase its viscosity. To modify subsurface flow, pneumatic and hydraulic fracturing have been applied during in situ remediation to create pathways for treatment chemical transport in the subsurface. In a field study, Scheutz et al. (2010) used hydraulic fracturing to facilitate the transport of the treatment chemical through low-permeability soils, which led to more complete degradation of the chlorinated solvents present at that site.

Active spreading techniques are another option for modifying subsurface flow. These techniques use pre-defined injections and extractions of water at wells surrounding the contaminant plume to generate flow fields that spread the plumes of groundwater contaminant and treatment chemical in a manner that increases their contact. Neupauer and Mays (2014) simulated an injection of treatment chemical into a plume of sorbing contaminant, followed by extractions of clean water at well locations surrounding the plume to draw the treatment chemical through the contaminated region. Results demonstrated that this active spreading approach achieves nearly complete contaminant degradation for fast rates of contaminant sorption and desorption relative to the treatment period and high reaction rate coefficients, but the approach was less effective for contaminants with slow rates of sorption and low reaction rate coefficients (Neupauer and Mays, 2014).

In this study, a multi-objective evolutionary algorithm (MOEA) is used to optimize active spreading during in situ remediation to remediate a sorbing contaminant in a two-dimensional, isotropic, confined aquifer. We consider both homogeneous and heterogeneous aquifers. To represent a variety of different types of sorbing contaminants, six cases are optimized in this study, each with a different combination of reaction and sorption properties. Three design parameters — the mass of treatment chemical injected, the rate of treatment chemical injection, and the duration of its injection — are optimized to maximize contaminant degradation while minimizing material and energy requirements. Each solution to the optimization problem is comprised of a unique set of design parameter values. Additionally, optimization of the in situ remediation system is conducted for three different ambient velocities and for two different remediation time frames to determine how the solutions to the optimization problem vary under these conditions. All optimal designs (i.e. solutions) are analyzed to understand how the design parameters of the solutions relate to the remediation objectives and to the reaction and sorption properties of the contaminant.

The remainder of this paper is structured as follows. Section 2 introduces the active spreading system considered in this work and provides the governing equations used to model advection, dispersion, sorption, and reaction during in situ remediation. Section 3 introduces multi-objective optimization in the context of groundwater applications and then describes the specific optimization framework used in this study, which includes objective function equations and design parameters definitions. Section 4 presents the results of the multi-objective optimizations, and analyzes how the sorption and reaction rates affect the in situ remediation system design and performance. Section 5 discusses the applicability of the results to the current practice of in situ remediation. Section 6 provides conclusions.

2. Reactive transport modeling

This study simulates in situ remediation of a two-dimensional circular plume of sorbing groundwater contaminant, which has an initial mass of m_1° and an initial plume radius of r_{init} (Fig. 1a). The contaminated aquifer is assumed to be confined, isotropic, and two-dimensional. At the start of remediation, the contaminant is assumed to have partitioned to equilibrium between the aqueous and sorbed phases. Although some contaminants can require weeks to months to reach equilibrium (Pignatello and Xing, 1996), the preparation and implementation of remedial action plans for contaminated groundwater sites are rarely completed in that time frame; thus, the assumption of equilibrium between phases at the start of remediation is valid.

The approach used here to remediate a sorbing contaminant with active spreading is to inject a non-sorbing treatment chemical into a well located at the center of the contaminant plume, forming a circular plume of treatment chemical surrounded by the contaminant plume following the injection phase approach of Neupauer and Mays (2014). During this injection, the treatment chemical and contaminant plumes move radially away from the injection well. Because the contaminant movement is retarded due to sorption, the treatment chemical plume moves more rapidly and overlaps the contaminant plume (Fig. 1b), which provides the opportunity for contaminant degradation. Injection occurs for a time T until the outer edge of the treatment chemical plume has passed beyond the outer edge of the contaminant plume. If no reaction were to occur, the positions of the treatment chemical and contaminant plumes after the injection would be as shown in Fig. 1b, with final radii r_{tc} and r_f for the treatment chemical and contaminant plumes, respectively.

Since the contaminant moves radially away from the injection well during the injection period, treatment chemical injected near the end of the injection period never encounters contaminant. For this reason, it is not necessary to inject the treatment chemical throughout the entire injection period. Instead, the treatment chemical is injected for a duration of $T' < T$, and clean water is injected for the remainder of the injection period. The treatment chemical and contaminant plumes at time T are shown in Fig. 1c without reaction and Fig. 1d with reaction.

For this system, reactive transport with bimolecular reaction is governed by the advection-dispersion-reaction equation, given by

$$\frac{\partial C_1}{\partial t}+\frac{\rho_b}{n}\frac{\partial S_1}{\partial t}=-\nabla\cdot(\mathbf{v}C_1)+\nabla\cdot(\mathbf{D}\nabla C_1)-kC_1C_2 \tag{1a}$$

$$\frac{\partial C_2}{\partial t}=-\nabla\cdot(\mathbf{v}C_2)+\nabla\cdot(\mathbf{D}\nabla C_2)-kFC_1C_2+\frac{Q}{b}C_{2I}\delta(\mathbf{x}-\mathbf{x}_w) \tag{1b}$$

$$\frac{\partial S_1}{\partial t}=\alpha_s(K_dC_1-S_1) \tag{1c}$$