Many-Objective Algorithm to Optimize Contaminant Degradation during In Situ Remediation by Engineered Injection and Extraction

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ABSTRACT

Although in situ treatment methods exist for remediation of contaminated groundwater, the rate of contaminant degradation that occurs is often limited. During in situ remediation, the treatment solution (e.g. chemical oxidant injected to degrade the contaminant) should ideally be spread throughout the contaminated region, leading to more opportunities for degradation reactions. However, for traditional in situ remediation methods, where the treatment solution is transported only by ambient groundwater flow, spreading is poor, and thus the contact and reaction between treatment solution and contaminant is limited. Spreading can be enhanced using engineered injection and extraction (EIE), in which transient flow fields are induced using a sequence of injections and extractions of clean water at wells surrounding the contaminant plume. Simulations of in situ remediation using one particular sequence of EIE have shown that spreading due to EIE can enhance reaction; however, a new approach is needed to design high-quality EIE sequences that consider multiple engineering performance objectives. This study uses a multi-objective evolutionary algorithm (MOEA) to determine a set of EIE sequences that balance multiple objectives, such as maximizing the amount of reaction while minimizing the volume of treatment solution required and the mass of treatment solution extracted. Because the MOEA can be used for any contamination scenario, (e.g. for sites with various degrees of aquifer heterogeneity, aqueous versus sorbing contaminants, numbers of wells, and locations of wells), it is a valuable tool that expands the relevance and applicability of EIE.

MOTIVATION

Around the world, people rely on groundwater resources to meet their basic freshwater needs; however, groundwater is frequently contaminated by industrial and agricultural sources. While prevention of groundwater contamination is undoubtedly preferable, instances of groundwater contamination are inevitable in today's industrialized world; therefore, a clear need exists for groundwater remediation methods. In situ remediation is one approach to treating contaminated groundwater, where a treatment solution (usually a chemical oxidant) is injected into an aquifer to degrade the groundwater contaminant. However, the degradation that occurs during in situ remediation is limited to areas where the treatment solution and groundwater contaminant contact each other. Natural phenomena, such as ambient groundwater flow and aquifer heterogeneity, provide a degree of spreading which can influence the position of the treatment solution relative to the contaminant, allowing for degradation reactions to occur. Engineered injection and extraction (EIE) is a novel technique that can enhance spreading significantly, using a sequence of injections and extractions of clean water at wells that surround the groundwater contaminant plume and the added treatment solution. The EIE sequence is designed to stretch and fold the plume within the contaminated zone. Spreading induced during EIE (i.e. plume reconfiguration due to advection and macrodispersion) provides increased contact between reactants, which thereby promotes mixing of these reactants by the molecular diffusion and pore-scale dispersion that only operate over small characteristic length scales (Weeks and Sposito, 1998; Bellin et al., 2011). In consequence, EIE leads to more contaminant degradation and ultimately reduces the duration of treatment (Piscopo et al., 2013).

ENGINEERED INJECTION AND EXTRACTION

Piscopo et al. (2013) simulated EIE in a two-dimensional, confined, isotropic aquifer with ambient groundwater flow traveling from east to west. Homogeneous and heterogeneous aquifers were modeled. The treatment solution and contaminant were assumed to be aqueous, and their reaction was modeled as a complete, instantaneous reaction. Figure 1 shows the conceptual model, where four wells are located around the plume of treatment solution and contaminant, each at a distance of L=25m from the origin. The 12-step sequence of EIE is given in Table 1, where each step of the sequence lasts 6.25 days. The sequence was designed such that no net injection or extraction of clean water occurs.

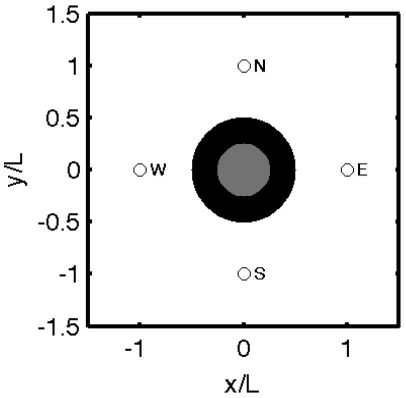

Figure 1. Plan view of model aquifer showing the initial positions of the treatment solution (gray) and contaminant (black) particles. The small open circles denote the four wells, identified by cardinal direction.

Step	Active Well	Injection Rate, Q (m^3/d)
1	W	875
2	E	875
3	W	-250
4	E	-750
5	W	-400
6	E	-350
7	S	875
8	N	875
9	S	-250
10	N	-750
11	S	-400
12	N	-300

Table 1. Engineered injection and extraction sequence used in this study. Negative injection rates represent extraction.

Simulations have shown that EIE can increase the amount of contaminant mass reacted during in situ remediation by six to seven times in homogeneous and heterogeneous aquifers respectively, as compared to in situ remediation without EIE (Piscopo et al., 2013).

OPTIMIZATION

All previous work by Piscopo et al. (2013) considered the same unique EIE design, comprising the 12-step sequence of pumping rates and well locations given in Table 1. In the current phase of work, we optimize the EIE design to maximize the contaminant mass reacted, while considering the following secondary objectives:

- Minimize treatment solution extracted: This objective is to reduce in-well reactions between the treatment solution and contaminant, which can lead to clogging.
- Minimize groundwater contaminant extracted: This objective is to promote in situ remediation, rather than pump-and-treat, which avoids certain regulatory requirements.

- Minimize mean pumping rate: This objective is to save energy.
- Minimize volume of treatment solution required: This objective is to reduce cost.

The objectives of the multi-objective problem formulation are often conflicting, and could evolve as we learn more about the problem. The algorithm is constrained such that the pumping rate magnitudes sum to zero to insure that there is no net injection or extraction during EIE. Multiple constraints can be used iteratively to develop multiple problem formulations as we advance with the optimization work (Kasprzyk et al., 2012).

The optimal design will likely depend on factors such as the contaminant distribution, aquifer properties, and chemical properties of the contaminant. We initially conduct the optimization for a basic aquifer scenario similar to the one described in the previous section, focusing on homogeneous aquifers without ambient flow. Later stages of work will investigate different possible aquifer contamination scenarios. Finally, we will also consider conducting the optimization for different design parameters, like the number of wells, the orientation of the wells, or the number of steps in the EIE sequence.

METHODS

The optimization will be conducted using an evolutionary algorithm, a search algorithm based on the mechanics of natural selection and genetics. Evolutionary algorithms use a simulation-optimization approach, by embedding a simulation model directly into the search process itself (Labadie, 2004). Starting with an initial population of known solutions, evolutionary algorithms measure the fitness of the solutions based on defined objectives, then generate new solutions from the current population using probabilistic operators (reproduction, crossover, and mutation) that mimic biological systems. As the process is repeated with the strongest solutions, the population should become increasingly fit until the process terminates (Goldberg, 1989). For a single objective evolutionary algorithm search, the search process terminates when one achieves an approximation to the single optimal solution for the problem.

However, in the presence of conflicting objectives, the analyst desires to find a tradeoff between the conflicting objectives. To solve such a problem, in this study we use a multi-objective version of an evolutionary algorithm, termed a MOEA (Nicklow et al., 2010; Coello Coello, 2007). The solution to a multiple objective problem is not a single optimal design for the system. Instead, we generate a high-quality approximation to the set of Pareto optimal solutions. A Pareto optimal set contains the solutions for which no other solutions perform better in all objectives. In other words, improving the performance of one objective for a solution in the Pareto optimal set requires diminishing the performance of another objective. For instance, in order to achieve higher contamination degradation for a solution in the Pareto optimal set, the pumping rate magnitudes must increase.

To determine the objective functions of the EIE designs generated by MOEA, the reactive transport of each design must be modeled. Reactive transport during simulations is governed by the advection-dispersion-reaction equation (ADRE)

$$\frac{\partial C_j}{\partial t} = -\nabla \cdot (\mathbf{v} C_j) + \nabla \cdot \mathbf{D} \nabla C_j - R \quad , \qquad (1)$$

where C_j is the concentration of the j^{th} species (j = 1 for the treatment solution, j = 2 for contaminant, and j = 3 for the reaction product), t is time, R is the reaction rate, $\mathbf{v}=(v_x,v_y)$ is the groundwater velocity vector, and $\mathbf{D}$ is the dispersion tensor. The velocity in (1) is based on flow fields in the aquifer, which reflect either injection or extraction at the specified well location and ambient groundwater flow.

We use random walk particle tracking methodology to simulate EIE during in situ remediation. Because we are considering homogeneous aquifers without ambient flow for the initial stages of optimization, we can use analytical solutions to model transport by advection. The movement of treatment solution and contaminant towards or away from the active well is given by

$$r = \sqrt{\frac{Q\Delta t}{\pi nb} + r_o^2} \quad , \tag{2}$$

where r_o is the initial distance from the active well, r is the final distance from the active well, Q is the injection rate, b is the aquifer thickness, n is the porosity, and Δt is the duration of the EIE step.

We calculate the dispersion component of (1) by adding random displacements to the particle positions. Random displacements in the direction of the local velocity vector and in the direction perpendicular to the local velocity vector are normally-distributed with zero mean and variances of $2\alpha_L \left|\mathbf{v}\right| \Delta t$ and $2\alpha_T \left|\mathbf{v}\right| \Delta t$, respectively, where α_L and α_T are the longitudinal and transverse dispersivities, respectively.

Reaction is modeled as an instantaneous irreversible reaction given by

$$C_1 + C_2 \rightarrow C_3 \quad , \tag{3}$$

where reactants C_1 and C_2 are the concentrations of the treatment solution and groundwater contaminant, respectively, and C_3 is the concentration of the reaction product, which is assumed to be inert. An instantaneous reaction allows us to evaluate how reaction is enhanced by stretching and folding, not by chemical kinetics. For convenience, the 1:1 stoichiometric ratio in (2) is assumed to imply a 1:1 mass ratio as well.

SUMMARY

Previous work demonstrates that EIE increases the amount of reaction that occurs during in situ remediation relative to passive in situ remediation techniques, where the injected treatment solution is transported only by ambient flow. The present work uses a MOEA to find a set of EIE sequence designs that balance specified objectives, such as maximizing the amount of contaminant mass reacted. Because the MOEA can ultimately be used for any contamination scenario, it is a valuable tool that expands the relevance and applicability of EIE.

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