then presenting for comment and revision. A single objective optimization problem is thereby posed and solved. An iterative process then occurs, at each step revising the objectives and constraints to address the concerns and requirements of various parties. Mathematical optimization methods are used increasingly to obtain the design, given the objective and constraints. Simulation models are generally used to predict the effect of a given design. In some cases, the response is approximated using response surfaces or artificial neural networks, for example.

There have been several prior reviews of the state of optimization in groundwater remediation problems. These include Gorelick (1983), Willis and Yeh (1987), Wagner (1995), Ahlfeld and Mulligan (2000), and Pinder et al. (2002). The latter contains a description of a number of issues and recent applications of optimization in groundwater remediation and monitoring. Additional background information may be found in USDOE (2002) and USEPA (2000).

A project entitled "Application of Flow and Transport Optimization Codes to Groundwater Pump-and-Treat Systems" is being funded by the Environmental Security Technology Certification Program to demonstrate optimization-simulation methods at three sites. Both transport optimization, based on contaminant transport models, and flow optimization, a simpler but more limited approach based only on groundwater flow models, are being performed by different parties using the same problem objective and constraints. The results of transport and flow optimization are being compared. Following completion of the optimization-simulation modeling, assistance will be provided to the sites in implementing the suggested modifications to the pump and treat system, and actual cost savings from recommendations that are implemented will be tracked for 2 years. It is expected that the draft final report for the project will be delivered by March 2003. An unattributed, informal, verbal personal communication has said that transport optimization led to 15 to 20% improvements over flow optimization, which in turn is a measurable improvement over the baseline designs.

The methods and applications reviewed above apply to the case of a single objective function. In real-world applications, multiple objectives are the rule, however. The presence of multiple objectives usually promotes a conflict situation, because the improvement in one objective is associated with the deterioration in another. Not only are these objectives or criteria competitive or conflicting, they are often noncommensurable. Specialized multiobjective methods have been developed to deal with such problems. Cohon and Marks (1975) classify these techniques as follows:

- generating techniques that determine only the non-inferior or pareto-optimal solutions
- techniques that rely on a priori articulation of preferences between different objectives and criteria
- techniques that rely on progressive articulation of preferences

Selection of a particular approach and technique depends upon the nature of the problem.

Evolutionary algorithms appear to be gaining a significant foothold in the solution of such problems. Erickson et al. (2001) describe a "niched Pareto" genetic algorithm for multi-objective design involving tradeoffs between cost minimization and mass removal. The best set of tradeoffs is the so-called Pareto curve. "Niching" ensures that the tendency of genetic algorithms to converge to a single optimum is suppressed, thereby obtaining a distribution of points along the Pareto curve. The niched Pareto genetic algorithm and similar evolutionary algorithms seem well-suited to the multi-objective problem. This line of research has been under investigation for several years, and there are no published reports for remediation process optimization of field-scale application.

Methodology

The starting point for choosing the method appropriate for determining optimal well locations for a groundwater extraction network focused on the question: "how do I select the decision from a set of alternatives so that a group of stakeholders with different criteria, objectives, and goals are best satisfied." A family of multi-criteria assessment methods described in the late 1960s for water resources management, called the Electre methods (Roy, 1968), and descendents (e.g., see Brans et al., 1984) formed the basis for the decision-making approach. It was implemented using a graph-theoretic strategy.

Once the set of evaluation criteria were established (although before the actual weighting of different criteria is decided), the key technical problem for using the method was generating a set of alternatives that reasonably span the multiple objectives of the stakeholders. This was accomplished using the Latin hypercube method with expert opinion weighting to select candidate well and pumping configurations.

Each candidate configuration was simulated using a three-dimensional model of groundwater flow and dual porosity transport for the entire planning period. In the application below, each simulation produced over 150 megabytes (MB) of output data. These were condensed, using the evaluation criteria, into about 150 kilobytes (KB) of data for each candidate configuration. These results were further condensed by applying some additional criteria, which are discussed in the Application section.

After generating the archive of solutions for the generated candidate configurations, the configurations were ranked in accordance with a specific set of weights for the evaluation criteria. This was accomplished using an Electre method.

Application

A groundwater extraction and treatment network (GWEN) has been deployed to recover and treat dissolved contaminants in the T-25 area of the U. S. Army SSC facility located in Natick, Massachusetts. The major constituents of concern are tricholorethene (TCE) and tetrachlorethene (PCE). The GWEN comprised two extraction wells, which are designated as MW-90B-4 and MW-15B, plus treatment facilities. These wells typically extracted around 10000 and 3500 cubic feet per day (roughly 52 and 18 gallons per minute), respectively. Subterranean Research, Inc. collaborated with HydroGeoLogic, Inc. on a project relating to the design of future GWEN system components. For this paper, TCE was used as the indicator chemical of concern, with an MCL of 5 ppb.

The purpose of this project was to devise groundwater pumping plans for the groundwater extraction and treatment network (GWEN) that are constrained by the total rate at which extracted water can be treated (in this case 130 gallons per minute, gpm) and by a maximum total number of GWEN well installations (in this case either 4 or 5 wells). It is anticipated that the GWEN system will operate until the end of calendar year 2007 and monitored natural attenuation (MNA) will be implemented between 2008 and the end of 2024. This study focuses on selection of wells for the time period covered by the GWEN system, and assesses the plume behaviors through the MNA period. Because the environmental restoration program involves multiple stakeholders and multiple objectives, the suitability of the resulting groundwater pumping plans was determined by considering four different performance functions:

- at specified Points of Compliance (POCs) that correspond to existing monitoring wells, what is the concentration as a function of time.
- at specified map locations that correspond to portions of the SSC property line and through the aquifer depth, what are the concentrations as a function of time.
- for the portion of the aquifer that is not part of the SSC property (off-site region), what is the mass remaining in the aquifer as a function of time.
- for the portion of the aquifer that is part of the SSC property (on-site region), what is the mass remaining in the aquifer as a function of time.

Because more than 20 years remained in the restoration plan, it was important to focus on key time-related milestones. Here we have focussed on two: at the end of calendar year 2007 (end of GWEN pumping) and the end of calendar year 2024 (end of MNA).

These were made more specific, and allowed computed results to be further condensed, by applying some additional criteria:

- Because of the need to meet conditions in the draft Record of Decision (ROD), TCE concentrations in a candidate set of Points of Compliance wells (POCs) must not exceed the MCL of 5 ppb at the end of 2024.
- There is a very strong preference for configurations that take POC concentrations to MCL before the end of 2007.
- There is a very strong preference for configurations that take off-site maximum concentrations to MCL by the end of 2024.
- There is a strong preference for configurations that take on-site maximum concentrations to MCL by the end of 2024.
- There is a strong preference for configurations that take off-site maximum concentrations to MCL by the end of 2007.
- There is a preference to exploit at least one of the existing GWEN wells.

Any selected design option should also be both flexible and robust (e.g., insensitive to reasonable changes in estimated initial conditions), because there are uncertainties intrinsic in every subsurface system.

Many different groundwater extraction (GWEN) configurations employing four or five pumping wells were considered. After clustering neighboring potential well locations and removing duplicates with a self-organizing map (Kohonen, 1987), a subset of candidate configurations were examined carefully. Each candidate configuration used four or five out of ten candidate wells, two of which were the existing MW-90B-4 and MW-15B wells. (The locations of these ten candidate wells are indicated in Figure 1.) A total pumping rate not exceeding 130 gpm was required, as stated previously. Deliverable well pumping rates were based on a experience at the existing wells and simulation results (with a suitable safety factor). For this project, the planning is based on the GWEN system operating until the end of calendar year 2007, followed by MNA until the end of 2024. Only on-site GWEN well locations were permitted under this project.

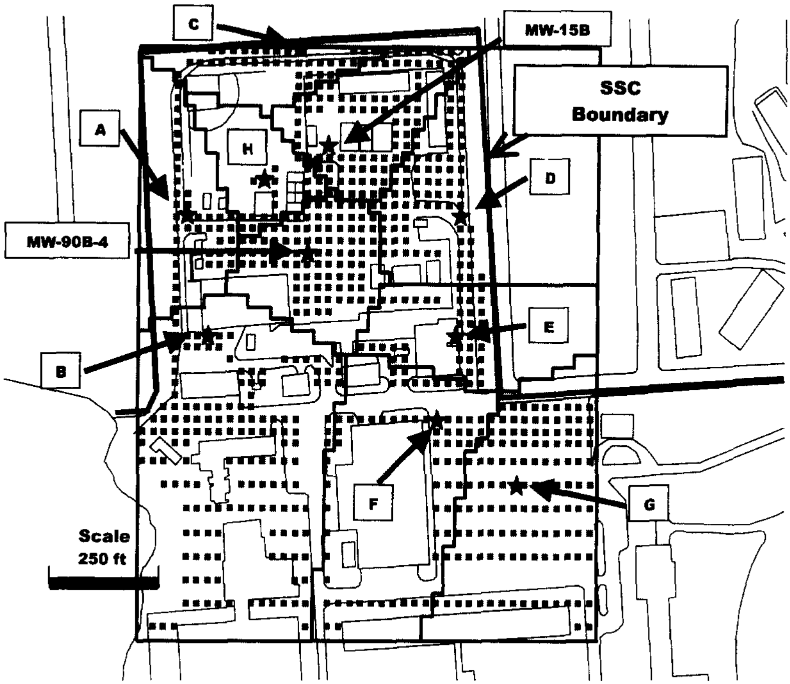

Figure 1. Site map showing potential well locations (square markers), candidate wells from clustering (stars), and property line.

Representative Results

The Electre method is not particular "visually friendly", so it is informative to plot the behavior of archived solutions for the several evaluation criteria. Because all but one candidate configuration shown here attains MCL at the POCs at the end of 2024, the maximum POC concentration at the end of 2007 is considered more informative. Candidate configurations were therefore numbered in sorted order, with 1 indicating the lowest maximum POC concentration at the end of 2007 and increasing with maximum POC concentration at the end of 2007. The resulting numbers are called "Run IDs".

The data were then sorted from least to highest peak off-site concentration at the end of 2024. Using this sorting, the maximum POC concentrations at 2007 and 2024, the maximum 2024 off-site concentration, and the 2024 amounts of TCE mass remaining at the end of 2024 were plotted against the Run IDs. The result is shown in Figure 2. below. (NOTE: When reading the figure, the following notations are used: Cmax_OffSite_2024 is the maximum aqueous phase concentration found offsite in a simulation, Cmax_POC_2007 is the maximum aqueous phase concentration found at any POC at the end of 2007, Cmax_POC_2024 is similar except at the end of 2024, and TotalMassRemaining2024 is the TCE mass in aqueous and solid (i.e., sorbed) phases in the model at the end of 2024.)

Among numerous points of interest observed in the many alternative solutions are the following:

- There are many good GWEN configurations.
- All but one of the presented candidate configurations were predicted to achieve 5 ppb at all POCs by the end of 2024.
- 22 of these candidate configurations were predicted to successfully achieve 5 ppb at all POCs by the end of 2007.
- Over half of the candidate configurations were predicted to attain off-site peak concentrations of 5 to 6 ppb at the end of 2024, even though no off-site candidate GWEN wells were considered. Simulated values of peak off-site 2024 TCE concentration were less than 5.1 ppb for 4 candidate configurations, and 2 of these used 5 GWEN wells.
- A low POC concentration in 2007 was not required to attain low POC concentration in 2024. (e.g., compare Run IDs 11 and 71).
- Mass remaining in the ground (or the mass removed from the ground) at the end of 2024 appeared to be well correlated with the maximum concentration at the POCs at the end of 2007.

New groundwater extraction well locations were proposed and, after public discussions and review, the new well locations were, with minor adjustments, those recommended by this methodology. These new groundwater extraction wells were given regulatory approval and were installed in late 2002.

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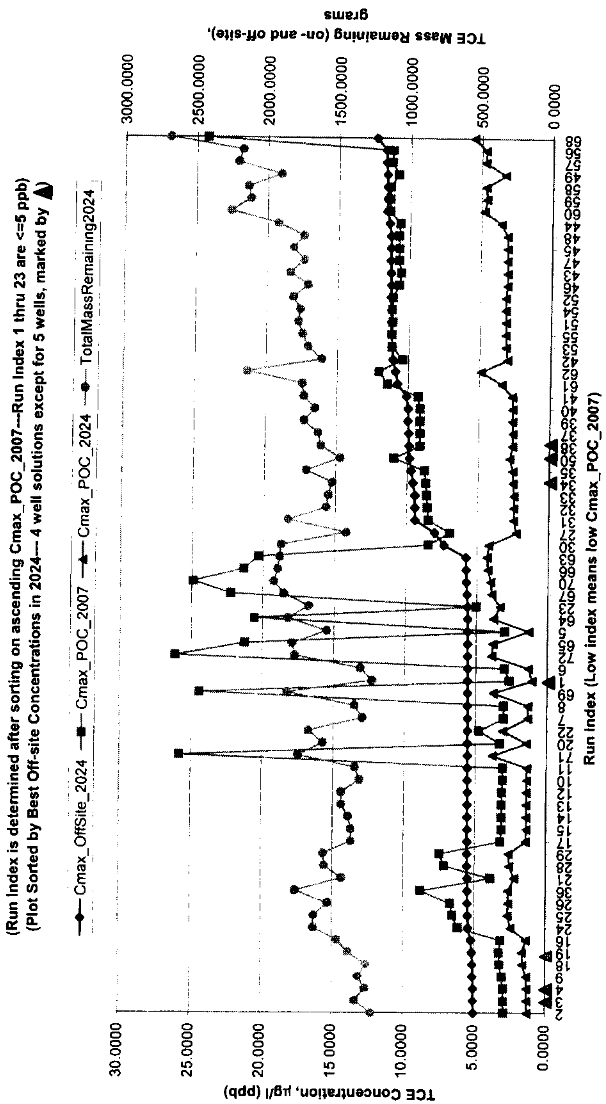

Figure 2. Display of performance of multiple candidate configurations in terms of different evaluation criteria.

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Analytical Method for Optimal Source Reduction with Monitored Natural Attenuation in Contaminated Aquifers

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Abstract

A method is developed for optimizing monitored natural attenuation (MNA) and the reduction in the aqueous source zone concentration (ΔC) required to meet a site-specific regulatory target concentration. The mathematical model consists of two one-dimensional equations of mass balance for the aqueous phase contaminant, to coincide with up to two distinct zones of transformation, and appropriate boundary and intermediate conditions. The solution is written in terms of zone-dependent Peclet and Damköhler numbers. The model is illustrated at a chlorinated solvent site where MNA was implemented following source treatment using in-situ chemical oxidation. The results demonstrate that by not taking into account a variable natural attenuation capacity (NAC), a lower target ΔC is predicted, resulting in unnecessary source concentration reduction and cost with little benefit to achieving site-specific remediation goals.

Introduction

Monitored Natural Attenuation (MNA) is best implemented with removal or remediation of the contaminant source (EPA 1999). MNA is designed to primarily control the migration of aqueous phase contaminant plume, and source treatment is thought to reduce the mass flux and time of remediation at the origin of the plume. Thus, MNA can be optimized if the level of source remediation is optimized to meet site-specific regulatory goals.

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Chapelle and Bradley (1998) presented a method to determine a target level of source concentration treatment based on a uniform natural attenuation capacity (NAC) within the aquifer and demonstrated its use for meeting regulatory compliance concentrations at locations downgradient of the source. The NAC is defined as the sum of all physical/chemical/microbial processes that contribute to the attenuation of an aqueous-phase steady-state contaminant plume. With this approach, the Department of the Navy successfully implemented a remediation strategy combining chemical oxidation and MNA. Fenten's reagent was injected into the unconfined aquifer to meet the target reduction (ΔC) in the aqueous concentration of tetrachloroethene (PCE) at the source of a 200-m long chlorinated ethene plume. Contaminant concentrations in the post-treatment plume have declined downgradient of the source, and the plume is shrinking and restabilizing (Chapelle et al. 2003).

At chlororethene contaminated sites, the effectiveness of MNA is highly dependent on the rate and extent of reductive dechlorination (Chapelle 2001). Specifically, strongly reducing conditions provide the most effective environmental for transformation of PCE and trichloroethene (TCE) to chlorinated daughter products (i.e., trichloroethene, cis-DCE, and vinyl chloride, VC). Spatial changes in redox (i.e., zonation) have been observed in ground-water systems where chlororethene plumes are attenuated, and this zonation is thought to influence the rate of reductive dechlorination and the relative role of direct oxidation in attenuating chlorinated daughter products (Bradley et al. 1998).

At chlororethene contaminated sites where redox zonation is present in the ground-water system (i.e., variable rate of biodegradation with space), the assumption of a single-zone NAC may result in poor estimation of □C required to meet site-specific regulatory compliance concentrations at downgradient locations. In this paper, we present a method to determine an appropriate level of source zone concentration reduction combined with MNA to meet site-specific regulatory compliance concentrations in a ground-water system with variable redox conditions. A two-zone analytical model for optimizing MNA and □C that accounts for spatial variability in NAC based on site conditions is presented.

Natural Attenuation Capacity

Following the approach presented in Chapelle and Bradley (1998), the NAC is defined when a contaminant plume has reached approximate steady-state conditions. The concentration profile along the centerline of the plume may be represented by the solution to the one-dimensional transport equation assuming uniform groundwater velocity and first-order decay. With this approach, the NAC, as defined in Chapelle and Bradley (1998), is calculate from the log change in concentration per unit length of flowpath.

The application of the single-zone NAC to determine the level of source concentration reduction is illustrated in Figure 1. The steady-state, centerline concentration profiles of two pre-treatment aqueous phase plumes are shown for a relatively high NAC (0.06 m^{-1}) and for a ground-water system with a lower NAC (0.03 m^{-1}), based on values reported by Chapelle and Bradley (1998). Both plumes have identical source (boundary) concentrations (10 mg/L), and the contaminant concentration exceeds the regulatory compliance level (MCL = 2 μg/L) at a prescribed distance downgradient of the source (75 m). As shown in the figure at the boundary, the source concentrations for the post-treatment plumes are dependent on the NAC for the same MCL and location along the flowpath. Although significant source treatment would be expected in either case, for the more attenuated plume (NAC = 0.06 m^{-1}) to meet the downgradient MCL, the required source concentration is 180 μg/L. Because the plume is less attenuated in the second ground-water system, the source concentration must be reduced to 19 μg/L.

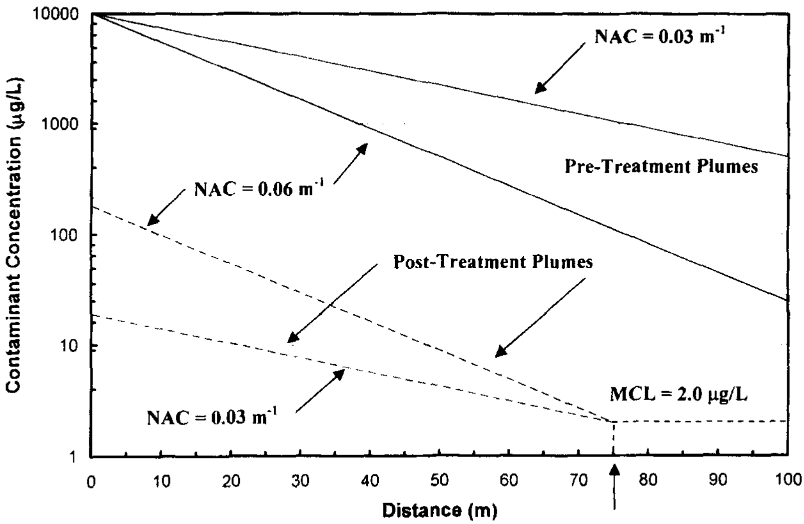

Figure 1. Schematic of contaminant concentrations in pre-treatment aqueous phase plumes with differing natural attenuation capacity (NAC) values and restabilized plumes following source treatment. The point of compliance is located 75 m from the source.

Mathematical Model and Analytical Solution

For a two-zone model, a system of two ordinary differential equations is given by the solute transport equations:

$$-v\frac{\partial C_1}{\partial x}+D\frac{\partial^2 C_1}{\partial x^2}-\lambda_1 C_1=0 \qquad 0\le x\le L \qquad (1)$$

$$-v\frac{\partial C_2}{\partial x}+D\frac{\partial^2 C_2}{\partial x^2}-\lambda_2 C_2=0 \qquad L\le x\le \infty \qquad (2)$$