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Radial basis function simulation of slow-release permanganate for groundwater remediation via oxidation

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ABSTRACT

An emerging strategy for remediation of contaminated groundwater is the use of permanganate cylinders for contaminant oxidation. The cylinders, which are only a few inches in diameter, can be placed in wells or pushed directly into the subsurface. This work focuses on the modeling and simulation of the reactive process to better understand the design of a group of cylinders for large scale contaminated sites. The underlying model is a coupled system of nonlinear partial differential equations accounting for advection, dispersion, and reactive transport for a contaminant and the permanganate in two spatial dimensions. Radial Basis Functions collocation method is used to simulate different spatial arrangements of the cylinders to understand the behavior of the system and gain insight into designing a remediation strategy for a large-scale contaminated region. Since the radial basis function collocation method is a meshless method, the locations of the cylinders are not tied to a numerical grid, making it an attractive choice for determining optimal placement. Our focus is to (1) identify a domain of influence measuring the effectiveness of the injected cylinders, (2) understand the placement for multiple cylinders required to effectively clean-up a given domain, and (3) determine a protocol for injecting multiple cylinders over time. We provide numerical results showing that domain of influence is a way to measure the effectiveness of installed cylinders. Domain of influence of one through three sources are simulated. Placement of two cylinders for an area of 13*ft* by 3*ft* and three sources for an area of 26*ft* by 6*ft* are sufficient to clean the contaminant within a reasonable time period. The average concentrations of oxidant and contaminant are simulated for the cases of a third cylinder is installed at different time and locations.

1. Introduction

In Situ Chemical Oxidation (ISCO) with permanganate (MnO_4^-) is a common technology used to treat contaminated groundwater. ISCO is the delivery of chemical oxidants, typically via injection, to groundwater to degrade contaminants. One challenge with traditional ISCO is the rapid dissolution and reaction of the oxidant in the environment. Often, the oxidant concentration is very high immediately after injection, but decreases rapidly over time due to reaction with reduced

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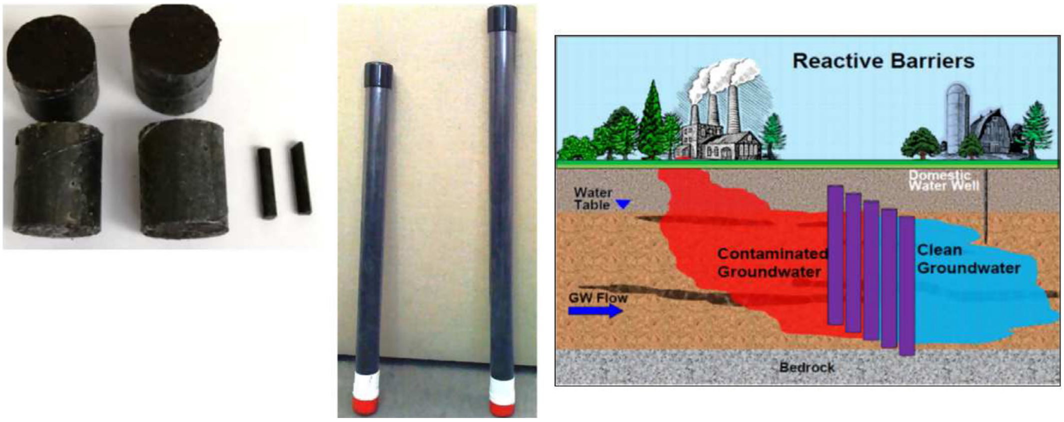

Fig. 1. MnO_4^- cylinders and their use in the field courtesy of Carus Corporation.

subsurface constituents, which is referred to as natural oxidant demand (NOD). Many injections typically need to be used in succession to fully treat a contaminated site, thereby driving up costs [1]. Also, there are several design challenges for ISCO (and other technologies involving delivery of liquid amendments). The first challenge occurs when a heterogeneous contaminated site contains finer textured soils that do not accept liquid injections. When this happens, the chemical will flow through the more permeable layers because this path offers the least resistance.

An approach to address these challenges is through the use of a encapsulated passive, slow-release oxidant, which is inserted and allowed to dissolve and intercept the contaminant over numerous years. Encapsulation prevents instant dissolution of the entire oxidant mass into the environment [2–4,1,5,6]. Studies have been conducted by Kang et al. [4] on the most effective, least reactive coating. They determined that paraffin wax polymer can best extend the oxidation lifespan. Some benefits of paraffin wax include that it is an environmentally benign product, it is safe to work with, it is solid at ambient temperatures, and it is insoluble in water. Its insolubility in water ensures that the oxidant contained within the shell is shielded from nonproductive use.

The first Slow Release Permanganate Cylinders (SRPCs) were manufactured in 2007. Now they are commercially available and manufactured through Carus Corporation, see Fig. 1. The cylinders can be installed in new or existing vertical and horizontal wells or installed using direct push technology. They can be vertically stacked and installed horizontally next to each other to cover the width and depth of a contaminant plume. Much headway has already been made towards the modeling of oxidant release into groundwater.

Mathematical modeling and simulation can be used to gain insight into the design of remediation strategies. Reactive transport models have found increased application in recent years in porous media [7,8]. This kind of models aims to provide reaction and transport dynamics of multicomponent system [9,8]. Early studies developed the theoretical basis of such models and necessary numerical tools to solve them. Some applications to problems of reactive contaminant transport in groundwater and flow through reacting hydrothermal systems are introduced in [10,11]. Work was conducted by Wolf (2013) [12] and Slaugh (2015) [13] to develop a slow-release oxidant design tool focused on the release of oxidant from cylinders and its reactive transport in 1-D. The tool was based on the analytical solutions to two interactive chemical unsaturated groundwater flow models. Laboratory data were used to verify the oxidant release term. The tool was developed in Microsoft Excel, which was used because of its universal acceptance and its ease-of-use (Wolf, 2013) [12]. A draw back in [12] is the restriction to one spatial dimension since the lateral interaction between cylinders was not considered.

In this paper, the reaction between MnO_4^- and a single contaminant in an ISCO diffusion–transport reaction model is simulated by a system of coupled partial differential equations in two-dimensional space. Radial basis function collocation method (RBFCM) is used to simulate different spatial arrangements of the injection points when planning the system. RBFCM is a method that uses scattered points in domains and the function values at the points to approximate solutions to PDEs. Mesh and numerical integration are not needed in the discretization process. The first RBFCM was introduced by Kansa in 1990 [14]. Since then, RBFCM have been widely used for solving various kinds of science and engineering problems, including heat transfer [15], porous media flow [16], the classical De Vahl Davis natural convection problem [17] etc. [18–20]. The main attraction of RBFCM is its effectiveness in dealing with high dimensional problems and complicated domains.

To the best of our knowledge, the earliest application of radial basis function (RBF) to groundwater problems is in 2002 [21]. The authors applied RBFCM to a steady state problem and a single linear transport equation in 2D and 3D. Since then, many researchers applied meshless methods to groundwater modeling problems to overcome the difficulties from other numerical techniques such as the finite difference methods, the finite volume method, the finite element method and others [22,23]. The focus of this work is to apply RBFCM to a coupled system of transient nonlinear PDEs in groundwater problems. An oxidant source term is included to represent the slow release of the oxidation cylinder. There are more complex and robust cases of applications of RBF collocation method on nonlinear system of PDEs that have been previously reported in the literature. For example, [24] focuses on numerical performance of RBF method on different kinds of PDEs. [25] focuses