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Stochastic cost optimization of DNAPL remediation – Method description and sensitivity study

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A B S T R A C T

A modeling approach is described for optimizing the design and operation of groundwater remediation at DNAPL sites that considers uncertainty in site and remediation system characteristics, performance and cost model limitations, and measurement uncertainties that affect predictions of remediation performance and cost. The performance model simulates performance and costs for thermal source zone treatment and enhanced bioremediation with statistical compliance rules and real-time operational system monitoring. An inverse solution is employed to estimate model parameters, parameter covariances, and residual prediction error from site data and a stochastic cost optimization algorithm determines design and operation variables that minimize expected net present value cost over Monte Carlo realizations. The method is implemented in the program SCOToolkit. A series of applications to a hypothetical problem yielded expected cost reductions for site remediation as much as 85% compared to conventional non-optimized approaches, while also increasing the probability of achieving "no further action" status in a specified timeframe by more than 60%. Optimizing monitoring frequency for compliance wells used to make *no further action* determinations as well as operational monitoring used to make decisions on individual remediation system components reveals tradeoffs between increased direct costs for sampling and analysis versus decreased construction and operating costs that arise because more data increases decision reliability. Optimizing protocols for operational monitoring and heating unit shutdown protocols for thermal source treatment (incremental versus all-or-none shutdown, soil versus groundwater sampling, number and frequency of samples) produced cost savings of more than 20%. Defining compliance based on confidence limits of a moving time window regression decreased expected cost and lowered failure probability compared to using measured extreme values over a lookback period. Uncertainty in DNAPL source delineation was found to have a large effect on the cost and probability of achieving remediation objectives for thermal source remediation.

1. Introduction

Optimization methods have been used increasingly to improve performance and reduce costs associated with groundwater remediation design and monitoring (Teutsch et al., 2001). Considerable work has been performed on optimization of long-term monitoring sampling locations and frequency (Loaiciga et al., 1992; EPA, 2000; Reed et al., 2000; Cameron and Hunter, 2002; Reed and Minsker, 2004; EPA, 2005; Parsons, 2005; EPA, 2007). User-friendly long-term optimization software tools have been developed by Aziz et al. (2003) and Harre et al. (2009) that utilize statistical methods to eliminate redundant well locations and to reduce sampling frequency.

Many studies have been reported involving optimization of pump-and-treat system design using deterministic groundwater models to minimize total pumping rate as a surrogate for operating cost (Gorelick et al., 1984) or considering fixed and operating costs (McKinney and Lin, 1996), with regulatory criteria (e.g., plume containment, time limits, etc.) treated as an optimization constraint (Wagner and Gorelick, 1987; McKinney and Lin, 1996), as a "penalty cost" for non-compliance in the objective function (Rizzo and Dougherty, 1996; Chan-Hilton and Culver, 2005), or as a criteria in multi-objective optimization (Erickson et al., 2002; Singh and Chakrabarty, 2011). Cost savings over trial-and-error methods

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ranging from 5 to 50% have been reported Becker et al. (2006) reported that simulation-optimization methods were able to identify solutions that cost less than, translating to cost savings of $600K to $10M for the sites studied.

Deterministic cost optimization identifies designs that minimize predicted costs if model parameters correspond to their best estimates. However, such an approach provides no "safety factor" for adverse deviations of model predictions from best estimates. Due to large uncertainties in groundwater model parameters and their predictions, deterministic optimization is thus likely to yield designs that have an unacceptably high probability of failure to meet design criteria. A number of authors have described stochastic optimization methods to take prediction uncertainty into consideration in the optimization process (Andricevic and Kitanidis, 1990; Lee and Kitanidis, 1991; Tucciarelli and Pinder, 1991; Wagner et al., 1992; Aly and Peralta, 1999; Teutsch and Finkel, 2002; Mugunthan and Shoemaker, 2004; Chan-Hilton and Culver, 2005; Feyen and Gorelick, 2005; Ricciardi, 2009).

Remediation of sites with dense nonaqueous phase liquid (DNAPL) source zones is particularly difficult due to their low solubility and long persistence (Cohen and Mercer, 1993; National Research Council, 1994). These sites often require source treatment to reduce the mass of DNAPL by excavation or in situ treatment via thermal or chemical oxidation, surfactant flushing or enhanced source biodecay (Liang and Falta, 2008; Heron et al., 2009; Thomson et al., 2007). Unfortunately, there is often a great deal of uncertainty in the location, total mass and spatial distribution of DNAPL within a site, which can introduce large uncertainty in design performance predictions. ITRC (2004) reviewed methods for identification and characterization of DNAPL source zones. Ayvaz (2010) and Datta et al. (2011) have described methods for source identification and parameter calibration using inverse modeling methods. Parker et al. (2010b) demonstrated that for a given data set available for model calibration, uncertainty in predicted source depletion exhibited increased above a minimum when model complexity increased or decreased from an optimum level. The optimum complexity increased and prediction uncertainty decreased when the information content of calibration data increased. Dokou and Pinder (2009, 2011) described a stochastic optimization method to design a sampling strategy to minimize uncertainty in DNAPL source parameters.

Dissolved plume containment or "polishing" of residual DNAPL source contamination in many cases will be accomplished more cost-effectively by introducing amendments to enhance in situ contaminant biodecay (Wymore et al., 2006) than by pump-and-treat methods. Mayer and Endres (2007) studied cost tradeoffs between source mass removal and dissolved plume remediation using a deterministic approach. In practice, optimal DNAPL site remediation may require a combination of technologies with tradeoffs among design variables for different systems. In addition to increasing the number of design variables, models capable of simulating multiple remediation technologies will require additional model parameters that will add to performance prediction uncertainty.

Cardiff et al. (2010) presented a semi-analytical model for DNAPL site remediation using thermal source treatment and/or electron donor injection for enhanced bioremediation with an optimization module to determine design variables to minimize expected cost to meet specified compliance criteria. Hypothetical cases were considered to optimize the duration of thermal source treatment and electron donor injection. Parker et al. (2010a) extended the approach to employ adaptive remediation termination criteria based on operational monitoring and investigated effects of monitoring frequency on expected cost.

In the present study, we extend the work of Cardiff et al. (2010) and Parker et al. (2010a) to consider the following:

- Effects of DNAPL source delineation uncertainty on thermal treatment performance reliability. In previous modeling efforts, we effectively assumed perfect source delineation knowledge, with no possibility of DNAPL mass outside of the specified thermal treatment area. Realistically, inaccurate source delineation is the most significant factor affecting the performance of thermal source treatment technologies. In this paper, we explicitly consider uncertainty in source delineation on thermal system performance.
- Methods of dealing with statistical outliers in compliance rules. In our previous efforts, "no further action" decisions were sensitive to outlier data. In the present work, we consider the effect of a compliance rule that employs regression confidence limits on a moving time window to attenuate the influence of outliers.
- Enhanced bioremediation model extensions. The current work considers model refinements to consider enhanced DNAPL dissolution associated with electron donor injection upgradient of source zones and nonequilibrium electron donor reactions.

Other improvements include revised cost models that explicitly treat costs for compliance and operational monitoring, an improved thermal mass removal model, and options to consider transport with nonlinear streamlines and multiaquifer plumes associated with localized vertical leakage. The methodology is implemented in the Stochastic Cost Optimization Toolkit (SCO-Toolkit) written in MATLAB.

The objective of this paper is to describe the methodology and present selected hypothetical case studies to demonstrate the interactions of operational and compliance monitoring strategies, compliance rules, and model and parametric uncertainty and their effects remediation design, cost and reliability.

2. Description of stochastic cost optimization approach

A comprehensive description of the modeling approach is available in a report by Parker et al. (2011), which can be retrieved online or from the authors on request. In the following, we present an overview that emphasizes previously unpublished features. A summary of symbols and acronyms used herein is given in Kim et al. (2011).

2.1. DNAPL source depletion and thermal treatment

The simulation model considers multiple DNAPL sources that may have different initial masses and dissolution kinetics. Considering the possibility of engineered manipulation in upscaled mass transfer kinetics, we describe the rate of contaminant mass dissolution in a given source zone, J [MT^{-1}], versus time, t, by

$$J(t) = F_{\mathrm{mt}}(t)J_{\mathrm{cal}}\left(\frac{M(t)}{M_{\mathrm{cal}}}\right)^{\beta} \quad (1)$$

where $J_{\mathrm{cal}} = J(t = t_{\mathrm{cal}})$ and $M_{\mathrm{cal}} = M(t = t_{\mathrm{cal}})$ in which t_{cal} denotes a reference date used for model calibration, M is the source contaminant mass remaining, β is a depletion exponent that reflects the DNAPL source "architecture," and F_{mt} is a time-dependent dimensionless mass transfer enhancement factor. The reference date is arbitrary since the $J(t)$ function is scalable with J and M values corresponding to any $t_{\mathrm{cal.}}$ within the span of time DNAPL is present. Integration of a source mass balance equation