2004

Optimal design of pump and treat remediation systems : treatment modeling, source modeling and time as a decision variable

Karen L. Endres
Michigan Technological University

Follow this and additional works at: https://digitalcommons.mtu.edu/etds
Part of the Civil Engineering Commons

OPTIMAL DESIGN OF PUMP AND TREAT REMEDIATION SYSTEMS:

Treatment Modeling, Source Modeling and Time as a Decision Variable

by

Karen L. Endres

A thesis submitted in partial fulfillment of the requirements for the degree of

Doctorate of Philosophy

Environmental Engineering

Michigan Technological University

May 6, 2004

This dissertation "Treatment Modeling, Source Modeling and Time as a Decision Variable" is submitted in partial fulfillment of the requirements for the degree of DOCTORATE OF PHILOSOPHY in the field of Environmental Engineering

Program: Environmental Engineering

Approved by ____

Dr. Alex Mayer

Chairperson of Committee- Department of Geological and Mining Engineering and Sciences, Michigan Technological University

Department Chair ____

Date ____

MICHIGAN TECHNOLOGICAL UNIVERSITY

ABSTRACT

OPTIMIZATION OF COMPLEX REMEDIATION SYSTEMS

Groundwater optimization and simulation is a maturing science. Research work contained in this thesis extends into areas that have not been fully explored. The incorporation of source and treatment systems selection and design produces information to help decision makers. Further insight is gained by evaluating some of the requirements and standards enforced by regulations such as, remediation time.

The technical aspects of a remediation system are set by the physical properties and the regulatory constraints enforced. As an example, the addition of a realistic treatment system gives more accurate cost estimates, but the pump and treat (PAT) systems parameters do not change. Only when changes to the aquifer, contaminant, or constraint are applied, do the technical (i.e. pumping rates or technology selection) parameters change. The effects of remediation should not be viewed only in terms of costs. The effects of time and source remediation impact the aquifer in both contaminant and hydrologic areas. A framework to evaluate these effects is presented in the hope of furthering our knowledge.

TABLE OF CONTENTS

ACKNOWLEDGMENTS

This research was supported by NSF grant BES-0083112 and USEPA grant CR826614-01-0 and Department of Education GAANN Fellowship.

Thanks to Reed Maxwell, Lawrence Livermore National Laboratory; Mark Erickson, AMEC Earth & Environmental, Inc.; and Jeff Horn, Northern Michigan University for help and source code.

The author wishes to thank my committee for all their insights and all those who helped makes this possible. Special thanks to my advisor Alex Mayer, for getting me through it all.

Dedication

This thesis is dedicated to Horace G. Stafford, who started me down this path so many years ago. Who would have thought it would have brought me here.

Overview

This dissertation is organized into four chapters detailing related research projects on groundwater remediation and optimization. The first chapter, the overview provides a general overview of the research projects. The second chapter presents an enhanced approach to modeling treatment systems in the form of a manuscript to be submitted to the *Journal of Environmental Engineering, ASCE*. The third chapter develops a source model and integrates in with the groundwater flow and transport simulator to optimize technology selection. This manuscript will be submitted to the *Journal of Water Resources Planning and Management, ASCE*. The final chapter investigates the assumption of fixed remediation time and the impact that it has on the remediation cost and operation of the system. This paper has been accepted for publication in *Computational Methods in Water Resources, 2004*.

1.0 Problem Statement

The remediation of the nation's contaminated soil and groundwater is a multi-billion dollar problem. Optimization using computer simulations to determine parameters is a useful tool for subsurface remediation system design. Application of mathematical optimization to remediation design problems has been shown to produce significant cost savings over conventional design methods, as well as adding to our knowledge of the underlying physical system.

Pump and treat (PAT) remediation is the most prevalent and studied groundwater plume technology. Underlying the PAT optimization framework are simulators of groundwater flow and contaminant transport that are based on numerical approximations of the governing flow and transport models. Development and execution of a typical simulator involves the solution of systems of equations with thousands to millions of unknown variables. To solve this dilemma, in most remediation optimizations studies done to date, only a portion of the system is selected to be optimized and the rest of the system is either ignored or simplified.

To determine how these modeling assumptions affect the accuracy and effectiveness of the designs produced is the goal of this work. The enhanced models will provide guidelines to help decision makers in the remediation process. The three main topics of this research are:

- Optimization of plume and treatment model
- Optimization of source and plume model
- Time as a decision variable

The most common treatment for dissolved organic contaminant is adsorption by granular activated carbon (GAC). The cost of using GAC has typically been modeled by using simple equilibrium processes. However, it is known that the process of adsorption is complex and varies by many factors resulting in non-equilibrium carbon usage rates.

Treatment capital and operational costs have a significant impact on the system design, but most studies have used treatment models that assume that the carbon adsorption can be treated as an equilibrium process, allowing the use of a Freundlich isotherm model. However, mass transfer limitations can be significant in the carbon adsorption process, leading to earlier breakthrough than that predicted by equilibrium models. Costs associated with the GAC system are dependent on flow rates, type of contaminant, concentration of contaminant, mass loading, required effluent concentration, site conditions and timing requirements. The incorporation of a treatment model will allow for these factors to be considered.

PAT focuses exclusively on the removal of contaminants in the groundwater plume. This plume emanates from a source that is frequently considered to be removed. However, complete source removal is frequently a poor assumption due to technical, economic or regulatory factors. In many sites where engineered source removal has been implemented, the efforts were incomplete, either because of poor design or because not all of the source material was identified. In other sites, engineered source removal was not implemented because it was deemed technically infeasible or economically impractical.

Most single objective investigations focus on minimizing cost while meeting the cleanup requirements within a given time frame. This period of time is normally set by regulatory processes. This constraint leads to a single set of parameters that may not be optimal when variable time frames are considered. The ability to visualize the trade-off between cost and remediation time will help decision makers in taking informed actions. The effect of time on remediation costs has not been explored in depth.

2.0 Optimization of Plume and Treatment Model

This work incorporates a state-of-the-art GAC adsorption model with a groundwater simulation model to predict remediation costs and optimize both the hydraulic and treatment portions of the system. The carbon model is based on pore diffusion kinetics using variable flow and concentration data from the groundwater model. The system of simulation models predicts optimal non-equilibrium carbon usage rates, hydraulic parameters and treatment column design parameters. The parameters are optimized using an evolutionary algorithm resulting in an decision variable that correspond to pumping rates and source remediation allocations. The simulation of the treatment process is critical in the optimization of PAT. With an equilibrium model only the total mass of contaminant is used to determine the amount of carbon used in the treatment of the extracted water. This approach ignores the influent concentration as a driving force for the adsorption rate as well as the variability in the flow rate. The non-equilibrium approach accounts for the realistic variation in the influent concentration and the current state of the carbon. The total cost of the carbon is a function of the usage rate and the volume of water treated. The effect influent concentration on optimal solutions is explored by varying the degree of heterogeneity in the aquifer producing the effect of tailing. The effect of this phenomenon can only be assessed using a non-equilibrium simulator that takes influent concentration in the account. The use of a non-equilibrium model also allows for the exploration of empty bed contact time (EBCT) on the optimal design.

Improvements in simulation of aquifer contaminant transport have been ongoing to closer simulate tracer study results and natural field conditions. One method currently under study is the dual domain method. The dual domain method can be considered as two first-order processes driven by the concentration gradient between the zones of mobile and immobile water. Incorporation of this method into the flow and transport simulator simulates natural aquifer heterogeneity.

2.1 Methods

A hypothetical contaminated aquifer system is used to assess the significance of including a sophisticated carbon simulator, by comparing the results for optimal designs found with equilibrium and mass transfer GAC treatment simulators. In our remediation design optimization framework, the objective consists of a single objective minimize cost function. The cost function includes capital and operating costs, which are a function of design variables and state variables. The design variables are the constant pumping rates at fixed-location extraction wells and the length of the GAC bed(s). The state variables are aquifer concentrations and hydraulic heads. A groundwater flow and transport simulator predicts the state variables. The aquifer cleanup goal is incorporated as a constraint on the groundwater concentration at monitoring locations. The treatment goal for the GAC model is incorporated directly into the GAC simulator.

We couple a conventional, subsurface flow and transport simulator with a state-of-the-art GAC simulator, developed by our collaborator, Dr. David Hand, and his group at MTU. The GAC simulator is based on a fully dynamic mass transfer, pore diffusion model, which can account for multiple contaminants, the impact of NOM fouling of the GAC, and variable flow. Given the influent contaminant composition and concentration, the influent NOM concentration, the carbon type, the absorber configuration, and the flow rate, the GAC simulator predicts a rate of carbon utilization. The rate of carbon utilization is then used to determine the treatment cost.

The effect of treatment design parameters on the cost of the remediation system is explored by using the empty bed contact time (EBCT) as a variable in the optimization process. Size of the treatment train is usually done using the highest contaminant concentration using steady state pumping rates, as these concentrations decline the mass transfer zone changes, changing the optimal EBCT.

The optimization is done with a niched pareto genetic algorithm that uses evolutionary methods to produce optimal values of decision variables. The aquifer simulation is done with a finite difference numerical simulator with a particle tracking transport method.

2.2 Results

The first set of experiments was conducted to assess the relationship between the equilibrium process used in prior optimization studies and the use of the new dynamic GAC simulation model. Previous work done with a multi-objective genetic algorithm used Freundlich isotherms to predict carbon usage and was used as the equilibrium model for this comparison. The comparison of the GAC model to equilibrium model results in the pareto-optimal fronts and shows that the use of the equilibrium model differs from the dynamic model with the equilibrium model consistently lower. The greatest difference is seen in the low mass removal area, while the higher mass removal data matches well.

The second set of experiments was conducted to assess the effect of tailing phenomenon on carbon usage rate. The transport code was modified to include the mobile-immobile partitioning of the aquifer to simulate tailing. Several alpha parameters were used to assess a range of heterogeneity that may be encountered in natural aquifers. Alpha parameters control the rate mass transfer from one phase to the other. The dual phase model runs were made using low immobile phase and high immobile phase porosities. In the low immobile porosity runs, little difference was shown. However in high immobile runs dramatic differences in pumping rates and treatment costs were observed. The general trends associated with the alpha parameters are increased cost as alpha is lowered. The alpha parameter showed similar trends were seen in both the high and low immobility model runs.

The third set of experiments was used to assess the feasibility of simultaneous hydraulic and treatment system design. The addition of an optimization parameter in the chromosome of the genetic algorithm was used to determine the number of beds of fixed length that were used in the treatment train. The total bed length with the flow rate determines empty bed contact time, which affects carbon usage rate. The inclusion of the design of the treatment column size was done with no dual porosities present and with a moderate alpha and high mobility runs. The homogeneous runs allowed a more efficient design, including a smaller column size, to be found. The dual porosity model also found a more efficient design but selected column size is of equal value.

2.3 Conclusions

The use of the non-equilibrium model that considers the diffusive processes of carbon has shown insights into optimization of remediation processes. The comparison of the equilibrium method to the non-equilibrium process shows that the use of the equilibrium model under estimates carbon usage. The inclusion of the non-equilibrium model using the radial collocation methods does not dramatically change modeling efforts. The advantage of the treatment model is the inclusion of multiple contaminants, carbon selection, variable flow and contaminants concentrations which gives a more realistic carbon usage rate.

Use of the dual domain model causes the time steps of the modeling process to be dramatically decreased in order to use alpha values consistent with literature. The inclusion of this process changed the outflow concentrations to be consistent with the effect of tailing. The effect of this tailing caused dramatic differences in the optimal design and costs of the remediation.

The most noteworthy result of this work has been in the inclusion of the treatment process design along with a hydraulic design. The inclusion of the design process did not alter the runtime or modeling effort for the homogenous system. However, the inclusion of the heterogonous system using the alpha parameters necessitated the reduction in time steps resulting in higher run times. The results indicate that the inclusion of treatment design will make more robust and efficient remediation designs.

3.0 Optimization of Source and Plume

From a management perspective, there is a tradeoff between the degree of cleanup effort and funds dedicated to source removal and to the cleanup of the groundwater plume emanating from the source. The dense non-aqueous phase liquid (DNAPL) source is modeled as a temporally varying, but non-dimensional, mass release input to the contaminant plume. The factors influencing the mass release rate include the advective rate through the source area, which could be impacted by the regional groundwater flow and flow induced by plume cleanup efforts, the spatial distribution of the contaminant mass and hydraulic conductivity distribution within the source area, and the chemical composition of the source. Once the contaminant mass has entered the plume via dissolution, the spatial and temporal behavior of the plume is not only controlled by the advective rate and hydraulic conductivity distribution, but also by what have been loosely termed as attenuation factors, which include dispersion and degradation reactions. The degradation reactions could include both biotic and abiotic reactions.

A "bundle of tubes" model is used to simulate the dissolution of the DNAPL source and provide the source term. The same model is used to simulate source removal under ambient and engineered conditions. This model represents the heterogeneous DNAPL distribution, and consequent distribution of DNAPL rates of dissolution. The source model accounts for variability in the aquifer properties with the use of an inverse log-normal probability distribution resulting in time-variable source input to the flow and transport model.

3.1 Methods

The optimal allocation of costs for the remediation is produced using a niched-pareto genetic algorithm to guide the optimization, coupled with simulation models for the source and the plume remediation systems. In our remediation design optimization framework, the objective consists of a single objective minimize cost function. The cost function includes capital and operating costs, which are a function of design variables and state variables. The system is applied to a hypothetical aquifer containing both source and plume contamination. This process provides useful insight to the optimization of remediation systems that can present decision-makers with progressive tools for use in resource allocation.

The hypothetical aquifer scenario implemented will be of a homogeneous aquifer with constant head and no-flow boundaries. The source, assumed to be a NAPL, will be at a fixed location with concentration inputs varying over time. The location of the pumping wells will be fixed with selection by the optimization algorithm. The pumping rates will be decision variables with constraints on observation well concentrations and drawdown. The extracted water will be treated to a given standard by a GAC adsorption unit as modeled by Freundlich equilibrium isotherms. Disposal of the water is assumed to be to surface receiving waters at no cost.

Models of flushing technologies (e.g. surfactant, co-solvent, and steam flushing) for NAPL removal that account for variablity in the aquifer properties with the use of an inverse log-normal probability distribution result in time-variable source input to the flow and transport model. The models are relatively simple, but are capable of simulating the “tailing” behavior that is often observed with these technologies.

By “tailing,” here we mean that the rate of removal decreases significantly after the majority of the source mass is removed, such that the last, say, 10% of the source mass, is removed less and less efficiently. Low permeability units, heterogeneities and insoluble contaminants may impose limitations and increase tailing.

The flushing technology models are linked to the groundwater flow and transport simulator. In this way, the source term for the groundwater contaminant plume will be adjusted through time as the source is removed via the flushing technology. The groundwater flow and transport simulator is modified to include biodegradation of groundwater contaminants. Biodegradation of most common NAPL has been demonstrated to be affective in treating dissolved phase contamination; however, is not likely to take place directly in the nonaqueous phase. This modification allows the simulation of the full range of groundwater plume remediation options: from aggressive, engineered remediation to natural attenuation.

3.2 Results

The numerical experiments simulate four distinct stages: (1) source emplacement, (2) plume creation, (3) source remediation, and (4) plume remediation. The source emplacement is simulated as an instantaneous event.

The impact of the variability in the source is examined by changing the variance in tube lengths. The results of base case optimizations for a range of source (tube length) variances, show that source remediation was not chosen for any of the source variances and no feasible solution was found for the highest variance. These results indicate that source remediation is expensive relative to plume remediation and that plume remediation is sufficient for all but the highest variances.

The flushing capital and operating cost coefficient were varied to assess the impact of a 50% reduction in costs. The optimization results for the case where the capital costs of the flushing are reduced by 50%, shows that the costs of source remediation are low enough to compete with plume remediation costs, but the variations in source variances produce optimal designs consisting of various configurations of source and plume remediation. Reduction of the operational cost of flushing by 50% also results in lowering the costs of source remediation enough to compete with plume remediation costs.

The plume development time, t_p. was varied to simulate the length of time from spill to remediation and the effect of this timing on the remediation efforts. The period between the initial DNAPL release and the implementation of the source remediation can vary widely, because the time elapsed before discovery of the contamination and the decision to implement the source remediation varies from site to site. The variation in t_p does not affect the selection of PAT as the only remediation technology, since the source remediation is expensive relative to the plume remediation. When the flushing capital costs are reduced source remediation is chosen only for the base case plume development time.

Finally, the effects of biodegradation in the dissolved plume was examined by varying the first-order degradation rate constant, λ. The cost of source remediation is high enough, relative to the source remediation cost, such that only PAT is chosen in the optimal design. The overall costs for plume remediation decrease as the degradation rate increases, since less mass needs to be extracted and treated. At the highest degradation rate, PAT operation is not required, implying that natural attenuation is sufficient to meet the cleanup goal.

3.3 Conclusions

In this work, a framework for determining optimal designs of combined source and plume remediation efforts has been developed. The optimization framework has been developed to allow the remediation designer to analyze tradeoffs between degrees of effort and funds committed to source remediation and plume remediation. The presence of heterogeneity in the source distribution has been accounted for, such that the rate of mass release into the plume and the efficiency of source remediation efforts are controlled by the degree of heterogeneity.

As expected, the optimal allocation of funds to source or plume remediation is sensitive to the unit costs associated with the remediation technologies. Only plume remediation, in the form of PAT remediation, is selected when the base case, source remediation capital and operating costs are applied. In this case, the relationship between plume remediation costs and the source variance is not monotonic, revealing the complex relationship between the release rate from the source into the plume and the costs associated with pumping and treatment.

Degradation of the contaminant within the plume lowers the total cost of remediation. For the highest degradation rate, no remediation is required, implying that natural attenuation is sufficient to meet the cleanup goal. For mid-range degradation rates, source remediation is not required, since, even for relatively high source release rates, the mass residing in the plume is reduce to the point where plume remediation can meet the cleanup goal.

4.0 Time as a decision variable

Groundwater remediation is a lengthy process taking years or perhaps decades. The time frame used will affect the pumping rates and the removal efficiency of the system. Time is an important factor that has not been considered in optimization of these systems. Optimization of this parameter is undertaken with single and multi-objective optimization methods.

Multi-objective optimization attempts to simultaneously find the minimum of two conflicting objective functions, in this case time and cost. A tradeoff curve for these objective functions is produced by the procedure. This curve can be verified

by running multiple single objective optimization runs, while varying the other objective. In this process, the time variable was successively increased by small increments from the minimum time to the maximum time. This produced a series of optimal single objective points. The multi-objective optimization was then preformed to produce a true
pareto-optimal front.

The application of interest rates scenarios was used to determine how financial management decisions would affect the process. Two cases of interest rate calculations were used – annualized and present worth cost. The interest rate calculations for annualized cost assumed that a bond for the complete remediation costs was purchased at the beginning of the remediation period. The present worth interest run assumed that operating capital was used to pay for each operating costs period and capital investment was available for the purchase of the initial purchase of equipment and installation. The choice of these two interest rates applications encompasses both extremes of funding opportunities. The interest rate chosen was a nominal five percent.

4.1 Methods

A multi-objective problem is formulated to minimize the design cost while also minimizing the remediation time. The multi-objective approach utilized operates on the concept of "Pareto domination", which states that one candidate dominates another only if it is at least equal in all objectives and superior in at least one. The niched Pareto genetic algorithim (NPGA) relies on a ranking scheme that ordered the population according to each containment design's degree of domination. Tradeoff curves produced by the multi-objective optimization give decision makers the capability of making better-informed decisions.

4.2 Results

The multi-objective optimization results matched the single objective runs well, providing a confidence in the multi-objective results. However, the multi-objective results did not exhibit full coverage of all the remediation times examined by the single-objective runs and some regions of the curve produced infeasible results for both the single and multi objective runs. This is due to the limited feasible region of the problem caused by the mass remaining constraint and model limitations. The trade-off curve exhibits a weak relationship to the remediation time, as shown by the flattening of the curve as remediation time is increased.

The interest rate runs showed a difference in costs for each of the scenarios examined. The decision variables of the optimal designs did not change in any of the interest rate scenarios, which represent extremes in financial funding options. The first scenario examined, in which a well-funded company can offset the operational costs of the remediation by investments, produced a lower overall cost. This produced an overall reduction in the cost of the remediation that was further reduced with longer remediation times. The second one, in which a bond must be purchased and the total cost borrowed, sharply increases the total costs. This run showed a sharp increase in the remediation cost and more sensitivity to remediation time. Both single and multi-objective runs were preformed with multi-objective interest rate runs followed the single-objective results, but exhibited the same lack of completeness from previous the discussion.

4.3 Conclusions

The process of defining and documenting the application of multi-objective optimizations for complex processes such as groundwater remediation is a daunting task. The verification of the trade-off curve represents a shift in the mindset of decision makers. Cost is no longer the overriding consideration. The ability to consider remediation time, funding options, or aquifer impact is now an option. This work has shown the relative low impact of remediation time on overall cost and investigating other issues associated with remediation processes and modeling efforts, for the given simulation models and parameters used.

The effect of interest rate on the optimization process produced varying results dependent on the financial method used for funding. However, the decision variables selected for the remediation did not change. This leads us to the conclusion that interest rates are a managerial rather than a technical component of the remediation process.

The most interesting results of this process came from the analysis of the effects of the different remediation time scenarios on the aquifer. The detailed examination of the timing runs has lead to interesting results and allows for issues, other than just remediation time and cost, to be considered. The results clearly show that the effects on the aquifer and the efficiency of the system will be maximized by longer remediation times. The minimization of water extracted means less drawdown and less impact on surrounding hydrology. These results indicate that the longer remediation times produce a lesser impact on the aquifer and deliver higher concentrations to the treatment system. The higher concentration and lower volumes associated with longer remediation times are due to lower pumping rates, which in turn extract less surrounding clean water. The effect of higher concentrations will lead to better efficiency and lower capitol costs of the treatment system.

5.0 Summary

This body of research attempts to detail effects of various areas of groundwater remediation systems that have been simplified or ignored. This effort has lead to some overall insights for the remediation community.

First, the technical aspects of a remediation system are set by the physical properties and the regulatory constraints enforced. As an example, the addition of a realistic treatment system gives more accurate cost estimates, but the PAT systems parameters do not change. Only when changes to the aquifer, contaminant, or constraint are applied, do the technical parameters (i.e. pumping rates or technology selection) change.

Secondly, the effects of remediation should not be viewed only in terms of costs. The effects of time and source remediation impact the aquifer in both contaminant and hydrologic areas. The framework to evaluate these affects is presented in the hope of furthering our knowledge.

6.0 Presentation of Research

This work has been presented at the following conferences:

Optimization of Plume and Treatment

Endres, KL, Mayer AS, Hand, D, Optimization of Pump and Treat Systems by Genetic Algorithm Incorporating a Carbon Pore Diffusion Simulator, Environmental and Water Resources Institute, ASCE Orlando, Fla, Spring 2001 Oral Presentation.

Endres, KL, Mayer AS, Hand, D, Optimization of Plume and Treatment Systems, Environmental and Water Resources Institute, ASCE Reston, Va, Spring 2002 Oral Presentation.

Optimization of Source and Plume

Endres, KL, Mayer AS, Enfield, C, Analysis of Tradeoffs Between Optimal Source and Dissolved Plume Remediation, American Geophysical Union, Fall 2001, Oral Presentation.

Endres, KL, Mayer AS, Enfield, C, Optimization of Source and Plume Remediation, American Chemical Society, New Orleans, Spring 2003 Poster Presentation.

Time as a decision variable

Endres, KL, Mayer AS, Using Time as an Objective Function & Decision Variable in Remediation Optimization, American Geophysical Union, Fall 2003, Oral Presentation.

Endres, KL, Mayer AS, Using remediation time as an optimization variable in groundwater remediation systems, Computational Methods in Water Resources, 2004 International Conference, Chapel Hill, North Carolina, June 13 - 17, 2004.

The research has also been or will be submitted to :

Optimization of Plume and Treatment

Endres, KL, Mayer AS, Hand, D, Optimization of Pump and Treat Systems by Genetic Algorithm Incorporating a Carbon Pore Diffusion Simulator, Environmental and Water Resources Institute, ASCE Orlando, Fla, Spring 2001 EWRI Conference Proceedings.

Endres, KL, Mayer AS, Hand, D, Optimization of Plume and Treatment Systems, Environmental and Water Resources Institute, ASCE Reston, Va, EWRI Conference Proceedings, Abstract Publication.

Endres, KL, Mayer AS, Hand, D, Optimization of Plume and Treatment Systems, Full Paper to be submitted to Journal of Environmental Engineering

Optimization of Source and Plume

Endres, KL, Mayer AS, Enfield, C, Analysis of Tradeoffs Between Optimal Source and Dissolved Plume Remediation, American Geophysical Union, Fall 2001, EOS Transactions of AGU, Abstract Publication.

Endres, KL, Mayer AS, Enfield, C, Optimization of Source and Plume Remediation, American Chemical Society, New Orleans, Spring 2003 Extended Abstract Publication, ACS Conference Proceedings.

Endres, KL, Mayer AS, Enfield, C, Optimization of Source and Plume Remediation, American Chemical Society, New Orleans, Spring 2003 Poster Presentation.

Endres, KL, Mayer AS, Enfield, C, Optimization of Source and Plume Remediation

Full Paper to be submitted to Journal of Water Resources Planning and Management.

Time as a decision variable

Endres, KL, Mayer AS, Using Time as an Objective Function & Decision Variable in Remediation Optimization, American Geophysical Union, Fall 2003, EOS Transactions of AGU.

Endres, KL, Mayer AS, Using remediation time as an optimization variable in groundwater remediation systems, Computational Methods in Water Resources, 2004 International Conference, Chapel Hill, North Carolina, June 13 - 17, 2004.

Groundwater Treatment Modeling in the Optimal Design of Pump-and-Treat Groundwater Remediation Systems

Karen L. Endres

Department of Civil and Environmental Engineering

Michigan Technological University, Houghton, Michigan

ABSTRACT

A common treatment for dissolved organic contaminants is adsorption by granular activated carbon (GAC). The GAC treatment process typically has been modeled by assuming equilibrium between the contaminant in the aqueous and solid phases. When non-equilibrium processes are considered, breakthrough can occur before the adsorptive capacity of the GAC is exhausted. The present work incorporates an advanced groundwater treatment model into PAT optimization that results in more realistic costs and better-engineered remediation systems. The goal of this work is to extend previous investigations of optimal PAT design to consider non-equilibrium processes of groundwater treatment systems.

The use of the non-equilibrium model that considers the diffusive processes of carbon has shown insights into optimization of remediation processes. The comparison of the equilibrium method to the non-equilibrium process shows that the use of the equilibrium model underestimates the carbon usage at all levels of mass removal. Through the inclusion of the treatment process design along with a hydraulic design, it is shown that the selection of the column length exhibits savings in treatment design and costs.

INTRODUCTION

Pump and treat (PAT) technologies have become a standard for groundwater remediation. Optimization of these systems has primarily focused on design of the hydraulic components of the system; however; the treatment component of the remediation usually comprises at least half of the total cost (e.g. Culver and Shoemaker,1997; Culver and Shenk,1998). A common treatment for dissolved organic contaminants is adsorption by granular activated carbon (GAC). The GAC treatment process typically has been modeled by assuming equilibrium between the contaminant in the aqueous and solid phases. The equilibrium assumption allows the use of simple, algebraic models of GAC treatment that depend on a limited number of GAC-contaminant properties. However, it is well known that the process of the absorption onto GAC is complex and that mass-transfer limitations can be significant (e.g. Sontheimer et al., 1988). The use of equilibrium methods has been to predict carbon usage has been shown to be inadequate by Hand et al. (1989, 1998) and Crittenden et al.(1986, 1987b, 1988).

Operational costs for a GAC groundwater treatment system are based primarily on the GAC usage rate, given that once breakthrough of the contaminant occurs in the treatment system, the GAC must be replaced. With equilibrium modeling of the GAC system, the replacement rate is based on the assumption that the entire adsorptive capacity of the GAC is exhausted at the time of breakthrough. Residence time in the adsorption unit does not need to be considered. When non-equilibrium processes are considered, breakthrough can occur before the adsorptive capacity of the GAC is exhausted. The time to breakthrough depends on many factors, such as the influent contaminant concentration, the length and cross-sectional area of the adsorption unit, the flow rate into the adsorption unit, and the contaminant treatment goal (Crittenden, et al., 1986, 1987b, 1988; and Hand, et al., 1989, 1998)).

The illustrations in Figure 1 emphasize that the equilibrium approach supposes that the GAC adsorptive capacity is completely used at the time when the effluent concentration (C_e) from the GAC unit reaches an operating limit (C_L), whereas the non-equilibrium approach supposes that some fraction of the adsorptive capacity remains at the time when $C_e \rightarrow C_L$. In the non-equilibrium approach, the greater the difference between the influent concentration (C_0) and the operating limit (C_L), the greater the amount of unused capacity that remains at the point when the GAC must be replaced. Since the operating limit is usually fixed at, for example, a drinking water standard, the efficiency of carbon usage can be maximized by attempting to maintain high influent concentrations.

Hand and Jarvie (2004, in press) have demonstrated that using an equilibrium approach to model GAC adsorption can greatly underestimate the rate of carbon usage by comparing models that account for non-equilibrium and equilibrium behavior. Hand and Jarvie (2004) modeled groundwater treatment scenarios with a range of chemical types and concentrations, influent flow rates, target effluent concentrations and background groundwater compositions with natural organic matter. They found that the equilibrium approach underestimated carbon usage by a factor of 2 to 10 without the effect of natural organic matter and up to 20 times with when it was considered.

The present work proposes that the incorporation of advanced groundwater treatment models into PAT optimization will result in more realistic costs and better-engineered remediation systems. The goal of this work is to extend previous investigations of optimal PAT design to consider advanced models of groundwater treatment systems. We first consider the effect of treatment system modeling on the optimal design by analyzing the relationship between cost and cleanup performance. We compare cost and cleanup performance using both equilibrium and non-equilibrium based models.

We also assess the significance of aquifer system heterogeneity on the optimal design while considering a non-equilibrium model of the treatment system. We expect the optimal design to be sensitive to heterogeneity, since we expect that the greater the degree of aquifer heterogeneity, the more severe the tailing will be in the extracted groundwater. With more severe tailing, the influent concentration to the treatment system will decrease, resulting in less efficient use of the treatment system. Finally, we extend PAT optimization to include the design of the treatment system, by considering the number of absorber units as a design variable. We hypothesize that, if the design of the GAC treatment system is not fixed, the optimal solutions will be more efficient overall.

METHODOLOGY

The goal of the computational framework is to determine optimal values of decision variables while satisfying multiple objectives and constraints. The framework, summarized in Figure 2, includes objective functions and models for simulating groundwater flow and transport processes and for simulating the groundwater treatment process. The two objective functions are to minimize capital and operational costs and to minimize the contaminant mass remaining in the aquifer and are given by:

$$\min f_1 = \min\left[a_1 N_{ew} + a_2 N_{GAC} + \sum_{k=1}^{N_{ew}} \sum_{l=1}^{N_t} \left(a_3 Q_k H_k t_l + a_4 \dot{M}_{GAC} t_l \right) \right] \tag{1}$$

$$\min f_2 = \min\left[\frac{1}{M_0} \left(\int_{\Omega_D} C(\mathbf{x},t)\, dV \right) \right] \text{ at } t = t_f \tag{2}$$

where f_1 is the total cost; a_1 is the cost coefficient associated with the extraction well installation; N_{ew} is the number of active extraction wells; a_2 is the cost coefficient associated with the treatment system installation; N_{GAC} is the number of GAC adsorption units; N_t is the number of time steps within the remediation horizon; k and l are the well and time indices, respectively; a_3 and a_4 are the cost coefficients associated with the pumping and groundwater treatment operating costs, respectively; Q_k is the pumping rate at well k; H_k is the head that the pump in extraction well k must overcome to deliver water to the treatment system; t_l is the incremental time period used to evaluate the PAT operational costs, $\dot{M}_{GAC}$ is the carbon usage rate; f_2 is the normalized mass remaining in the aquifer; M_0 is the initial contaminant mass; and C is the contaminant concentration in the aquifer, as a function of location and time.

The terms in equation (1) represent, in order of appearance, capital costs associated with well installation, capital costs associated with the treatment system, operational costs associated with pumping, and operational costs associated with groundwater treatment by GAC. Equation (2) essentially represents the objective of maximizing cleanup performance, measured by the contaminant mass remaining in the aquifer, normalized by the initial contaminant mass. The decision variables are the pumping rates at fixed-location extraction wells, Q_k, and the number of GAC adsorption units, N_{GAC}.

The constraints on the decision variables and state variables are

$$0 \le Q_k \le Q^{\max} \quad \text{for } k = 1, \ldots N_{ew} \tag{3}$$

$$N_{GAC} \le N_{GAC}^{\max} \tag{4}$$

$$h \ge h_{\min} \quad \text{over } \Omega_D \tag{5}$$

$$\sum_{l=1}^{N_t} t_l = t_f \tag{6}$$

where $Q^{\max}$ is the maximum, individual pumping rate; $N_{GAC}^{\max}$ is the maximum number of GAC adsorption units in series, $h_{\min}$ is the minimum head allowed over the model domain, Ω_D; and t_f is the remediation horizon. Equation (5) effectively constrains the maximum drawdown in the aquifer.

The subsurface simulation processes used in this work is based on the two-dimensional steady state flow equations and contaminant mass balance equations. The steady-state, confined groundwater flow equation for a non-deforming, saturated, aquifer system is

$$\nabla\left(\mathbf{K}\cdot\nabla h\right)=\sum_{k=1}^{N_{ew}}Q_k'\delta\,(x-x_k,y-y_k) \tag{7}$$

where **K** is the hydraulic conductivity tensor, Q_k' is the extraction rate per unit aquifer volume from well k located at x_k and y_k, and δ is the Dirac delta function. The hydraulic head, h, is related to the head that the pump in extraction well k must overcome to deliver water to the treatment system, H, by $H = z_{gs} - h + h_l$ where z_{gs} is the ground surface elevation and h_l is the estimated head loss in the treatment train. Contaminant concentrations are determined by solving the contaminant mass balance equation, given by

$$\frac{\partial C}{\partial t}+\nabla[\mathbf{v}-\nabla\left(\mathbf{D}\cdot\nabla C\right)]=-\sum_k\frac{C_k}{n}Q_k'\delta\,(x-x_k,y-y_k) \tag{8}$$

where **v** is the pore velocity vector, C_k is the aqueous concentration removed from well k, and n is the porosity. The hydrodynamic dispersion tensor, **D**, is defined as:

$$\mathbf{D}=\left(\alpha_T\left|\mathbf{v}\right|+D^*\right)\mathbf{I}+\left(\alpha_L-\alpha_T\right)\frac{v_iv_j}{\left|\mathbf{v}\right|} \tag{9}$$

where α_L and α_T are the effective longitudinal and transverse dispersivity coefficients, respectively; **I** is the unit tensor; and D^* is the molecular diffusivity. The pore velocity, **v**, is given by Darcy's law as

$$n\mathbf{v} = -\mathbf{K}\nabla h \tag{10}$$

Equation 10 represents a constant homogenous aquifer that has a constant mean value, symbolizing a sand aquifer. To better represent contaminant transport in heterogeneous systems, we modify equation (8) by utilizing the dual domain concept. This concept considers the aquifer as partitioned into mobile and immobile zones, such that the total contaminant concentration in the aquifer and the total porosity is divided into mobile and immobile pore volumes, as in $nC = n_m C_m + C_{im} n_{im}$, where the subscripts *m* and *im* refer to the mobile and immobile domains. The exchange of mass between the pore volumes is driven by the concentration gradient between the zones of mobile and immobile water. The origin of the conceptual model and its mathematical representation can be traced to Coats and Smith (1964) and has been applied in the last two decades to simulate transport under natural and engineered field conditions (e.g. Harvey and Gorelick,1994 and Feehley et al.,2000). Equation (8) is replaced with mass balance equations for the mobile and immobile pore volumes, as in

$$\frac{\partial\left(n_m C_m\right)}{\partial t} + \frac{\partial\left(n_{im} C_{im}\right)}{\partial t} + \nabla[n_m \mathbf{v} - \nabla\left(n_m \mathbf{D} \cdot \nabla C_m\right)] = -\sum_k C_{m,k} Q'_k \delta\,(x - x_k, y - y_k)$$

(11)

$$\frac{\partial\left(n_{im} C_{im}\right)}{\partial t} = \alpha(C_m - C_{im}) \tag{12}$$

where α is the first-order rate constant controlling the rate of exchange between the mobile and immobile domains. This approach allows for each grid of the aquifer system to be considered as homogenous, while accounting for sub-grid heterogeneity, such as would be seen by a sandy aquifer with clay lenses.

We employ a 2-D finite difference approximation to solve the groundwater flow equation (equation (7)) and a particle-tracking method to solve the mobile zone mass transport equation (equation (11)). The numerical codes have been validated by Maxwell (1998). Additional background information pertaining to the development of this numerical simulator can be found in LaBolle et al. (1996). The transport code of Maxwell (1998) has been modified to include mobile-immobile mass exchange following the approach of

Valocchi(1985), where particle transfers between the pore volumes is based on a normal probability distribution with a variance calculated from the first-order rate constant, α, and the fractional porosities, n_m and n_{im}.

Two approaches are taken to estimate the carbon usage rate, $\dot{M}_{GAC}$. The "equilibrium" approach relies on the assumption that the contaminant in the groundwater and GAC are in instantaneous equilibrium. This approach is the traditional approach taken in previous PAT optimization efforts. The carbon utilization rate for the equilibrium approach is based on using a Freundlich isotherm to describe partitioning between the groundwater and GAC, or

$$q = K_{AB} C^{1/n} \tag{13}$$

where q is the concentration on the GAC (mass contaminant/massGAC), K_{AB} and $1/n$ are Freundlich isotherm constants, which are particular to the groundwater-GAC-contaminant system. Given equation (13), we can determine the GAC utilization rate for the equilibrium approach as

$$\dot{M}_{GAC} = Q_k \frac{C_k}{K_{AB} C_k^{1/n}} \tag{14}$$

The "non-equilibrium" approach accounts for kinetic interactions between the contaminant, groundwater, and GAC. This approach is based on the pore and surface diffusion model (PSDM) developed and verified by Crittenden and Hand (Crittenden, et al., 1986, 1987b, 1988; and Hand, et al., 1989, 1998) to describe fixed-bed, GAC adsorption. The PSDM incorporates the following assumptions: (a) plug-flow conditions exist in the GAC bed; (b) a linear driving force describes the mass flux from the bulk, flowing phase to the exterior surface of the adsorbent particle; (c) intra-particle mass flux is described by surface and pore diffusion; and (d) local adsorption equilibrium exists between the solute adsorbed onto the adsorbent particle and the intra-aggregate stagnant fluid. A graphical depiction of the water-contaminant-GAC processes is given in Figure 3, along with mathematical descriptions of the mass flux from the bulk phase to the surface of the particle and the intra-particle mass flux.

In the PSDM, the differential equations describing transport in the bulk phase and fluxes to an inside the GAC particles are solved using radial and lateral collocation techniques. The radial collocation defines diffusion across the bed and the lateral defines the length of the bed, which gives the solutions to the space derivatives. Time derivatives are solved using the DGEAR solution method. The GAC utilization rate for the non-equilibrium approach is calculated as an output of the PSDM. The most significant factors controlling $\dot{M}_{GAC}$ in this work are the influent concentration and the treatment goal (effluent concentration), but $\dot{M}_{GAC}$ also depends on factors such as the residence time in the GAC absorber unit (empty bed contact time, or EBCT), contaminant properties (e.g. free liquid diffusivity and density), GAC properties (e.g. particle radius, intra-particle porosity), and contaminant-GAC interactions (e.g. Freundlich isotherm constants).

Obtaining optimal solutions to equations (1) and (2) is a multi-objective problem, which is solved using a niched-Pareto genetic algorithm (NPGA). When equations (1) and (2) are considered simultaneously, the optimal solutions are represented in the form of a tradeoff curve of cost vs. mass remaining. The NPGA uses evolutionary methods to search for optimal design candidates based on a fitness evaluation of each candidate. The fitness is based on evaluating each candidate solution with respect to how many other solutions dominate the solution in a Pareto optimal sense. McKinney and Lin (1994), Ritzel et al. (1994), and Huang and Mayer (1997) give detailed descriptions of the traditional GA selection, reproduction, and mutation operators and a general overview of the GA as applied to single-objective groundwater problems. The NPGA also uses a "niching" operator to force the solutions to span the limits of the tradeoff curve. Erickson et al. (2002) gives a complete description of the application of the NPGA to multi-objective groundwater remediation design.

In this work, the NPGA also was used to find single-objective optimal solutions, where the objective function described equation (1) was considered but equation (2) was transformed into a constraint with a fixed, target value of the mass remaining. This constraint is formulated as :

$$\frac{1}{M_0}\left(\int_{\Omega_D} C(\mathbf{x},t)\,dV\right) \le MR' \quad \text{at } \ t = t_f \tag{15}$$

The constraint was enforced by using a standard penalty approach Erickson et al. (2002). The mass remaining target relates to an approximate maximum concentration in the aquifer of 0.00007 mg/L for the variance of 0.6 without source remediation.

NUMERICAL EXPERIMENTS

The hypothetical aquifer used in this set of experiments is homogenous with respect to hydraulic conductivity. A graphical description of the hypothetical aquifer is given in Figure 4. Each simulation begins with the development of a plume over a 500-day period. The plume emanates from a continuous source and is transported by groundwater flow imposed by constant head boundary conditions on the west and east boundaries of the aquifer. At the end of the 500-day period, the source is removed and PAT remediation begins using a single extraction well. All groundwater from the extraction well is treated in the GAC system, unless the concentration in the extraction well falls below the treatment objective. The remediation continues for a 5,000-day period.

The aquifer, contaminant, and treatment system parameters are given in Table 1. The rates given for pumping exceed the capture zone rates of 247 m^3/day in order to meet the mass removal constraints of the optimization method. The capture zone calculation was done using type curves as a reference. The hypothetical contaminant has properties similar to trichloroethylene, one of the most frequently found groundwater contaminants associated with hazardous waste disposal. The GAC properties are based on Calgon Filtrasorb® 400, which is a commercially available GAC and is widely used in groundwater treatment systems. The coefficients associated with the cost objective function (equation (1)) are given in Table 2. The well installation, pumping, and GAC unit cost coefficients are taken from Erickson et al. (2002). The GAC absorber unit costs are based on the purchase of a unit cost excluding carbon. The parameters used in the NPGA are given in Table 3. These parameter values were determined to give optimal performance in previous PAT optimization work by Erickson et al., (2002).

Three sets of numerical experiments were conducted. The purpose of the first set of experiments was to compare multi-objective optimal solutions obtained with the equilibrium and non-equilibrium GAC models, while solving objective functions (1) and (2) simultaneously. The solutions are obtained in the form of cost vs. mass remaining tradeoff curves. In these experiments, the effects of the mobile-immobile mass exchange were not considered and the number of absorber units was fixed at one ($N_{GAC} = 1$).

The second set of experiments was conducted to assess the effects of mobile-immobile mass exchange on optimal PAT designs. These experiments were single objective experiments, where cost was minimized (equation (1)) and the mass remaining was treated as a constraint (equation (15)). A range of mobile-immobile zone mass exchange rates and mobile-immobile zone porosities were used to assess the sensitivity of the optimal solutions to the parameters controlling mobile-immobile zone exchange. The values of the parameters are given in Table 4 and were selected based on values in the literature (Feehley et al, 2000, Sardin, et al, 1991, Zhang and Brusseau, 1999, Haggerty and Gorelick, 1999). Decreasing values of α and n_m correspond to greater degrees of heterogeneity and hence, the expectation of greater tailing in the concentrations in the extraction well. The number of absorber units was fixed at one ($N_{GAC} = 1$).

The third set of experiments was used to assess the feasibility of simultaneous design of the pumping system and treatment system by considering the number of absorber unit in series (N_{GAC}) as a decision variable. In the other experiments the EBCT was explicitly set according to 15 minutes for the average flow rate of the simulation. These experiments were conducted with the non-equilibrium PSDM model and with both homogeneous (no mobile-immobile mass exchange) and heterogeneous aquifer systems. Using more than one absorber units in series could lead to more efficient use of the GAC, since the successive units can manage the breakthrough concentrations from the preceding units, allowing for more of the capacity of the GAC to be utilized in the preceding units.

RESULTS

Tradeoff curves for the equilibrium and non-equilibrium GAC models are shown in Figure 5. Each point in the tradeoff curve represents a Pareto optimal design obtained with either the equilibrium or non-equilibrium GAC model. In general, the costs obtained with the non-equilibrium approach are higher than those obtained with the equilibrium approach, with the greatest differences occurring at the lowest and highest levels of mass remaining. For the low mass remaining targets, the concentrations in the extracted groundwater, decrease sharply as the bulk of the contaminant has been removed. Figure 6 shows that, during the latter stages of remediation, the concentration decrease is greater for lower mass remaining targets. The low concentrations in the extracted groundwater translate directly into low concentrations in the water delivered to the treatment system, and hence less efficient use of the GAC per mass of contaminant removed. The non-equilibrium model accounts for this lower efficiency, while the equilibrium model does not. Figure 7 shows the mass of GAC used as a function of mass removal for the equilibrium and non-equilibrium GAC models. As expected, GAC usage increases sharply as mass removal decreases, for the non-equilibrium model results; whereas the GAC usage for the equilibrium model results remains relatively constant. However the pumping rates did not vary with the inclusion of the non-equilibrium model.

Figure 8 shows the costs for the optimal designs obtained with the mobile-immobile mass exchange modeling approach. These results were obtained with single objective optimization, where the mass remaining target was fixed at *MR'* = 0.001. The costs obtained for $\alpha = 0$ day^{-1} and $n_m = n = 0.25$ correspond to costs obtained for homogeneous aquifer properties. The costs for the mobile zone porosity of $n_m = 0.2$ increase slightly as α decreases, and are similar to the costs obtained for homogeneous aquifer properties. However, for the lower mobile zone porosity, the total costs increase sharply as α decreases, due to sharp increases in treatment costs. For the lowest value, $\alpha = 0.002$ day^{-1}, no feasible solution was obtained, meaning that the mass remaining constraint could not be met.

Figure 9 shows a profile of mass remaining in the aquifer for the case where α = 0.002 day^{-1} and n_m = 0.05, along with a mass remaining profile for the homogeneous case for reference. These results show that, for the heterogeneous case, excessive tailing in the mass removal low concentrations occurs due to the slow release of contaminant mass from the immobile zone during pumping. The tailing in mass removal results in the delivery of low concentration water to the treatment system, inefficient use of the GAC, and high treatment costs. For the infeasible case, corresponding to $\alpha = 0.0002$ day^{-1} and $n_m = 0.05$, the mass release from the immobile zone is considerably slower. The result is extreme tailing, such that the mass remaining target cannot be achieved within the remediation horizon of 5,000 days, even at the maximum pumping rate.

In Figure 10, costs are shown for the optimal designs obtained with the number of adsorption units in series as a decision variable. For the homogeneous case, the maximum number of three adsorption units was selected. The GAC treatment costs for the case where the number of adsorption units is a decision variable are less than those for the case where the number of units is fixed. Since the cost per adsorption unit is relatively low, the total cost for the case where the number of adsorption units is a decision variable is lower. This result implies that when the design of the treatment system is optimized simultaneously with the design of the pumping, more efficient solutions can be found. However, for the heterogeneous case ($\alpha = 0.002$ day^{-1} and $n_m = 0.05$), there is no difference in the designs obtained when the number of adsorption units in series is or is not a decision variable. This result is explained by the excessive tailing (see Figure 9) and consequently very low influent concentration to the GAC treatment system for the homogeneous case. Even when multiple units in series are considered, the efficiency of the GAC usage is not improved.

CONCLUSIONS

The use of the non-equilibrium model that considers the diffusive processes of carbon has shown insights into optimization of remediation processes. The comparison of the equilibrium method to that it to the non-equilibrium process shows that the use of the equilibrium model underestimates the carbon usage at all levels of mass removal. The inclusion of the non-equilibrium model does not dramatically change modeling efforts, but when compared to the equilibrium model, gives more realistic usage rates.

To use of the mobile-immobile model causes the time steps of the modeling process to be dramatically decreased in order to use alpha values consistent with literature, resulting in longer simulation times. The inclusion of this process did change the outflow concentrations to be consistent with the effect of tailing. The effect of this tailing caused dramatic differences in the optimal design and costs of the remediation.

The most noteworthy result of this work has been in the inclusion of the treatment process design along with a hydraulic design. The homogeneous and heterogeneous optimizations that select the column length show a difference in treatment design and costs that vary with the treatment design. The inclusion of the design process in the optimization did not alter the runtime or modeling effort. The results indicate that the inclusion of treatment design will make more robust and efficient remediation possible.

ACKNOWLEDGEMENTS

This research was supported by NSF grant BES-0083112, USEPA grant CR826614-01-0 and the Statistical and Applied Mathematical Sciences Institute, Research Triangle Park, North Carolina.

REFERENCES

Coats, K.H., and Smith, B.D, Dead-end pore volume and dispersion in porous media: Journal of the Society of Petroleum Engineers, 4, p. 73-84, 1964.

Crittenden, J.C., D.W. Hand, H. Arora, and B.W. Lykins Jr., "Design Considerations for GAC Treatment of Organic Chemicals," Jour. of AWWA, 79 (1), 74-82, 1987b.

Crittenden, J.C., N.J. Hutzler, D.G. Geyer, J.L. Oravitz, and G. Friedman, "Transport of Organic Compounds with Saturated Groundwater Flow: Model Development and Parameter Sensitivity," Water Resources Research, 22 (3), 271-284, 1986.

Crittenden, J.C., R.D. Cortright, B. Rick, S.R. Tang, and D. Perram, "Using Granular Activated Carbon to Remove Volatile Organic Chemicals from Air Stripping Off-Gas," Jour. of AWWA, 80 (5), 73-84, 1988.

Crittenden, J.C., T.F. Speth, D.W. Hand, P.J. Luft, and B. Lykins, "Evaluating Multi-component Competition in Fixed Beds," Journal of Environmental Engineering, 113 (6), 1363-1375, 1987a.

Culver TB, Shenk GK, Dynamic Optimal Ground Water Remediation By Granular Activated Carbon, Journal of Water Resources Planning and Management, Jan/Feb, 59-64, 1998.

Culver TB, Shoemaker C, Dynamic Optimal Ground-water Reclamation with Treatment Costs, Journal of Water Resources Planning and Management, Jan/Feb, 59-64,1997.

Erickson M, Mark, Mayer AS, Horn J, Multi-objective optimal design of groundwater remediation systems: application of the niched Pareto genetic algorithm, Advances in Water Resources, Vol 25, 51-65, 2002.

Feehley C.E., C. Zheng, and F.J. Molz, A dual-domain mass transfer approach for modeling solute transport in heterogeneous porous media, application to the MADE site, Water Resources Research, 36(9), 2501-2515, 2000.

Hand and Jarvie In press, 2004

Hand, D. W., J. C. Crittenden, and W. E. Thacker, “Simplified Models for Design of Fixed-Bed Adsorbers,” Jour. of Env. Eng. Div., Proceedings of ASCE, 110 (EE2), 1984.

Hand, D. W., J. C. Crittenden, H. Arora, J. Miller, and B.W.Lykins Jr., “Design of Fixed-Beds to Remove Multi-component Mixtures of Volatile and Synthetic Organic Chemicals,” Jour. of AWWA, 81(1) 1989.

Hand, D. W., John Crittenden, Dave Hokanson, and John Bulloch, “Predicting the performance of fixed-bed granular activated carbon adsorbers,” Water Science and Technology, 35 (7), pp. 235-241,1997.

Haggerty R,Gorelick SM. Design of multiple contaminant remediation: sensitivity to rate-limited mass transfer. Water Resour Res, 30(2):435–46,1994.

Haggerty, R. and Gorelick, S. M. Multiple rate mass transfer for modeling diffusion and surface reactions in media with pore-scale heterogeneity. Water Resources Research.
31(10):2383-2400,1995.

Huang C,Mayer AS. Pump-and-treat optimization using well locations and pumping rates as decision variables. Water Resour Res 33(5):1001–12,1997.

LaBolle Em, Fogg GE, Thompson AFB, Random-walk simulation of transport in heterogeneous porous media. Water Resour Res. 32(3),583-593, 1996.

McKinney DC, and Linn M, genetic algorithim solutions of groundwater management models, Water Resour Res. 1994;30(6),1897-1906

Ritzel BJ,Eheart JW,Ranjithan S. Using genetic algorithms to solve a multiple objective groundwater pollution containment problem. Water Resour Res 1994;30(5):1589–603.

Sardin, M.; Schweich, D.; Leij, F. J.; and van Genuchten, M. Th.. Modeling the nonequilibrium transport of linearly interacting solutes in porous media: a review. Water Resources Research. 27(9):2287-2307,1991.

Sontheimer, H., J.C. Crittenden, and R.S. Summers, "Activated Carbon for Water Treatment," DVGW-Forschungsstelle, Engler-Bunte-Institut, Univ. Karlsruhe, Fed. Rep. of Germany (1988).

Valocchi, A.J., 1985, Validity of the local equilibrium assumption for modeling sorbing solute transport through homogeneous soils: Water Resources Research, v. 21, no. 6, p. 808-820.

Zhang, Z. and Brusseau, M. L, Nonideal transport of reactive solutes in heterogeneous porous media Simulating regional-scale behavior of a trichloroethene plume during pump-and-treat remediation. Water Resources Research. 35(10):2921-2935, 1999.

APPENDIX

Table A-1: Parameters used in PSDM model simulations

Parameter	Value
Void Fraction of the particle, unitless	0.667
Apparent Density, g/cm^3	0.650
Particle Radius, cm	0.042
Length, m	3.00
Weight of adsorbent in bed, kg	50.0
Adsorber diameter, m	0.3
Operating temperature, Celsius	24.0
Number of radial collocation points	5
Number of axial collocation points	10
Number of axial elements	1
Molecular weight of adsorbate, g/gmol	119.38
Molar volume of adsorbate, cm^3/gmol,	87.5
Freundlich K_{AB}, of adsorbate $(umol/g)(L/umol)^{1/n}$	11.285
Freundlich exponent 1/n, of adsorbate, unitless	0.78
Surface to Pore Diffusion Flux Ratio number, unitless	4.0
Tortuosity constant of adsorbate, unitless	1.0

Table 1: Base case parameters for flow, transport and treatment simulations

Parameter	Symbol	Value	Units
Aquifer properties			
total porosity	n	0.25	(-)
mobile zone porosity*	n_m	0.25	(-)
immobile zone porosity*	n_{im}	0.00	(-)
hydraulic conductivity	K	3.82×10^{-5}	m/s
background pore velocity	v	2.7×10^{-2}	m/d
longitudinal dispersivity	α_L	10	m
transverse dispersivity	α_T	2	m
mobile-immobile zone exchange rate*	α	0	day^{-1}
Groundwater treatment system properties			
GAC adsorption coefficient	K_{AB}	28.4	$(mg/gm)(L/mg)^{1/n}$
GAC adsorption coefficient	$1/n$	0.48	(-)
effluent treatment goal	C^*	0.005	mg/L
other GAC properties	See Appendix, Table A-1		

*this parameter is varied in numerical experiments; the value given is for the base case

Table 2: Base case values used in objective function and constraints

Parameter	Symbol	Value	Units
Cost coefficients in objective function			
well installation cost coefficient	a_1	10,800	\$/well
adsorber unit cost coefficient	a_2	1,000	\$/adsorber unit
pumping operation cost coefficient	a_3	1.05	$\$/m^4$
treatment cost coefficient	a_4	2.14	\$/gm GAC
Constraint values			
maximum extraction rate	$Q^{\max}$	250	m^3/day
maximum number of adsorption units	$N_{GAC}^{\max}$	3	(-)
remediation horizon	t_f	5,000	days
maximum mass remaining	MR'	0.001	(-)

Table 3: Optimization algorithm parameters used in NPGA.

Parameter	Value
population size	50
tournament selection size	2
niche radius	0.5
probability of crossover	0.9
probability of mutation	0.001

Table 4: Parameter values for the mobile-immobile zone simulations

Mobile-Immobile Zone Exchange rate, α (day^{-1})	Mobile Zone Porosity, n_m	Immobile Zone Porosity, n_{im}
0.02	0.05	0.20
0.02	0.20	0.05
0.002	0.05	0.20
0.002	0.20	0.05
0.0002	0.05	0.20
0.0002	0.20	0.05

FIGURE CAPTIONS

Figure 1: Description of equilibrium and non-equilibrium GAC models.

Figure 2: Schematic of computational framework.

Figure 3: Illustration and mathematical description of GAC adsorption processes.

Figure 4: Illustration hypothetical aquifer system.

Figure 5: Cost vs. mass remaining tradeoff curves for equilibrium and non-equilibrium GAC models.

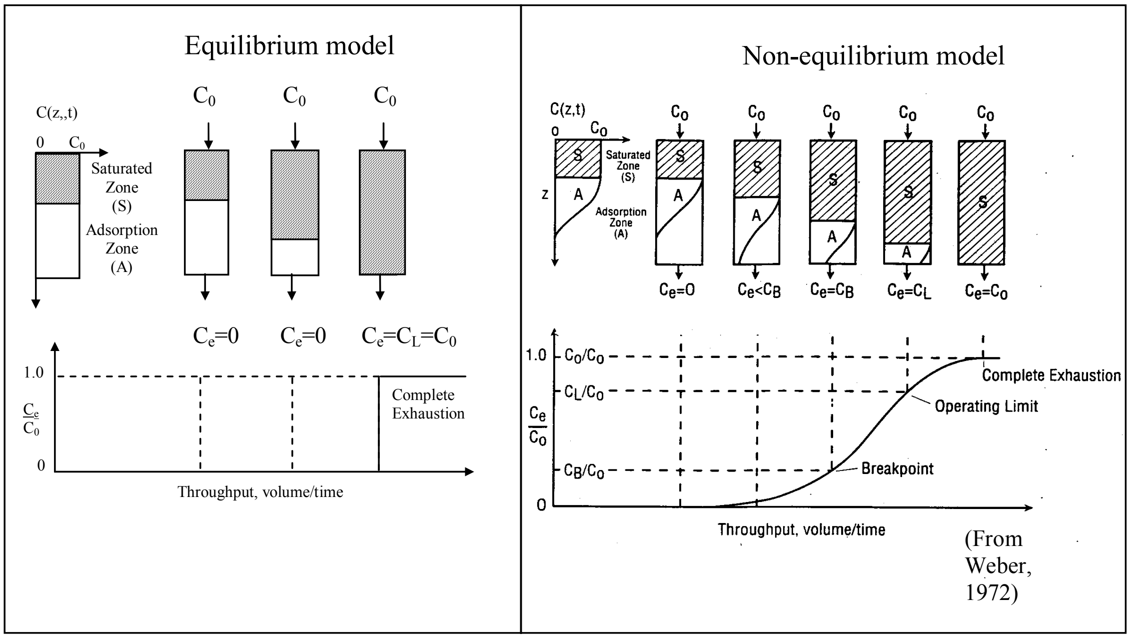
Figure 6: Concentration at extraction well vs. time for range of cleanup performances, measured as mass remaining, (*MR*').

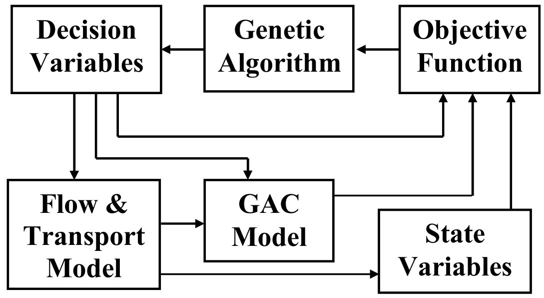
Figure 7: GAC usage rate (gm GAC used/volume of water treated) vs. mass remaining for equilibrium and non-equilibrium GAC models.

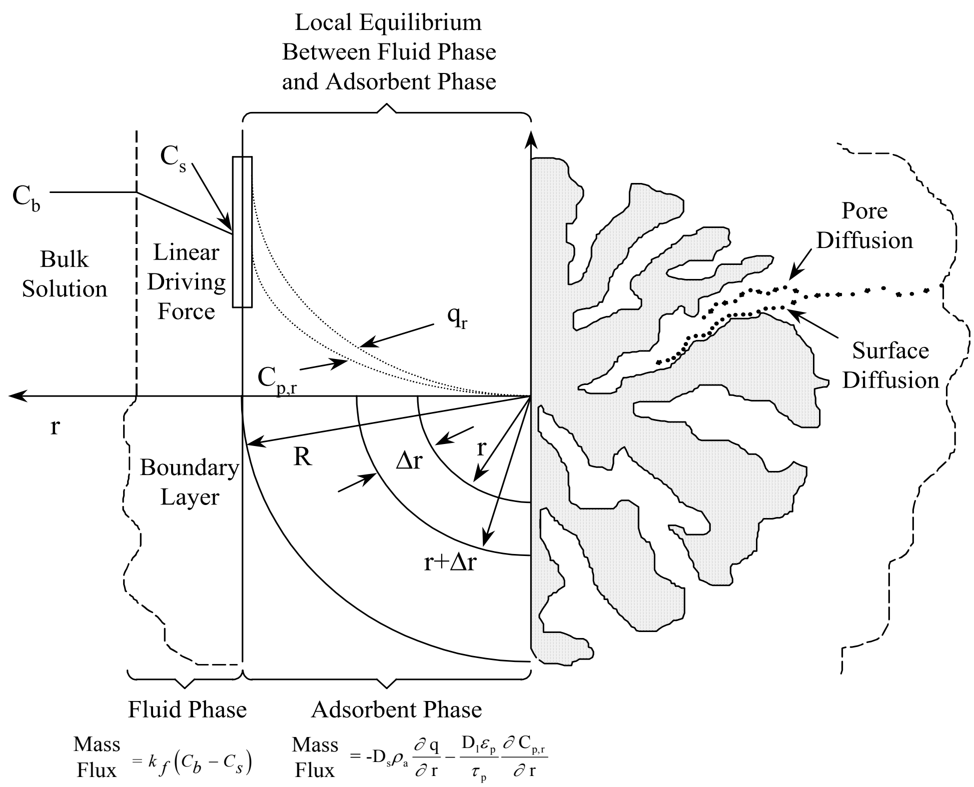
Figure 8: Treatment and pumping costs for a range of mobile-immobile zone exchange rates and for high and low mobile zone porosities.

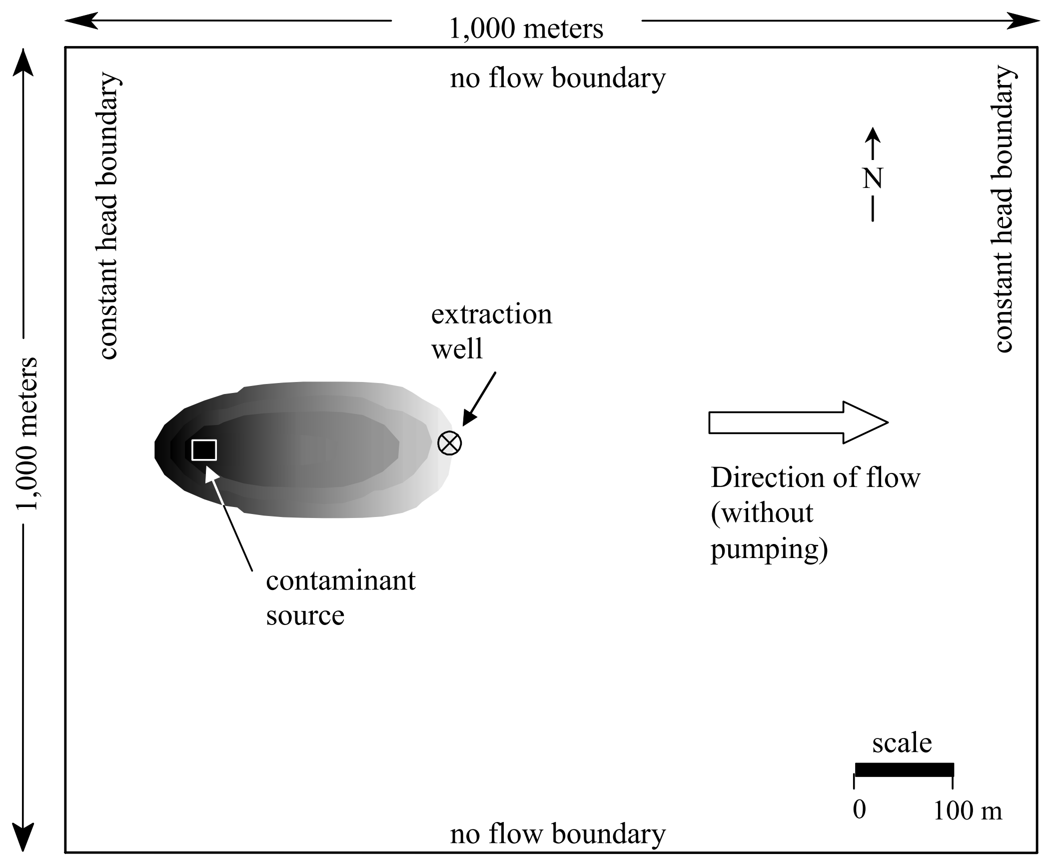
Figure 9: Contaminant mass in mobile and immobile zones and total contaminant mass vs. time for mobile-immobile zone exchange rate $\alpha = 0.002$ day^{-1} and mobile zone porosity $n_m = 0.05$. Contaminant vs. time for the homogeneous case is provided for reference.

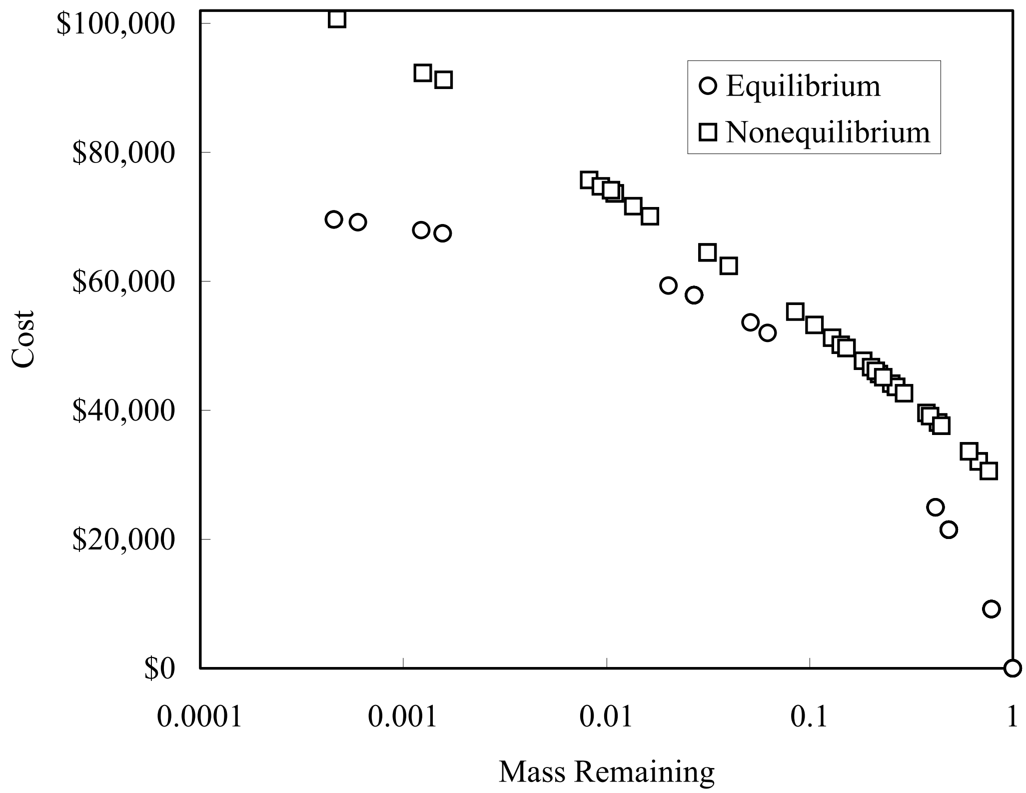
Figure 10: Treatment and pumping costs for cases where the number of adsorber units was and was not considered as a decision variable for homogeneous and heterogeneous systems. Heterogeneous system has a mobile-immobile zone exchange rate of $\alpha = 0.002$ day^{-1} and a mobile zone porosity of $n_m = 0.05$.

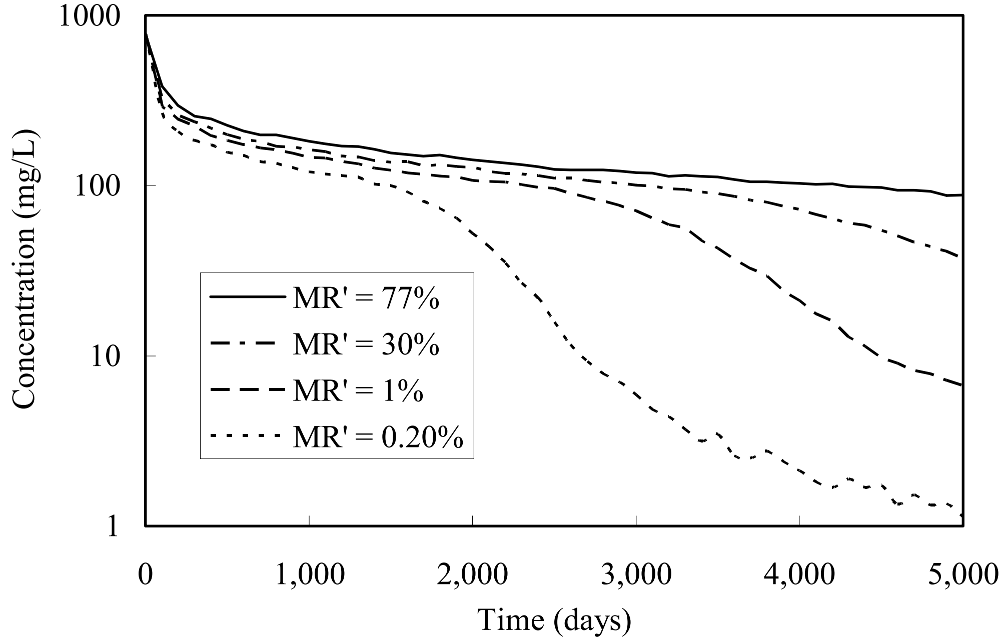

Equilibrium model
C(z,,t)
0
C_0
Saturated Zone (S)
Adsorption Zone (A)
C_0
C_0
C_0
C_e=0
C_e=0
C_e=C_L=C_0
1.0
$\frac{C_e}{C_0}$
0
Complete Exhaustion
Throughput, volume/time
Non-equilibrium model
C(z,t)
o
C_o
Saturated Zone (S)
Adsorption Zone (A)
z
S
A
C_e=O
C_e<C_B
C_e=C_B
C_e=C_L
C_e=C_o
1.0
C_o/C_o
C_L/C_o
C_B/C_o
$\frac{C_e}{C_o}$
0
Complete Exhaustion
Operating Limit
Breakpoint
Throughput, volume/time
(From Weber, 1972)


Decision Variables
Genetic Algorithm
Objective Function
Flow & Transport Model
GAC Model
State Variables

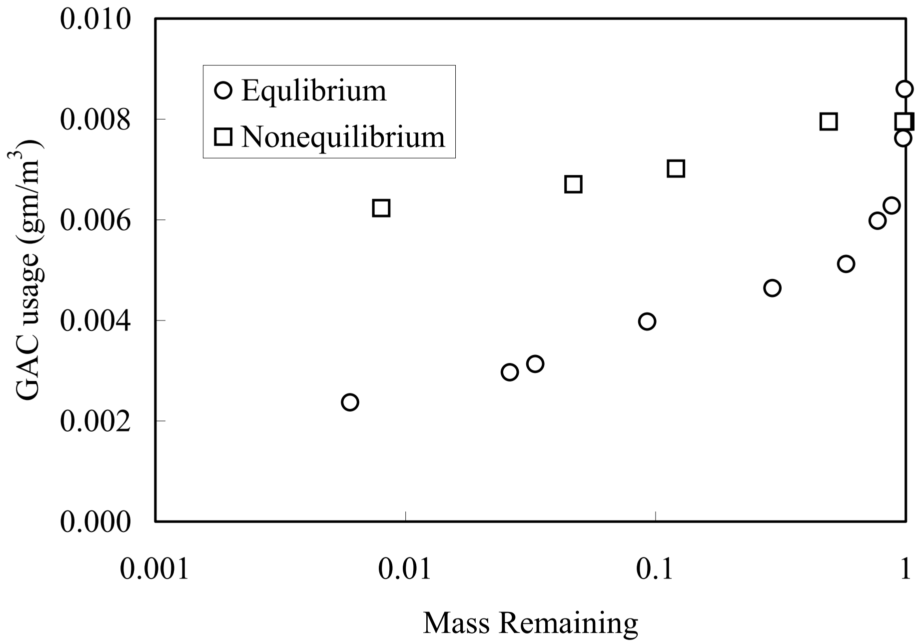

Local Equilibrium
Between Fluid Phase
and Adsorbent Phase
C_s
C_b
Bulk
Solution
Linear
Driving
Force
q_r
$C_{p,r}$
Pore
Diffusion
Surface
Diffusion
r
R
Δr
r
r+Δr
Boundary
Layer
Fluid Phase
Adsorbent Phase
Mass
Flux $= k_f(C_b - C_s)$
Mass
Flux $= -D_s\rho_a \frac{\partial q}{\partial r} - \frac{D_l \varepsilon_p}{\tau_p}\frac{\partial C_{p,r}}{\partial r}$


1,000 meters
no flow boundary
constant head boundary
N
constant head boundary
1,000 meters
extraction
well
Direction of flow
(without
pumping)
contaminant
source
scale
0
100 m
no flow boundary

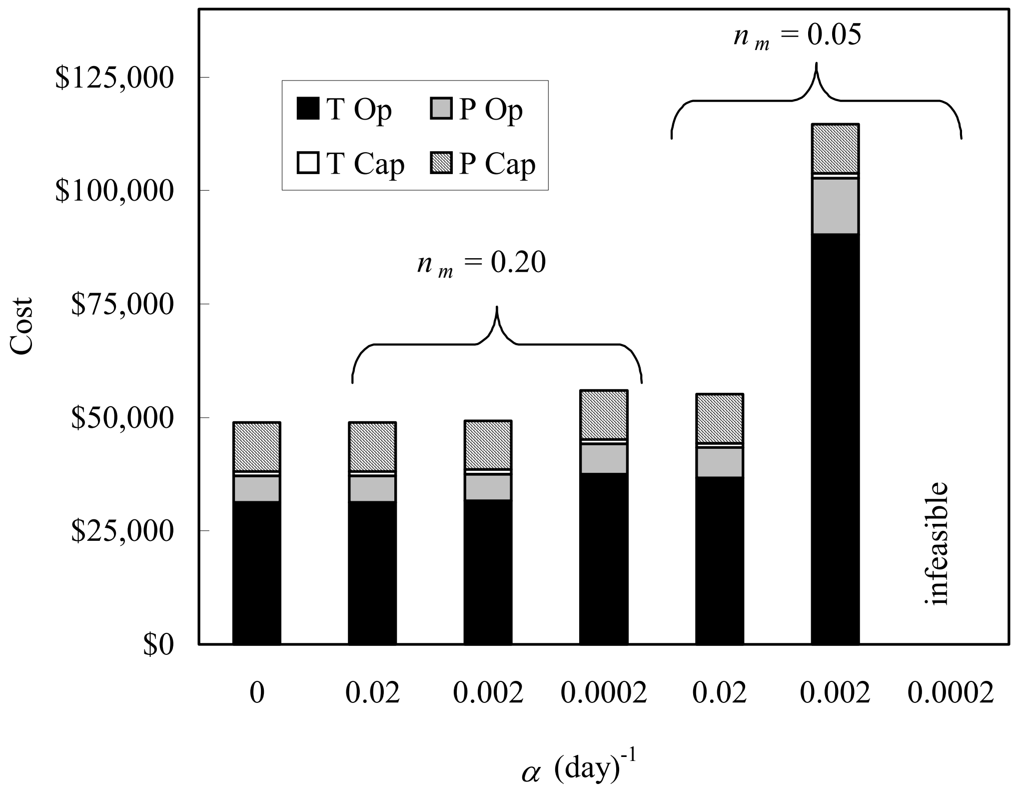

$100,000
$80,000
$60,000
$40,000
$20,000
$0
Cost
0.0001
0.001
0.01
0.1
1
Mass Remaining
Equilibrium
Nonequilibrium



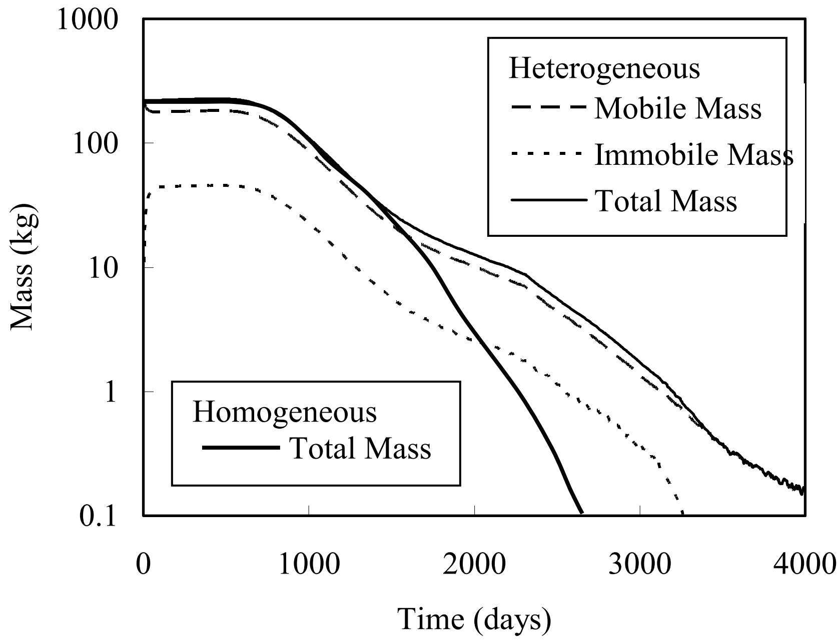
1000
100
10
1
Concentration (mg/L)
0
1,000
2,000
3,000
4,000
5,000
Time (days)
MR' = 77%
MR' = 30%
MR' = 1%
MR' = 0.20%

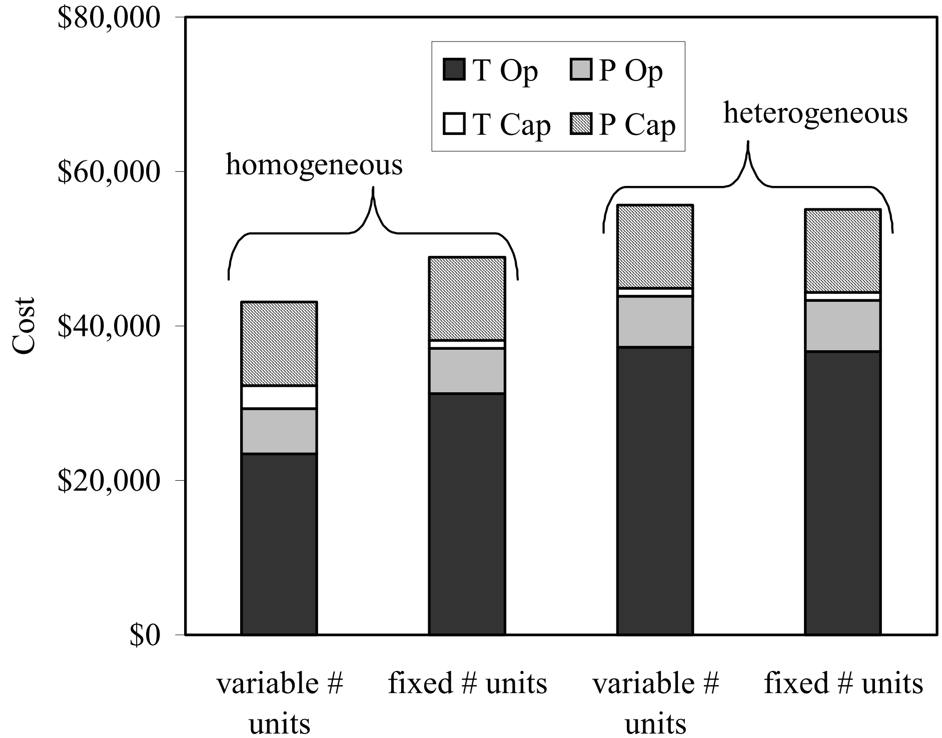


0.010
0.008
0.006
0.004
0.002
0.000
Equlibrium
Nonequilibrium
GAC usage (gm/m3)
0.001
0.01
0.1
1
Mass Remaining



n_m = 0.05
$125,000
$100,000
$75,000
$50,000
$25,000
$0
Cost
T Op
P Op
T Cap
P Cap
n_m = 0.20
infeasible
0
0.02
0.002
0.0002
0.02
0.002
0.0002
α (day)$^{-1}$


1000
100
10
1
0.1
Mass (kg)
0
1000
2000
3000
4000
Time (days)
Heterogeneous
Mobile Mass
Immobile Mass
Total Mass
Homogeneous
Total Mass


$80,000
$60,000
$40,000
$20,000
$0
Cost
T Op
P Op
T Cap
P Cap
homogeneous
heterogeneous
variable # units
fixed # units
variable # units
fixed # units

Optimization of Source and Plume Remediation

Karen L. Endres

Department of Civil & Environmental Engineering, Michigan Technological University, Houghton, Michigan

ABSTRACT

Most optimization efforts are based on the assumption that the source material has been eliminated before the PAT efforts begin and focus exclusively on the removal of contaminants in the groundwater plume. However, complete source removal is frequently a poor assumption. From management perspective, there is a tradeoff between the degree of cleanup effort and funds dedicated to source removal and to the cleanup of the groundwater plume emanating from the source. A framework is developed for determining optimal designs of combined source and plume remediation efforts. The framework accounts for the presence of heterogeneity in the source distribution, such that the rate of mass release into the plume and the efficiency of source remediation efforts are controlled by the degree of heterogeneity. The relationship between plume remediation costs and the source variance is not monotonic, revealing the complex relationship between the release rate from the source into the plume and the costs associated with pumping and treatment. Only when the source remediation capital or operating cost are reduced does source remediation become competitive with plume remediation, particularly in lower source variances. Degradation of the contaminant within the plume lowers the total cost of the remediation. For the highest degradation rates, no remediation is required, implying that natural attenuation is sufficient to meet the cleanup goal.

INTRODUCTION

Over the last two decades, groundwater quality control and remediation have been the focus of optimization efforts in the literature. The design of pump-and-treat (PAT) systems is the most frequent technology considered (Mayer et al., 2002). Underlying the PAT optimization framework are simulators of groundwater flow and contaminant transport that are based on numerical approximations of the governing flow and transport models. Development and execution of a typical simulator involves the solution of thousands to millions of unknowns. The simulators also require the determination of physical and chemical parameter distributions; however, these parameters are usually poorly characterized. The large computational burden and parameter variability leads to the frequent use of simplified models, including two spatial dimensions, steady-state conditions, confined aquifers, simple reaction models, single species and local equilibrium between phases and simplified treatment of contaminant sources.

Since PAT focuses exclusively on the removal of contaminants in the groundwater plume, this technology only incidentally removes source material as it is released into the plume. All but a few remediation optimization studies (Lin and McKinney, 1995; Yu et al., 1998; Teutsch and Finkel, 2002) have neglected the contribution of sources to the remediation design problem by relying on the assumption that the source material has been eliminated. However, complete source removal is frequently a poor assumption, due to technical, economic or regulatory factors. In many sites where engineered source removal has been implemented, the efforts were incomplete, either because of poor design or because not all of the source material was identified or inaccessibility of the source material to treatment. In other sites, engineered source removal was not implemented because it was deemed technically infeasible or economically impractical.

Dense nonaqueous phase liquids (DNAPLs), such as chlorinated solvents or coal tars, are contaminant sources that particularly difficult to remove. DNAPLs act as contaminant sources as the groundwater flows through region containing the trapped DNAPL. The ultimate distribution of residual NAPL saturation is not uniform or predictable in the subsurface due to minute variations in the pore size distributions, soil texture, soil structure and mineralogy (ITRC, 2002). This highly irregular distribution makes both characterization and remediation difficult (Pankow and Cherry, 1996). However, as suggested by Sale and McWhorter (2001), near-complete removal of DNAPL source would be required to achieve meaningful improvements in groundwater quality.

Innovative technologies have been developed that focus specifically on DNAPL removal, e.g. surfactant and co-solvent flushing, in-situ chemical oxidation, and thermal methods.

EPA encourages the use of innovative technologies to eliminate or isolate DNAPL source zone, especially where operation and maintenance costs associated with conventional plume remediation technologies are prohibitive

(ITRC, 2002). Despite federal and state guidance citing the long-term benefits of source removal and recommending that NAPL sources be remediated to the extent feasible (EPA, 1996), there is still apprehension in the regulatory community over the presumed high cost and uncertain benefits of aggressive source zone treatment (ITRC, 2002).

A simplified conceptual model of the DNAPL source-contaminant plume system is proposed in Figure 1. In this model, the DNAPL source is modeled as a temporally varying, but non-dimensional, input to the contaminant plume, quantified with a mass release rate, $\dot{m}(t)$. The factors affecting the mass release rate include the advective rate through the source area, which could be impacted by the regional groundwater flow and flow induced by plume cleanup efforts, the spatial distribution of the contaminant mass and hydraulic conductivity distribution within the source area, and the chemical composition of the source. Once the contaminant mass has entered the plume via dissolution, the spatial and temporal behavior of the plume is again controlled by the advective rate and hydraulic conductivity distribution, but also what have been loosely termed as attenuation factors, which include dispersion and degradation reactions. The degradation reactions could include both biotic and abiotic reactions.

Figure 2 shows the timeline that accompanies the conceptual model in Figure 1. The DNAPL contaminant source is released into the aquifer at the beginning of the scenario. Until the contamination is discovered and cleanup efforts begin, mass is transferred via dissolution from the DNAPL source into the contaminant plume. In a global sense, some mass is lost via degradation reactions within the contaminant plume. At some point in time, the DNAPL source is remediated using, for example, chemical flushing or thermal technologies. The DNAPL source is either partially or completely remediated (although complete remediation is highly unlikely). The time period over which the DNAPL remediation occurs is assumed to be small relative to the total time.

Plume remediation can begin at the same time as the DNAPL remediation, but occurs over much longer time period. In the case of engineered remediation, contaminant mass in the plume is removed via physical (e.g. pump-and-treat) or biochemical (e.g. bioremediation) means. Alternatively, natural attenuation may be considered, where plume mass removal occurs via biochemical reactions. In either case, if the DNAPL source removal is incomplete, mass will continue to transfer from the source into the plume. The amount of mass entering the aquifer after source remediation is dependent on the efficiency of the source removal efforts and the properties of the source area.

From a management perspective, there is a tradeoff between the degree of cleanup effort and funds dedicated to source removal and to the cleanup of the groundwater plume emanating from the source. Many of these issues have been reviewed by Teutsch et al. (2001). For example, an aggressive source removal plan might be costly initially, but should reduce the amount of effort and cost needed to complete the cleanup of the groundwater plume, perhaps to the point of relying on natural attenuation. While the capital costs of installing a remediation system that focuses only on the groundwater plume may be more attractive from a net present value, the estimated life-cycle costs of operating a typical PAT system for possible 100 years or more are considerable (ITRC, 2002).

The investigators that have addressed the issue of simulating DNAPL source inputs have generally taken two approaches. The first approach involves explicitly modeling the DNAPL release, migration, and subsequent dissolution by solving multiphase flow and transport equations (e.g. Sleep and Sykes, 1993; Powers et al., 1994; Mayer and Miller, 1996). These efforts have given valuable insight into the behavior of DNAPL sources over time, such as extreme tailing when the source zone is heterogeneous (e.g. Mayer and Miller, 1996). However, these simulators are computationally expensive and require parameters that are usually unavailable at most field sites.

The second approach involves embedding time-variant models of DNAPL dissolution into single-phase (groundwater) contaminant transport simulators. These DNAPL dissolution models have included explicit modeling of NAPL blob dissolution (Powers et al., 1994), a simple analytical model of NAPL source release rates (Robinson and Bedient, 1991), and superposition of multiple DNAPL release rates into an analytical model (Sale and McWhorter, 2001). Enfield (2001) also has suggested that bundle of tube models can be used to characterize release rates from heterogeneous DNAPL sources, where the degree of heterogeneity is estimated from partitioning tracer tests.

The ultimate goal of this work is to provide guidelines for choosing the degree of effort and funds to dedicate to source removal vs. plume remediation, based on the conditions at the site. We approach this goal with the use of multiple simulation processes linked within an optimization framework. The optimal allocation of costs for the remediation is produced using a niched-Pareto genetic algorithm to guide the optimization, coupled with simulation models for the source and the plume remediation systems. The system is applied to a hypothetical aquifer containing source and plume contamination.

SIMULATION AND OPTIMIZATION APPROACH

The management of source-plume remediation is explored with the computational framework consisting of determining optimal values of decision variables by specifying an objective function and simulating flow and transport processes, including a specialized model for the source. The framework is summarized in Figure 3.

Optimization Problem

The optimization problem is stated as

$$\begin{aligned}&\text{find } \mathbf{w} \text{ while } \min f = \min\left(f_{cap}^{S} + f_{op}^{S} + f_{cap}^{P} + f_{op}^{P}\right)\\&\text{subject to: } \mathbf{z} \in \Omega_{\mathbf{z}} \text{ and } \mathbf{w} \in \Omega_{w}\end{aligned} \tag{1}$$

where **w** is the vector of decision variables; *f* is a cost objective function; the subscripts *cap* and *op* refer to capital and operational costs, respectively; the superscripts *S* and *P* refer to costs associated with source and plume remediation, respectively; **z** is the vector of state variables; and $\Omega_{\mathbf{z}}$ and $\Omega_{\mathbf{w}}$ represent constraints on the state and decision variables, respectively.

We assume that the source remediation will be conducted with a chemical flushing technology (e.g. surfactant or cosolvent flushing) and that the chemical flushing technology works by solubilization of the DNAPL, rather than mobilization. The capital costs for the chemical flushing are based on purchasing the flushing agent ant the associated remediation equipment such as pumps, wells and contaminant removal systems, such as air stripping towers.. The operational costs for the chemical flushing are based on the costs required to recycle the chemical flushing agent. We further assume that the plume remediation will be conducted with pump and treat (PAT). The capital costs for the PAT system include the cost of extraction well installation. Operating cost for the PAT system are based on the costs of replacing the adsorbent in a granular activated carbon (GAC) system.

Given the conceptualization of the source and plume remediation, the components of the cost objective functions can be defined as

$$
\begin{aligned}
&f_S^{cap} = a_1 V_f \\
&f_S^{op} = a_2 V_{nf} \\
&f_{cap}^{P} = a_3 N_{ew} \\
&f_{op}^{P} = \sum_{k=1}^{N_{ew}} \sum_{l=1}^{N_t} \left(a_4 Q_k H_k t_l + a_5 Q_k \frac{C_{k,l}}{K_{AB} C_{k,l}^{1/n}} t_l \right), \quad a_5 = 0 \text{ for } C_{k,l} \le C^*
\end{aligned}
\tag{2}
$$

where a_1 and a_2 are the cost coefficients associated with the capital and operating costs for the flushing system, respectively; V_f is the volume of flushing solution purchased; V_{nf} is the number of source area pore volumes flushed, expressed as an integer; a_3 is the cost coefficient associated with the extraction well installation; N_{ew} is the number of active extraction wells; N_t is the number of time steps within the remediation horizon; k and l are the well and time indices, respectively; a_4 and a_5 are the cost coefficients associated with the pumping and groundwater treatment operating costs, respectively; Q_k is the pumping rate at well k; H_k is the head that the pump in extraction well k must overcome to deliver water to the treatment system; t_l is the incremental time period used to evaluate the PAT operational costs; $C_{k,l,}$ is the average flow-weighted concentration removed by well k in time step l; and K_{AB} and $1/n$ are Freundlich GAC adsorption parameters for a given contaminant and carbon adsorbent. The cost coefficient for the groundwater treatment term is set to 0 when the influent to the treatment system falls below the treatment effluent concentration goal, C^*.

The decision variables appearing in equation (2) are the pumping rates at fixed-location extraction wells, Q_k and the number of flushes of the source area, V_{nf}. The constrains on the decision variables and state variables are

$$0 \le Q_k \le Q^{\max} \quad \text{for } k = 1, \ldots N_{ew} \tag{3}$$

$$V_{nf} \le V_{nf}^{\max} \tag{4}$$

$$h \ge h_{\min} \quad \text{over } \Omega_D \tag{5}$$

$$\sum_{l=1}^{N_t} t_l = t_f \tag{6}$$

$$\frac{1}{M_0}\left(\int_{\Omega_D} C(\mathbf{x},t)\, dV + \frac{1}{V} \int_{\Omega_D} nS_n(\mathbf{x},t)\, \rho_n dV \right) \le M'_{\max} \quad \text{at } t = t_f^{\max} \tag{7}$$

where $Q^{\max}$ is the maximum, individual pumping rate; $V_{nf}^{\max}$ is the maximum number of chemical flushes, $h_{\min}$ is the minimum head allowed over the model domain, Ω_D; t_f is the remediation horizon; C is the concentration in the plume, S_n is the DNAPL saturation in the source zone; ρ_n is the DNAPL density, V is the volume of the model domain; M_0 is the initial mass; and $M_{\max}$ is the maximum contaminant mass allowed in the aquifer at the end of the maximum remediation horizon. Equation (5) effectively constrains the maximum drawdown in the aquifer. Equation (6) sets the maximum length of time for the remediation horizon. Equation (7) is a normalized cleanup goal constraint. The two integral terms in equation (7) represent the contaminant mass in the plume (dissolved) and the contaminant mass in the source (DNAPL), such that maximum mass remaining at the end of remediation accounts for the contaminant mass in the plume and the source.

Flow and Transport Simulators

The state variables in equations (1) through (7) are the contaminant concentration in the plume, C, the mass of DNAPL, m, and the hydraulic head, h. The subsurface processes used in this work are based on the two-dimensional steady state flow equations and contaminant mass balance equations. The steady-state, confined groundwater flow equation for a non-deforming, saturated, aquifer system is

$$\nabla\left(\mathbf{K}\cdot\nabla h\right)=\sum_{k=1}^{N_{ew}}Q_k'\delta\left(x-x_k,y-y_k\right) \tag{8}$$

where $\mathbf{K}$ is the hydraulic conductivity tensor, Q_k' is the extraction rate per unit aquifer volume from well k located at x_k and y_k , and δ is the delta Dirac function. The hydraulic head, h, is related to the head that the pump in extraction well k must overcome to deliver water to the treatment system, H, by $H=z_{gs}-h+h_l$ where z_{gs} is the ground surface elevation and h_l is the estimated head loss in the treatment train. Contaminant concentrations are determined by solving the contaminant mass balance equation, given by

$$\frac{\partial C}{\partial t}+\nabla[\mathbf{v}-\nabla\left(\mathbf{D}\cdot\nabla C\right)]+R=-\sum_k\frac{C_k}{n}Q_k'\delta\left(x-x_k,y-y_k\right) \tag{9}$$

where $\mathbf{v}$ is the pore velocity vector, R is a contaminant degradation term, C_k is the aqueous concentration removed from well k, and n is the effective porosity. The hydrodynamic dispersion tensor, $\mathbf{D}$, is defined as:

$$\mathbf{D} = \left(\alpha_T \left|\mathbf{v}\right| + D^*\right)\mathbf{I} + \left(\alpha_L - \alpha_T\right)\frac{v_i v_j}{\left|\mathbf{v}\right|} \tag{10}$$

where α_L and α_T are the effective longitudinal and transverse dispersivity coefficients, respectively; $\mathbf{I}$ is the unit tensor; and D^* is the molecular diffusivity. The pore velocity, $\mathbf{v}$, is given by Darcy's law as

$$n\mathbf{v} = -\mathbf{K}\nabla h \tag{11}$$

Degradation of contaminants by biotic or abiotic pathways can be a complicated process. For example, the chemical species may follow higher order reaction rates, multiple species can be created or destroyed in the transformation process, and concentrations of ancillary chemicals may need to be considered (e.g. oxygen). In this work, we greatly simplify the degradation process by assuming that the chemical contaminant follows a single, first-order decay and that the concentrations of chemicals ancillary to the degradation are unlimited. In this case, the degradation term R in equation (9) can be represented as

$$R = -\lambda C \tag{12}$$

where λ is the first-order decay constant. This simplified approach to representing chemical degradation is often taken when the chemical of interest is a chlorinated solvent (e.g. Schwarzenbach et al., 1993), which are most frequently associated with DNAPL contaminant sources.

We employ a 2-D finite difference approximation to solve the groundwater flow equation (8) and a particle-tracking method to solve the contaminant transport equation (9). The numerical codes have been validated by Maxwell (1998).

These codes have been modified to include the reaction term (equation (12)) and a time-varying source term. Additional background information pertaining to the development of the numerical simulator can be found in LaBolle et al. (1996). The contaminant source is incorporated by specifying by a particle input term, $N_p(t)$, over a source zone that is specified numerically with a number of finite-difference cells. The value of $N_p(t)$, is updated every time-step, depending on the mass of DNAPL remaining in the source zone. The procedure for evaluating $N_p(t)$ is described in the following section.

Source Model

A "bundle of tubes" model is used to simulate the dissolution of the DNAPL source and provide the source term $C^*(\mathbf{x},t)$. The same model is used to simulate source removal under ambient and engineered conditions. This model represents the heterogeneous DNAPL distribution, and consequent distribution of DNAPL rates of dissolution. The source model accounts for variability in the aquifer properties with the use of an inverse log-normal probability distribution resulting in time-variable source input to the flow and transport model. The model is relatively simple, but is capable of simulating the "tailing" behavior that is often observed with these technologies. By "tailing," here we mean that the rate of removal decreases significantly after the majority of the source mass is removed, such that the last, say, 10% of the source mass, is removed less and less efficiently. Low permeability units, heterogeneities and insoluble contaminants may impose limitations and increase tailing.

The tube model also incorporates variability into the source remediation.

The source model is based on a log-normal probability distribution of n_ℓ tube lengths, with μ_ℓ as the mean of the $\log_{10}$-transformed tube lengths and σ_ℓ^2 as the variance of the $\log_{10}$-transformed tube lengths. The distribution of tube lengths is produced by sampling n_ℓ times from the cumulative distribution function ($\mathbf{cdf}(\mu_\ell = 1, \sigma_\ell^2)$) with numbers randomly generated from a uniform distribution with range (0,1).

The individual tube length, ℓ_i, is an indicator of the initial mass of DNAPL in the tube, as in

$$m_{i,0} = \ell_i a_i S_n \rho_n \tag{13}$$

where a_i is the area of the tube, S_n is the average DNAPL saturation in the source zone, and ρ_n is the DNAPL density. Note that we assume that S_n and ρ_n are uniform throughout the source zone. Also, all of the tube areas are equal and are computed from

$$n = \frac{\sum_{i=1}^{n_\ell} a_i}{A} \tag{14}$$

where A is the cross-sectional area of the source zone.

The mass rate of removal in each tube is

$$\dot{m}_i = q_i a_i C_s \tag{15}$$

where q_i is the flux through the tube and C_S is the saturated concentration of the DNAPL in the groundwater. The global source mass balance at time *t* is obtained by

$$m(t) = \sum_{i=1}^{n_\ell} \left(m_{i,0} - \int_0^t q_i a_i C_s dt \right) \tag{16}$$

Equation (16) implies that, at some time, the DNAPL in an individual tube can be exhausted. At this point, the tube is eliminated from the model; that is, the subscript *i* in equation (16) includes only the active tubes. Figure 4 shows a few examples of tube distributions and the corresponding DNAPL source mass as a function of time. The ranges of source variances are comparable to a homogenous sand aquifer at low variance to a aquifer containing clay lenses at the higher values.

During the time when the source zone is not being remediated, the saturated concentration, C_S, is equal to the solubility of the compound in equilibrium with pure water and all tube fluxes, q_i, is equal to the flow through the source zone as computed by the groundwater flow model. Over the period when source remediation occurs via chemical flushing, the saturated concentration, C_S, is set to the enhanced solubility, or the solubility that would occur when the DNAPL is in equilibrium with the flushing solution. During this period, the tube fluxes are set to the flow imposed by the flushing operations.

In order to link the source model with the transport model, the mass input to the aquifer over a time step, Δt, is converted to a corresponding number of mass-based particles, N_p, as in

$$N_p(t) = \frac{1}{m_p} \sum_{i=1}^{n_\ell} \left(\int_t^{t+\Delta t} q_i a_i C_s dt \right) \tag{17}$$

where m_p is the particle mass.

The hypothetical model aquifer model is based on a physical system of a sand matrix. The source model accounts for changes in the matrix indicative of clay lenses or organic matter.

Optimization Solution

The optimization problem is solved using a niched-Pareto genetic algorithm (NPGA). The NPGA uses evolutionary methods to search for optimal design candidates based on a fitness evaluation of each candidate. The size of the search space and the non-linear, non-convex nature of the optimization problem considered here lend themselves to the use of genetic algorithms. The NPGA is based on conventional GA tournament selection, reproduction, and mutation operators, which have been described by McKinney and Lin (1994), Ritzel et al. (1994), and Huang and Mayer (1997). The NPGA also uses a niching operator (Horn, 1997), which is intended to enhance diversity in the population of candidate solutions. The diversity enhancement occurs by giving preference to candidate solutions that have objective function values that are farther from the mean, for a given generation. The heuristic parameters for the NPGA are population size, tournament size, crossover probability, mutation probability and niche radius. Erickson et al. (2002) describes in detail the implementation of NPGA to subsurface remediation design problems. Erickson et al. (2002) also gives guidelines for the selection of the values of the NPGA parameters.

NUMERICAL EXPERIMENTS

The numerical experiments simulate four distinct stages: (1) source emplacement, (2) plume creation, (3) source remediation, and (4) plume remediation. The source emplacement is simulated as an instantaneous event. During the plume creation phase, groundwater passes through the DNAPL source at the regional groundwater velocity, dissolves the DNAPL, and transports the dissolved DNAPL. The source input to the plume is simulated with the tube model. The plume is created over the period $0 \le t \le t_P$.

At the plume development time ($t = t_P$), the source is remediated. Since the source remediation is expected to occur quickly, relative to the other stages, it is treated as an instantaneous event. The source remediation occurs by injection of chemical flushing agents through the source zone at a fixed flow rate. The flushing agents increase the solubility of the DNAPL over the solubility in pure water, as determined by a fixed multiplicative factor, x_f. The source remediation is simulated with the tube model.

In the final stage, the plume is remediated the plume by PAT over the period $t_P < t \leq t_f$, where t_f = 7,500 days. In the cases where the DNAPL source has not been completely removed in the source remediation stage, the source continues to dissolve into the plume during the plume remediation stage.

The hypothetical, two-dimensional aquifer is confined and homogenous and isotropic with respect to hydraulic conductivity. Boundary conditions are set to produce a west-to-east flow, as shown in the graphical depiction of the aquifer in Figure 5. There is one extraction well and one source location. The model aquifer is discretized into 10,000 square, equally-sized finite-difference cells. The aquifer, treatment system, and source properties are given in Table 1.

The decision variables are the pumping rates used in the extraction well, Q_k, and the number of source area pore volumes flushed, V_{nf}. The decision variables are constrained by maximum values, as indicated in Table 2. The remaining constraint values and the values of the cost coefficients are given in Table 2. The cost coefficients used for the chemical flushing are derived from costs for surfactant-enhanced aquifer remediation given by Krebs-Yuill et al. (1995) and Sabatini et al. (1996). The capital flushing cost coefficient, a_1, is based on the purchase of surfactant solution and capital costs associated with treatment of the recovered surfactant/DNAPL stream. The recovery stream treatment consists of recovery of the surfactant, such that the surfactant can be re-used, and removal and destruction of the dissolved DNAPL.

The operational flushing cost coefficient, a_2, is the cost associated with operating the flushing system injection and extraction wells and recycling the surfactant solution, on a source area pore volume basis. The remaining cost coefficients are based on PAT capital and operating costs given by Erickson et al. (2002). The parameter values used in the NPGA optimization are given in Table 3. The values in Table 3 were taken from a previous work (Erickson et. al., 2002) where optimal values of the NPGA parameters, with respect to convergence rates, were obtained.

We consider four sets of experimental variables. First, we examine the impact of the variability in the source by changing the variance in tube lengths. The base case tube length variance was 0.6. The tube-length variances used in these experiments are 0.01, 0.4, 0.6, 1.0, and 2.0. According to Enfield (2000), who fitted partitioning tracer curves to tube distributions, it is expected that the variance in tube distributions will not exceed 2.

Second, we vary the flushing capital and operating cost coefficient, a_1 and a_2. Chemical flushing is a relatively new and complex technology, such that the design of these systems, including the choice and concentration of the flushing chemical, is not straightforward. Since the choice of flushing chemical type and concentration is based not only economic considerations, but also on factors such as regulatory acceptability, site characteristics, and characteristics of the flushing solution-DNAPL mixture (Sabatini et al., 1996), the costs associated with the technology vary greatly from site to site. The flushing chemical capital and operating costs derived from Krebs-Yuill et al. (1995) and Sabatini et al. (1996) were used as base case cost coefficients for a_1 and a_2, respectively. To test the sensitivity of the optimal design to flushing remediation cost, we also used values of a_1 and a_2 corresponding to 50% of the base costs.

Third, we varied the plume development time, t_p. The period between the initial DNAPL release and the implementation of the source remediation can vary widely, because the time elapsed before discovery of the contamination and the decision to implement the source remediation varies from site to site. The plume development time partially determines the fraction of the mass held in the DNAPL source versus the mass dissolved into the plume. The residence time of the dissolved DNAPL impacts the distribution of the mass relative to the extraction well location, as determined by advection and distribution processes. The residence time also will impact the quantity of dissolved DNAPL mass lost due to degradation. The effort and funds dedicated to source or plume remediation are likely to be sensitive to the distribution of the mass between the source and the plume. In addition to the value used as a base case of $t_p = 500$ days, we used a minimum value of 100 days and a maximum value of 1,000 days.

Fourth, we investigated the effects of biodegradation in the dissolved plume by varying the first-order degradation rate constant, λ. The degradation rate constant is well known to vary widely from site to site (e.g. Wiedemeier et al., 1998). The constant is essentially a parameter fitted to quantify degradation processes that are distributed in both space and time and is a function of site and contaminant biogeochemistry. We expect that the rate of degradation in the plume will significantly impact the effort and funds used for plume remediation, such that the plume remediation effort will range from aggressive pumping (high extraction rates) to natural attenuation (zero extraction rates). We used a degradation rate of 0 as a base case, and tested rates of 0.01, 0.05, 0.1, and 0.25 day^{-1}. This range corresponds to a range tabulated for various sites by Schwarzenbach (1993) for chlorinated organic chemicals.

RESULTS

We first report the results of base case optimizations for a range of source (tube length) variances, given in Figure 6. The results in Figure 6 show that source remediation was not chosen for any of the source variances and no feasible solution was found for the highest variance. These results indicate that source remediation is expensive relative to plume remediation and that plume remediation is sufficient for all but the highest variances. The infeasibility of the highest variance is an indication of the length of time the source is released at in the natural aquifer. Release rates for natural and engineered systems are documented in Table 5. This table gives values for remediation times with source removal and the efficiency of the removal by source variance. The infeasible result for the highest variance is explained by the detailed results given in Table 4. First, although the maximum number of chemical flushes ($V_{nf}^{\max} = 3$) is selected, the mass removed from the source is insufficient to meet the cleanup goal. Second, while the maximum extraction rate in the pumping well is selected and is sufficient to clean the mass released into the plume, the release of the remaining DNAPL into the plume is slow enough such that, at the end of the maximum remediation horizon ($t_f^{\max} = 10$ years), the mass remaining in the source exceeds the cleanup goal.

The results in Figure 6 also show that the relationship between total cost and variance is not monotonic. Figure 7 shows the concentration at the pumping well vs. time for three variances. For both the $\sigma^2 = 0.4$ and $\sigma^2 = 0.6$ cases, the optimal design has the extraction rate reaching the maximum value ($Q^{\max} = 1000$ m^3/d), whereas for the homogeneous source case ($\sigma^2 = 0$), the extraction rate is about 60% of the maximum. The higher (but constant) pumping rates result in higher pumping costs for the $\sigma^2 = 0.4$ and $\sigma^2 = 0.6$ cases. However, as the variances increase, the average concentration reaching the extraction well decreases slightly, resulting in slightly lower treatment costs

Figure 8 shows optimization results for the case where the capital costs of the flushing are reduced by 50%. In this case, the costs of source remediation are low enough to compete with plume remediation costs, but the variations in source variances produce optimal designs consisting of various configurations of source and plume remediation. For the source variance of 0.001, the source remediation is efficient enough to reach the cleanup constraint, without any plume remediation. For the source variance of 0.4, pumping is required in addition to the source remediation to meet the cleanup goal. In this case, treatment is not required, since the concentration in extracted water is below the treatment goal of 0.005 mg/L. For the source variance of 0.6, the optimal design consists of pumping one pore volume of flushing solution through the source, followed by plume remediation. The source remediation is less efficient than for the higher variances, such that the concentration in the plume is high enough to impose treatment of the extracted water. For the source variance of 1.0, the flushing is inefficient, such that PAT is required to perform all of the remediation. As in the base case, the highest variance case is infeasible.

Reduction of the operational cost of flushing by 50% also results in lowering the costs of source remediation enough to compete with plume remediation costs, as shown in Figure 9. The operational cost reduction results in an optimal design that consists of one and two source area pore volumes for source variances of 0.001 and 0.4, respectively, indicating that the volume of flushing solution needed to meet the cleanup constraint increases as the heterogeneity in the source area increases. For the source variances of 0.6 and 1.0, the decrease in operating costs is not sufficient to overcome the inefficiency of the source remediation efforts at these higher variances, and PAT is required to perform all of the remediation. Again, as in the base case, the highest variance case is infeasible.

Figure 10 shows the optimization results where the length of time for plume development (t_p) was varied. For the base case flushing capital costs (a_1 = 150 $\$/m^3$), the variation in t_p does not affect the selection of PAT as the only remediation technology, since the source remediation is expensive relative to the plume remediation. The lower cost of the plume remediation for the t_p = 100 days case can be explained by the fact that the plume has not spread as far and so less pumping is required to capture the plume. The t_p = 1,000 days case is cheaper than the t_p = 500 days because the contaminant concentrations in the plume are lower, resulting in lower treatment costs.

When the flushing capital costs are reduced (a_1 = 75 $\$/m^3$), source remediation is chosen only for the base case plume development time. In the case of the lower plume remediation time (t_p = 100 days), the lower pumping requirements make the overall costs for PAT cheap enough to supplant the need for source remediation. In the case of the higher plume remediation time (t_p = 1,000 days), enough of the mass has dissolved from the source such that, again, PAT is sufficient to reach the cleanup criteria.

Figure 11 shows the optimal designs where the biodegradation rate was varied from 0 to a high rate of 0.25 day^{-1}, and all other parameters were taken from the base case. As noted in previous results, the cost of source remediation are high enough, relative to the source remediation cost, such that only PAT is chosen in the optimal design. The overall costs for plume remediation decrease as the degradation rate increases, since less mass needs to be extracted and treated. At the highest degradation rate ($\lambda = 0.25$ day^{-1}), PAT operation is not required, implying that natural attenuation is sufficient to meet the cleanup goal.

Figure 11 shows the results where the degradation rate is varied and the unit flushing capital costs are reduced ($a_1 = 75$ \$/m^3). For the lower biodegradation rates ($\lambda \leq 0.01$ day^{-1}),, the results are similar to previous results where the flushing capital costs were reduced: source remediation becomes cheap enough to compete with plume remediation. However, for the higher biodegradation rates ($\lambda \geq 0.05$ day^{-1}), source remediation is not needed. In these cases, plume remediation costs are relatively inexpensive, since a greater amount of mass is degraded and a correspondingly lower amount of mass is present in the plume.

CONCLUSIONS

In this work, we have developed a framework for determining optimal designs of combined source and plume remediation efforts. The optimization framework has been developed to allow the remediation designer to analyze tradeoffs between degrees of effort and funds committed to source remediation and plume remediation. We have accounted for the presence of heterogeneity in the source distribution, such that the rate of mass release into the plume and the efficiency of source remediation efforts are controlled by the degree of heterogeneity. The degree of heterogeneity is simulated as the variance of tube lengths in a bundle of tubes DNAPL dissolution model.

As expected, the optimal allocation of funds to source or plume remediation is sensitive to the unit costs associated with the remediation technologies. Only plume remediation, in the form of pump-and-treat remediation, is selected when the base case, source remediation capital and operating costs are applied. In this case, the relationship between plume remediation costs and the source variance is not monotonic, revealing the complex relationship between the release rate from the source into the plume and the costs associated with pumping and treatment. When the source remediation capital or operating costs are reduced, source remediation becomes competitive with source remediation, particularly for the lower source variances.

Degradation of the contaminant within the plume lowers the total cost of remediation. For the highest degradation rate, no remediation is required, implying that natural attenuation is sufficient to meet the cleanup goal. For mid-range degradation rates, source remediation is not required, since, even for relatively high source release rates, the mass residing in the plume is reduce to the point where plume remediation can meet the cleanup goal.

The results of this work are specific to the range of aquifer-contaminant properties and unit costs considered here. Although we have explored the sensitivity of the results to many of these variables, we expect that others would have an influence on the results. In particular, less stringent cleanup goals may make tend to favor source remediation for higher variances, and may allow for the highest variance case to be feasible.

ACKNOWLEDGEMENTS

This research was supported by NSF grant BES-0083112, USEPA grant CR826614-01-0 and the Statistical and Applied Mathematical Sciences Institute, Research Triangle Park, North Carolina.

REFERENCES

Brown, C. L., G. A. Pope, L. M. Abriola, K. Sepehrnoori, Simulation of surfactant-enhanced aquifer remediation, Water Resour. Res., Vol 30 #11, 2959-2978, 1994

Enfield C.G., Tracers forecast the performance of NAPL remediation projects, In P.L.Bjer, et al, eds. Groundwater 2000. Balkea, Copenhagen, Denmark

Erickson M, Mark, Mayer AS, Horn J, Multi-objective optimal design of groundwater remediation systems: Application of the niched Pareto genetic algorithm, Advances in Water Resources, Vol 25, 2002, 51-65

Finkel, M., Liedel, R., Tuetsch, T., Modelling of surfactant-enhanced remediation of polyciyclic aromatic hydrocarbons, Environmental Modeling and Software, Vol 14, 1999, 203-211

Horn J. The nature of niching: genetic algorithms and the evolution of optimal, cooperative populations. PhD thesis, University of Illinois at Champaign, Urbana, Illinois, 1997

Mayer,A.S, Kelly, C,T. Miller,Cass T., Optimal Design for problems involving flow and transport phenomena in staurated subsurface systems, Adv in Water

Resour, 2002

Maxwell RM, Understanding the effects of variability and variability on groundwater-driven health risk assessment. PhD dissertation, University of California, Berkley, Ca.1998

Krebs-Yuill, B. ,Harwell, J.H., Sabatini, D.A., and R.C. Knox, Economic Considerations in Surfactant-Enhanced Pump-and-Treat Remediation, in Surfactant-Enhanced Subsurface Remediation- Emerging Technologies edited by David A. Sabatini, Robert C. Knox and Jeffery H. Harwell ASC Symposium Series 594

Kavanaugh, M.C., P.S.C. Rao, and A.L. Wood. 2003. The DNAPL Remediation Challenge: Is There a Case for Source Depletion? (EPA/600/R-03/143)

Robinson, George C., and Bedient, Phillip B., Modeling a time-variant source of contamination, Petroleum Hydrocarbons and Organic Chemicals in Ground Water: Prevention, Detection and Restoration, November 20-22, 1991, Houston Texas

Sabatini, D.A., Knox, R.C., Harwell, J.H. 1996. Surfactant-Enhanced DNAPL Remediation: Surfactant Selection, Hydraulic Efficiency, and Economic Factors.

Environmental Research Brief. Environmental Protection Agency. Washington, D.C. EPA/600/S-96/002.

Sale Tom C, Mc Whorter David B., Steady state mass transfer from single-component dense nonaqueous phase liquids in uniform flow fields, Water Resources Research, Vol 37, # 2, Pages 393-404, 2001.

Schwarzenbach, R.P., Gschwend, P.M., and Imboden, D.I., Environmental Organic Chemistry, Wiley-Interscience, Hoboken, New Jersey, 1993.

U.S. Environmental Protection Agency, Guidance for evaluating the technical impracticability of groundwater restoration interim final report, Publ 9234.2-25, EPA540/R93/080, Office of Solid Waste and Emergency Response, Washington, D. C., 1993

U.S. Environmental Protection Agency, Guide to Principal Threats and Low Level Threat Wastes, Publ 9380.2-25, EPA540/R93/080, Office of Solid Waste and Emergency Response, Washington, D. C., 1991

U.S. Environmental Protection Agency, Presumptive Response Strategy and Ex-Situ Treatment Technologies for Contaminated Groundwater at CLERCA Sites 9283.1-12, Office of Solid Waste and Emergency Response, Washington, D. C., 1996

Interstate Technology and Regulatory Council, DNAPL Source Reduction: Facing the Challenge, Dense Nonaqueous Phase Liquids Team, April 2002

U.S. Environmental Protection Agency, Groundwater Cleanup: Overview of Operating Experience at 28 sites, EPA542/R/99/006, Technology Innovation Office, Washington, D. C., 1999

Wiedemeier, T.H., Swanson, M.A., Moutoux, D.E., Gordon, E.K., Wilson, J.T., Barbara, B.H., Kampbell, D.H., Haas, P.E., Miller, R.N., Hansen, J.E., and Chapelle, F.H., Technical Protocol for Evaluating Natural Attenuation of Chlorinated Solvents in Ground Water, United States Environmental Protection Agency, Washington DC, EPA/600/R-98/128, 1998.

Yu, M. ,Rizzo, D.M.,Dougherty, D.E., Multi-period Objectives and Groundwater Remediation using SAMOA: Tandem Simulated Annealing and Extended Cutting Plane Method For Containment with Cleanup, XII International Conference on Computational Methods in Water Resources, Greece June 15-19. 1998

Lin, M-D. and McKinney, D.C.,Optimization of Surfactant Enhanced Pump-and-Treat Remediation Systems Proc. ASCE Specialty Conference on Water Resour. Plan. and Mgt.,ASCE,1995

Sleep, B.E., and J.F. Sykes, Compositional simulation of groundwater contamination by organic compounds 1. Model development and verification, Water Resour. Res., 29(6), 1697-708, 1993.

Mayer, A.S. and C.T. Miller, "The Influence of Mass Transfer Characteristics and Porous Media Heterogeneity on Nonaqueous Phase Liquid Dissolution," *Water Resources* Research, 32(6), pp. 1551-1567, 1996.

Teutsch, G. & Finkel, M. (2002): Integrated Physico-Chemical-Economical Modelling for Optimal Plume Management at Contaminated Sites - A Decision Support System.- In: K. Kovar, Z. Hrkal (Eds.): Calibration and Reliability in Groundwater Modelling: A Few Steps Closer to Reality - Proceedings of the ModelCARE 2002 conference held at Prague, June 2002, IAHS Publ. no.277, 2002.

Teutsch, G., Rügner, H., Zamfirescu, D., Finkel, M. & Bittens, M. (2001): Source Remediation vs. Plume Management: Critical Factors Affecting the Cost-Efficiency.- In:

Land Contamination and Reclamation: The Sustainable Management and Remediation of

Contaminated Land, Vol. 9, No.1: 128-139.

Powers, Susan E., Linda M. Abriola, Joyce S. Dunkin, and Walter J. Weber, Jr., "Phenomenological Models for Transient NAPL-Water Mass Transfer Processes," Journal of Contaminant Hydrology, 16, 1-33, 1994. ,

Table 1: Base case parameters for flow, transport and treatment simulations

Parameter	Symbol	Value	Units
Aquifer properties			
porosity	n	0.30	(-)
hydraulic conductivity	K	3.82×10^{-5}	m/s
background pore velocity	v	2.7×10^{-2}	m/d
longitudinal dispersivity	α_L	10	m
transverse dispersivity	α_T	2	m
biodegradation rate*	λ	0	day^{-1}
Groundwater treatment system properties			
GAC adsorption coefficient,	K_{AB}	28.4	$(mg/gm)(L/mg)^{1/n}$
GAC adsorption coefficient	$1/n$	0.48	(-)
effluent treatment goal	C^*	0.005	mg/L
Source properties			
solubility in pure water	C_s	1500	mg/L
solubility increase with flushing agent	x_f	50	(-)
DNAPL saturation in source zone	S_n	0.2	(-)
DNAPL density	ρ_n	1.46	g/cm^3
number of tubes	n_f	100	
variance $\log_{10}$(tube length)*	σ_f^2	0.6	
length × width × depth of source area	$L \times W \times D$	10 × 10 × 30	m
length of time to establish plume*	t_P	500	days

*this parameter is varied in numerical experiments; the value given is for the base case

Table 2: Base case values used in objective function and constraints

Parameter	Symbol	Value	Units
Cost coefficients in objective function			
capital flushing cost coefficient*	a_1	150	\$/m^3 flushing solution purchased
operational flushing cost coefficient*	a_2	1,500	\$/pore volume
well installation cost coefficient	a_3	10,800	\$/well
pumping operation cost coefficient	a_4	1.05	\$/m^4
treatment cost coefficient	a_5	2.14	\$/gm GAC
Constraint values			
maximum extraction rate	$Q^{\max}$	1,000	m^3/day
maximum number of pore volumes	$V_{nf}^{\max}$	3	(-)
maximum remediation horizon	t_f	7,500	days
maximum allowable mass remaining	$M'_{\max}$	0.001	(-)

*this parameter is varied in numerical experiments; the value given is for the base case

Table 3: Optimization algorithm parameters used in NPGA.

Parameter	Value
population size	50
tournament selection size	2
niche radius	0.5
probability of crossover	0.9
probability of mutation	0.001
$M'_{\max}$ constraint violation weight	150

Table 4: Distribution of contaminant mass for base case with range of source variances

	Variance				
	0.001	0.4	0.6	1.0	2.0*
Normalized mass dissolved from source/ released into plume over interval $0 \le t \le t_P$	32.17	32.17	32.02	29.11	17.37
Normalized mass dissolved from source/ released into plume over interval $t_P < t \le t_f$	67.83	67.83	67.98	70.89	21.35
Normalized mass extracted from plume over interval $t_P < t \le t_f$	99.94	99.92	99.91	99.93	NA
Normalized mass extracted from source during source remediation	NA	NA	NA	NA	51.09

*Infeasible

Table 5: Time required for removal and mass removed for range of source variances

	Source Variance				
	0.001	0.4	0.6	1.0	2.0
Days to dissolve source under natural conditions	6,400	10,000	14,500	51,700	93,000
Mass removed in source remediation by 1 flush	100%	83%	62%	47%	38%
Days to dissolve source under natural conditions after source remediation	0	2,600	5,800	25,000	59,000
Mass removed in source remediation by 2 flushes	NA	100%	89%	63%	57%
Days to dissolve source under natural conditions after source remediation	NA	0	3,000	21,000	40,000
Mass removed in source remediation by 3 flushes	NA	NA	100%	81%	67%
Days to dissolve source under natural conditions after source remediation	NA	NA	NA	1100	37200
Number of flushes to remove all mass by source remediation	1	2	3	6	13

Table 6: Distribution of contaminant mass for case with 50% reduction in flushing capital cost and range of source variances

	Variance				
	0.001	0.4	0.6	1.0	2.0*
Normalized mass dissolved from source/ released into plume over interval $0 \le t \le t_P$	31.83	25.73	32.17	31.84	17.37
Normalized mass dissolved from source/ released into plume over interval $t_P < t \le t_f$	0.00	0.00	1.35	68.16	21.35
Normalized mass extracted from plume over interval $t_P < t \le t_f$	31.83	25.73	32.95	99.99	NA
Normalized mass extracted from source during source remediation	68.16	74.27	67.05	0.00	51.09

*Infeasible

Table 7: Distribution of contaminant mass for base case with range of degradation rates

	Degradation Rate (day^{-1})				
	0	0.0001	0.0005	0.001	0.0025
Normalized mass dissolved from source/ released into plume over interval $0 \le t \le t_P$	32.17	32.17	32.17	32.17	32.17
Normalized mass dissolved from source/ released into plume over interval $t_P < t \le t_f$	67.83	67.83	67.83	67.83	67.83
Normalized mass extracted from plume over interval $t_P < t \le t_f$	99.92	94.81	78.41	27.46	0.00
Normalized mass degraded over interval $0 < t \le t_f$	0.00	5.19	21.59	72.53	99.99

FIGURE CAPTIONS

Figure 1: Schematic illustration of contaminant source-plume conceptual model.

Figure 2: Sequence of events and contaminant mass history for source-plume conceptual model.

Figure 3: Simulation-optimization computational process.

Figure 4: Contaminant mass input from source and into plume as a function of variance

Figure 5: Graphical depiction of hypothetical aquifer system.

Figure 6: Remediation costs for base case and for range of source variances.

Figure 7: Concentrations in pumping well for base case as a function of time and source variances.

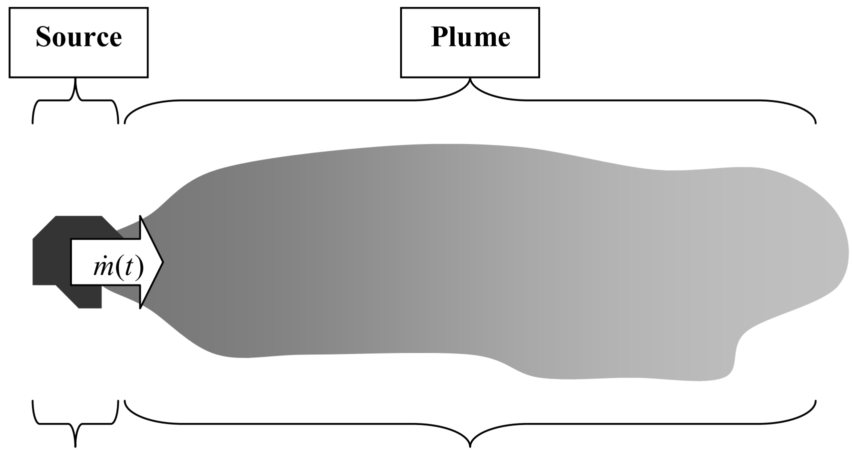
Figure 8: Remediation costs for case where flushing capital cost is reduced 50% for range of source variances.

Figure 9: Remediation costs for case where flushing operational cost is reduced 50% for range of source variances.

Figure 10: Remediation costs for case where for range of plume development times and flushing capital cost.

Figure 11: Remediation costs for range of degradation rates.

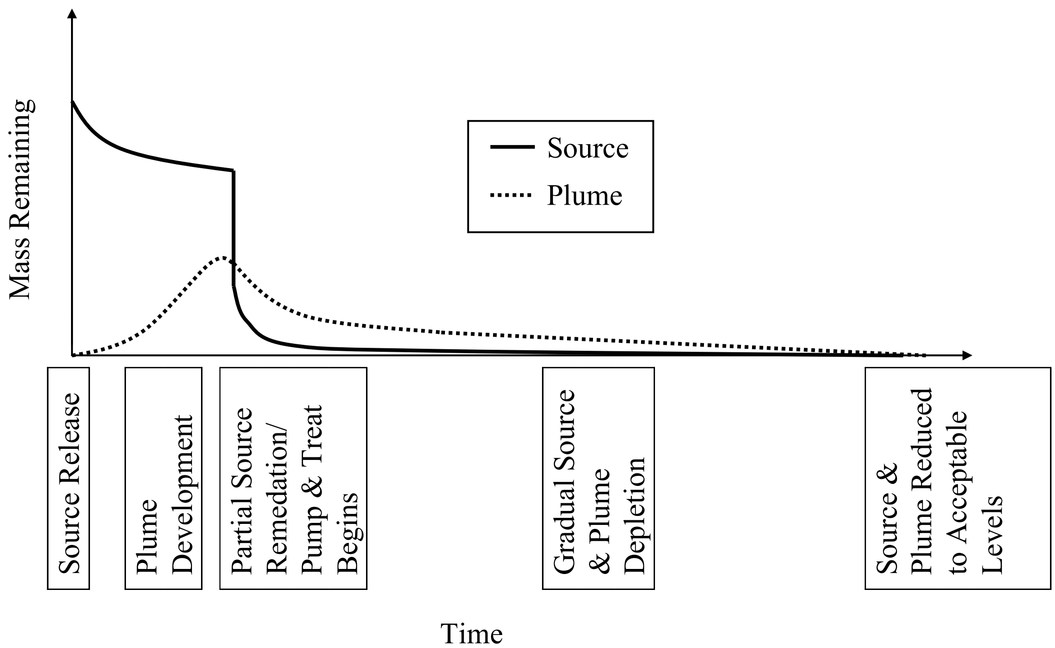
Figure 12: Remediation costs for range of degradation rates where flushing capital cost is reduced 50%.

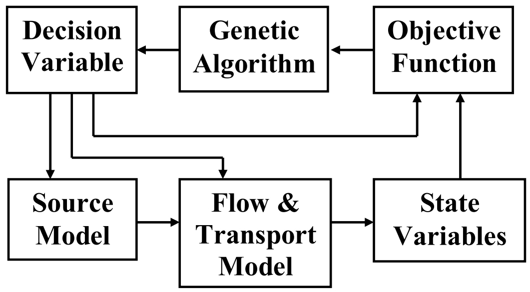


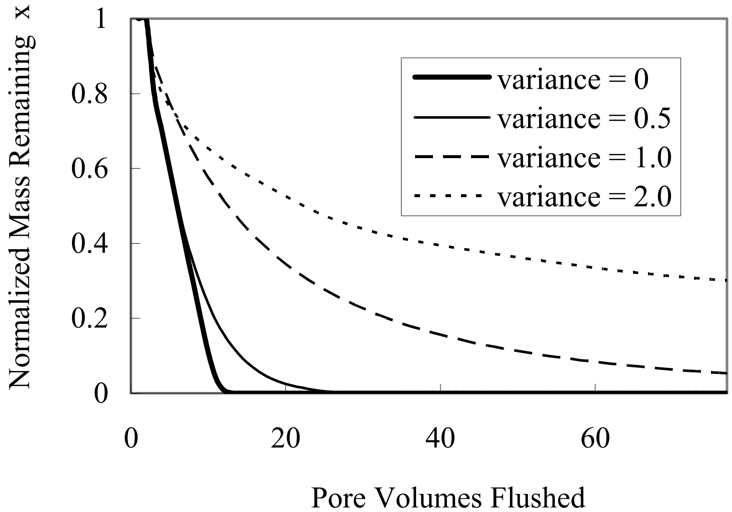
Factors impacting source-plume system

- Advection
- Source distribution
- Source Chemistry

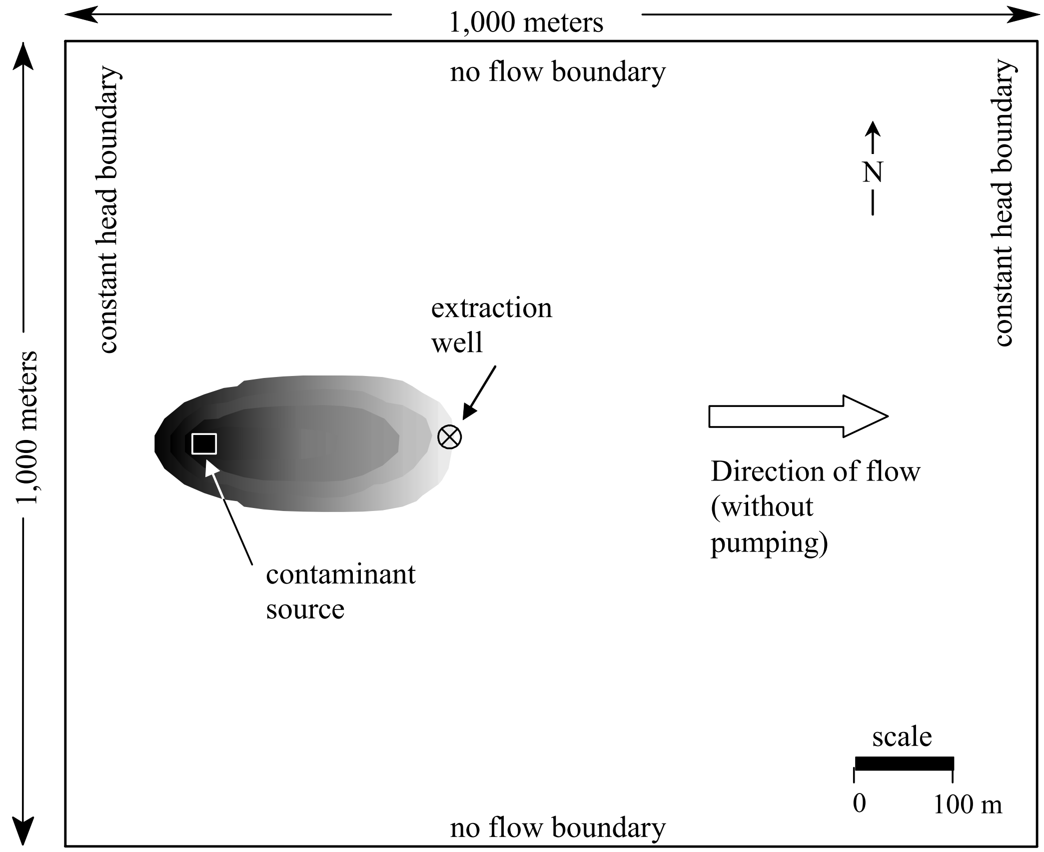
- Regional flow & pumping/injection-induced flow
- Dispersion
- Reactions

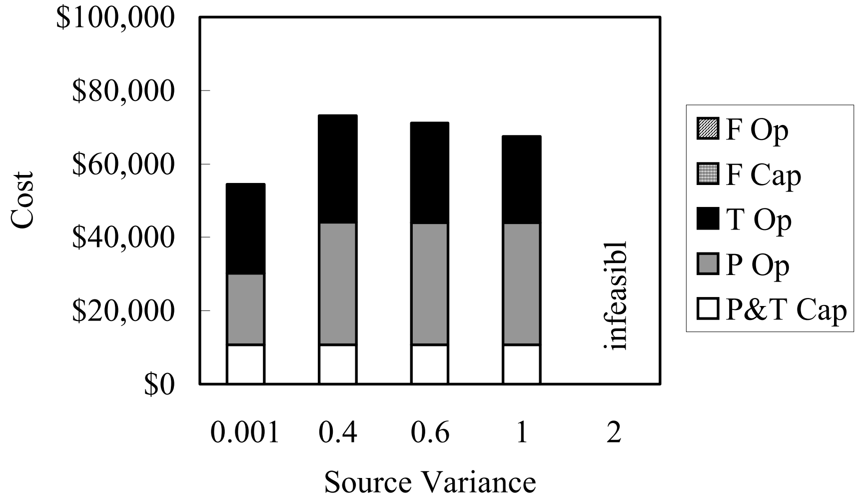

Mass Remaining
Source
Plume
Source Release
Plume Development
Partial Source Remedation/ Pump & Treat Begins
Gradual Source & Plume Depletion
Source & Plume Reduced to Acceptable Levels
Time

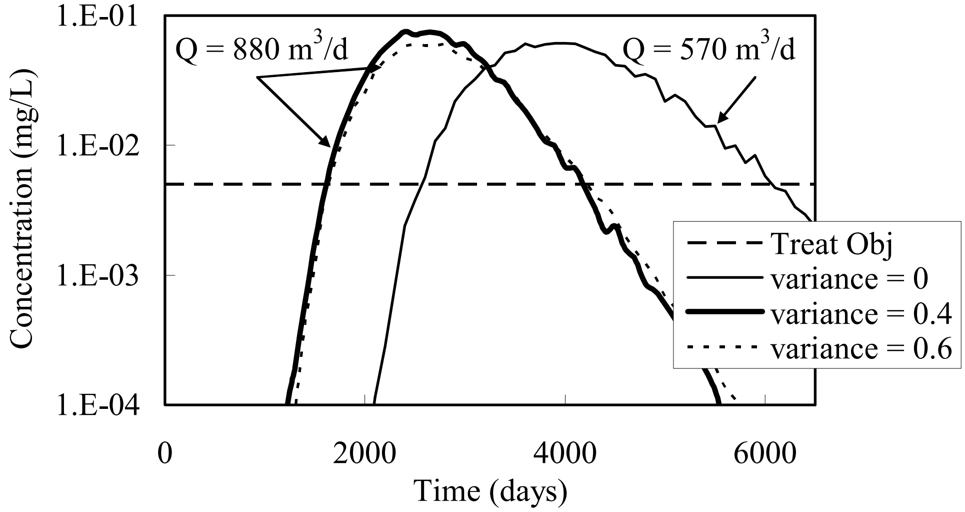

Decision Variable
Genetic Algorithm
Objective Function
Source Model
Flow & Transport Model
State Variables



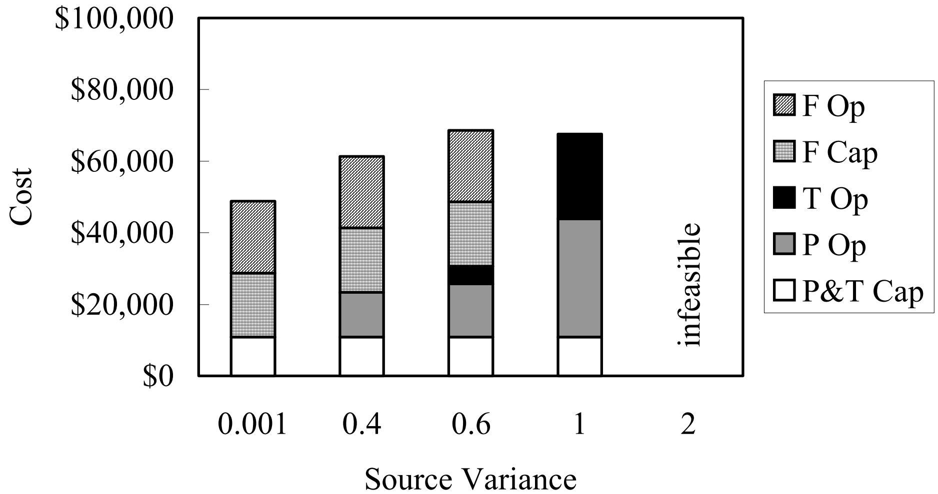
Normalized Mass Remaining x
1
0.8
0.6
0.4
0.2
0
0
20
40
60
Pore Volumes Flushed
variance = 0
variance = 0.5
variance = 1.0
variance = 2.0

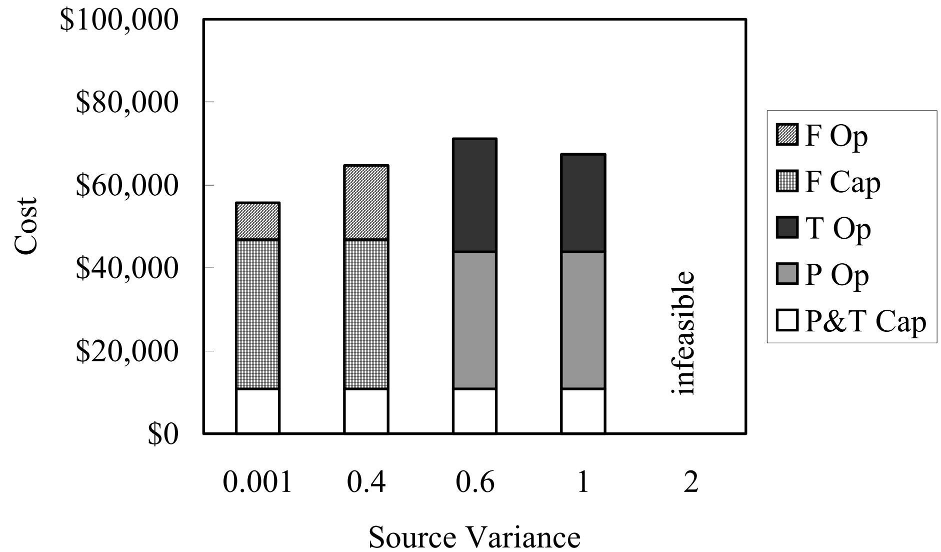

1,000 meters
no flow boundary
constant head boundary
constant head boundary
N
1,000 meters
extraction
well
Direction of flow
(without
pumping)
contaminant
source
scale
0
100 m
no flow boundary

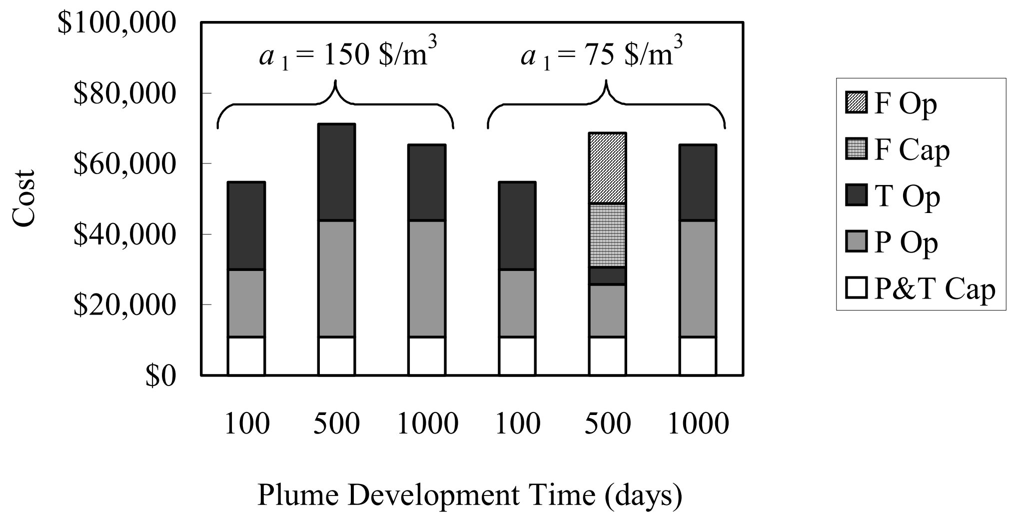

$100,000
$80,000
$60,000
$40,000
$20,000
$0
Cost
infeasibl
0.001
0.4
0.6
1
2
Source Variance
F Op
F Cap
T Op
P Op
P&T Cap



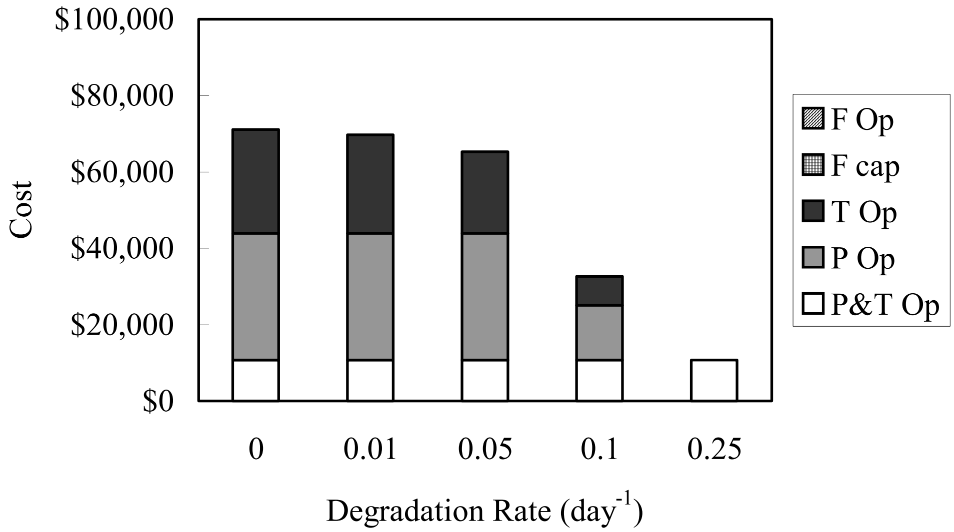
1.E-01
1.E-02
1.E-03
1.E-04
Concentration (mg/L)
0
2000
4000
6000
Time (days)
Q = 880 m3/d
Q = 570 m3/d
Treat Obj
variance = 0
variance = 0.4
variance = 0.6

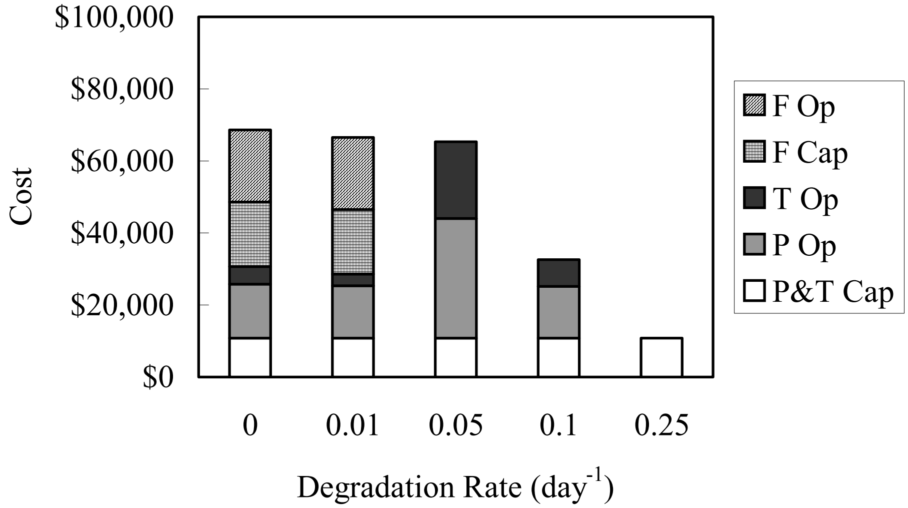

$100,000
$80,000
$60,000
$40,000
$20,000
$0
Cost
0.001
0.4
0.6
1
2
Source Variance
infeasible
F Op
F Cap
T Op
P Op
P&T Cap


$100,000
$80,000
$60,000
$40,000
$20,000
$0
Cost
infeasible
0.001
0.4
0.6
1
2
Source Variance
F Op
F Cap
T Op
P Op
P&T Cap



$100,000
$80,000
$60,000
$40,000
$20,000
$0
Cost
a 1 = 150 $/m3
a 1 = 75 $/m3
100
500
1000
100
500
1000
Plume Development Time (days)
F Op
F Cap
T Op
P Op
P&T Cap


$100,000
$80,000
$60,000
$40,000
$20,000
$0
Cost
0
0.01
0.05
0.1
0.25
Degradation Rate (day^{-1})
F Op
F cap
T Op
P Op
P&T Op



$100,000
$80,000
$60,000
$40,000
$20,000
$0
Cost
0
0.01
0.05
0.1
0.25
Degradation Rate (day-1)
F Op
F Cap
T Op
P Op
P&T Cap

Using remediation time as an optimization variable in groundwater remediation systems

Karen L. Endres

Department of Civil & Environmental Engineering, Michigan Technological University, Houghton, Michigan 49931-1295, USA

Alex S. Mayer[1]

Department of Geological & Mining Engineering & Sciences, Michigan Technological University, Houghton, Michigan 49931-1295, USA

Abstract

Optimization by the use of computer simulations is a useful tool for designing subsurface remediation systems. Most optimization studies focus on minimizing cost while meeting a cleanup goal within a given time frame. However, decision-makers may be interested in analyzing tradeoffs between cost and time. In this work, we employ a multi-objective optimization to minimize cost and time simultaneously. The optimization procedure uses a niched Pareto genetic algorithm with state variables (hydraulic head and concentration) generated from a finite difference flow stimulator and a particle tracking contaminant simulator.

Computational experiments were performed to verify the multi-objective trade-off curve with the use of single objective optimization runs. The effect of interest rate on cost-time tradeoffs was investigated with two financial management scenarios. The result of this work showed only a weak relationship between remediation cost and time. Further investigation of the results produced insight in to the aquifer and treatment efficiency impacts of remediation time. Interest rate experiments showed that the effect is dependent on the financial methodology and has little impact on the technical selection of the remediation design.

[1] Corresponding author, *E-mail address:* asmayer@mtu.edu (A.S. Mayer)

1 Introduction

Optimization and modeling of contaminant transport in subsurface porous medium systems has become commonplace [1]. Optimization by the use of computer simulations is a useful tool for designing subsurface remediation systems. Most subsurface remediation optimization investigations focus on as single objective: minimizing cost while meeting a specified cleanup goal within a given time frame. The remediation time is usually set by the investigator or by a regulatory agency. However, we suggest that viewing trade-offs between cost and remediation time will allow for more efficient decisions to be made. With cost vs. time tradeoff curves, decision makers simultaneously consider allocation of remediation funds and choosing the sites where remediation needs be accelerated.

The construction of cost vs. remediation tradeoff curves requires a multi-objective optimization approach. Essentially, the tradeoff curve consists of solutions (or design) that are Pareto optimal, or,in other word, solutions that are superior with respect to at least one objective function. The relationship between remediation cost and time has been investigated using cost as a single objective and using time as a constraint [5] [4]. In these investigations a series of single objective runs are conducted where the value of the time constraint is changed for each run. The work performed by [5] indicated that the relationship between cost and time depends on the severity of the cleanup goal. In [4], the authors considered the effects of hydraulic constraints, contaminant source removal, variable cleanup goals and variable interest rates. They find that the imposition of constraints on aquifer drawdown has the most significant impact on the cost vs. time relationship.

In the present work, we consider a true multi-objective approach, using a variation of the genetic algorithm that is especially suited for multi-objective optimization. This approach will allow for more flexibility in investigating the cost vs. time relationship. We focus on pump-and-treat remediation, where the design variables are the number, location, and rates for extraction and injection wells. Computational experiments are performed to produce and verify the multi-objective trade-off curve with the use of single objective optimization runs. The effect of interest rates on the cost vs. time relationship is investigated with financial management scenarios.

2 Methodology

In this work, we attempt to find the best design for a pump-and-treat (PAT) groundwater remediation system. In general terms, we determine optimal pumping rates with respect to the system cost and the total time required for the remediation while meeting a fixed cleanup goal.

The computational framework used in this work consists of linked optimization and simulation codes, as shown in Figure 1. The optimization code is based on the niched Pareto genetic algorithm (NPGA). [6] This algorithm is developed specifically to handle multi-objective optimization problems. The algorithm works by ranking candidate solutions according to their Pareto optimality. The highest ranking is accorded to solutions that are Pareto optimal; that is, the solution is superior to all other solutions with respect to at least one objective function. The next highest ranking is accorded to solutions that are superior to all but one solution with respect to at least one objective function, and so on. Niching is a genetic algorithm operator that attempts to spread solutions along the entire length of the Pareto, or tradeoff surface. With the niching operator, solutions are ranked according to the distance (in normalized objective function space) between solutions of the same Pareto optimality rank. More details on the NPGA can be found in [2].

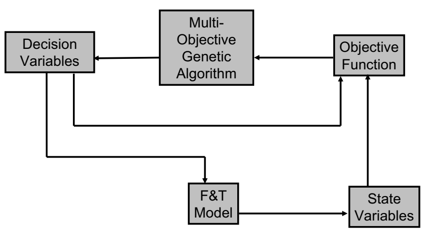


Fig. 1. Computational framework for groundwater simulation optimization procedure

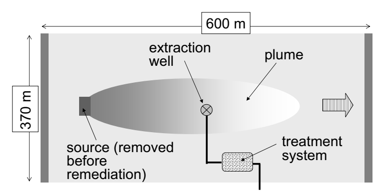


Fig. 2. Hypothetical aquifer system used in computational experiments

The objective functions are given by

$$\min J = \min \left\{ a_1 N_w + \sum_{k=1}^{N_w} \left[\sum_{l=1}^{n_t} \left(a_2 Q_k H_k t_l + a_3 Q_k \frac{C_{k,l}}{K_{AB} C_{k,l}^{1/n}} t_l \right) \right] \right\} \tag{1}$$

$$\min T = \min \sum_{l=1}^{n_t} t_l \tag{2}$$

where a_1, a_2, and a_3 are coefficients of the cost model, N_w, k is the well index, Q_k is the extraction rate at well k, H_k is the total lift needed to move the groundwater from the well to the treatment system effluent for well k, T is the total remediation time, n_t is the number of time intervals l that the treatment system costs are estimated, t_l is the time interval length for interval l, $C_{k,l}$ is the concentration at well k and time interval l, and K_{AB} and n are coefficients related to the performance of the treatment system. In equation (1), the three terms represent, in order, well installation capital costs, pumping well operational costs, and water treatment system operational costs. The operational cost term for water treatment is developed by applying granular activated carbon (GAC) to remove contaminants, assuming instantaneous equilibrium between the contaminants and the GAC.

In equations (1) and (2), the decision variables are the extraction rates at fixed location pumping wells, and the total remediation time, since n_t appears in equation (1). In the NPGA, the decision variables are formatted as binary numbers. The decision variables are discretized in real number space by specifying minimum and maximum values of the extraction rates (Q^{max} and Q^{min})and the number of bits, N_b, used to represent the pumping rate in binary notation, as in

$$\Delta Q = \frac{Q^{max} - Q^{min}}{2^{N_b} - 1} \tag{3}$$

The size of the decision variable space, N_p, is thus determined by the minimum and maximum values and precisions, as in

$$N_p = \left(2^{N_b}\right)^{N_w} \tag{4}$$

In equation(1), the state variables are concentration, C, and hydraulic head, h. The state of the physical system is represented by a mathematical model consisting of a set of conservation equations, which take the form of a set of differential equations. The conservation equations used in this work are based on the two-dimensional steady state flow equations and contaminant mass balance equations. The steady-state, confined groundwater flow equation for a non-deforming, saturated, aquifer system is

$$S_s \frac{\partial h}{\partial t} = \nabla \cdot (\mathbf{K} \cdot \nabla h) - \overline{\mathcal{S}} \tag{5}$$

where where S_s is a specific storage coefficient, $\mathbf{K}$ is a hydraulic conductivity tensor and $\overline{\mathcal{S}}$ is a fluid sink term. The hydraulic head, h, is related to H, the total lift needed to move the groundwater from the well to the treatment system, by $H = z_{gs} - h + h_l$, where z_{gs} is the ground surface elevation and h_l is the head loss in the treatment train. The fluid sink term, $\overline{\mathcal{S}}$, is related to the decision variables, Q_k as in

$$\int_{\Omega} \overline{\mathcal{S}}(t)\,\mathrm{d}\Omega = \sum_{k=1}^{N_w} Q_k(\mathbf{x}_k, t) \tag{6}$$

where Ω is the domain of the system and $\mathbf{x}_k$ is the location of well k.

Contaminant concentrations are determined by solving the conservative form of the contaminant mass balance equation, as in

$$\frac{\partial(\phi C)}{\partial t} = \nabla \cdot (\phi \mathbf{D} \cdot \nabla C) - \nabla \cdot (\mathbf{q} C) - \mathcal{S}^i \tag{7}$$

where $\mathbf{D}$ is a hydrodynamic dispersion tensor, q is the specific discharge, and $\mathcal{S}^i$ represents a mass sink. The classic dispersion tensor is written as

$$\mathbf{D} = D_{ij} = \delta_{ij}\alpha_t|\mathbf{v}| + (\alpha_l - \alpha_t)\frac{v_i v_j}{|\mathbf{v}|} + \delta_{ij}\tau D^* \tag{8}$$

where α_l and α_t are the longitudinal and transverse dispersivities, respectively, τ is the tortuosity of the porous medium, $\mathbf{v}$ is the pore velocity vector, and D^* is the free liquid diffusivity of species. The contaminant sink term is defined as

$$\int_\Omega \mathcal{S}^i(t)\,\mathrm{d}\Omega = \sum_{k=1}^{N_w} Q_k(\mathbf{x}_k, t) C_k(\mathbf{x}_k, t) \tag{9}$$

The pore velocity, $\mathbf{v}$, is given by Darcy's law as

$$\phi \mathbf{v} = \mathbf{q} = -\frac{\mathbf{k}}{\mu} \cdot (\nabla p + \rho g \nabla z) \tag{10}$$

where $\mathbf{k}$ is the effective permeability tensor; μ is the dynamic viscosity; p is the fluid pressure; g is the magnitude of gravitational acceleration, which is assumed to be oriented in the -**k** direction, and z is a spatial coordinate oriented aligned with **k**.

We employ a 2-D finite difference approximation to solve the groundwater flow equation and a particle-tracking method to solve the mass transport equation. The numerical codes have been validated by [7]. Additional background information pertaining to the development of this numerical simulator can be found in [3].

3 Numerical Experiments

Numerical experiments were performed with a hypothetical, two dimensional (aerial) aquifer-contaminant system, schematically described in Figure 1. The

Table 1
Hydrogeological parameters for the simulated test case.

Parameter	Symbol	Value	Units
Isotropic hydraulic conductivity	K	6.02×10^{-5}	m/s
Constant head on left-hand-side boundary		60	m
Constant head on right-hand-Side boundary		55	m
Porosity	ϕ	0.25	–
Longitudinal dispersivity	α_L	10	m
Transverse dispersivity	α_T	2	m
Molecular diffusivity	D^*	10^{-9}	m^2/s
Tortuosity	τ	0.4	–

Table 2
Parameters used in numerical models.

Parameter	Value	Units
Number of nodes in x-direction	60	–
Number of nodes in y-direction	37	–
Size of blocks in x-direction	10	m
Size of blocks in x-direction	10	m

aquifer properties are homogeneous are described in Table 1. One-dimensional groundwater flow in the 30-m thick confined aquifer is driven by constant head boundaries on the left- and right-hand side boundaries. No flow boundaries are imposed on the upper and lower boundaries. A constant concentration source (C = 1,000 mg/L) is used to produce a dissolved contaminant plume. The location of the constant concentration source and the approximate extent of the resulting plume are shown in Figure 1. The numerical parameters used in the flow and transport simulations are given in Table 2.

At the beginning of the remediation phase of the numerical experiments, the contaminant source is removed. The groundwater remediation system consists of a single extraction well (see Figure 1 for the approximate location) and a GAC treatment system. Table 3 gives the GAC-contaminant parameters used in equation (1).

Table 3
Parameters used in cost objective function (equation(1)).

Parameter	Symbol	Value	Units
Time step size	t_l	100	days
GAC adsorption coefficient	K_{AB}	28.4	(mg/gm) (L/mg)$^{1/n}$
GAC adsorption coefficient	$1/n$	0.48	–
Coefficient	a_1	10,800	\$/well
Coefficient	a_2	1.05	\$/(m^4)
Coefficient	a_3	2.14	\$/(gm GAC)

Multi-objective optimization experiments were conducted on the aquifer- contaminant system. The pumping rate for the single extraction well and the number of remediation time steps, n_t, were the decision variables and minimization of cost and time were the objectives (equations (1) and (2). The intended results of each multi-objective optimization is the Pareto-optimal front which gives a tradeoff curve for cost vs. remediation time.

Remediation times were allowed to float between 0 days and maximum of 5,000 days. The aquifer remediation goal was specified as a minimum global fraction of mass remaining in the aquifer, or

$$\frac{\int_\Omega (\phi C)_{t=T}\, \mathrm{d}\Omega}{\int_\Omega (\phi C)_{t=0}\, \mathrm{d}\Omega} \leq M \qquad (11)$$

where M is the maximum fractional mass remaining at time T. The aquifer remediation goal was enforced as a constraint using a multiplicative penalty coefficient on the cost function (equation (1)). The parameters used in the cost function (equation(1)) and the heuristic parameters controlling the NPGA are given in Table 3 and Table 4, respectively.

A series of single objective runs were performed to benchmark the multi-objective results. In the series of single-objective runs, the remediation time was specified as a constraint, varying over 100-day intervals between the minimum and maximum remediation times.

Finally, a series of multi-objective runs were conducted to examine the impacts of remediation cost financing. Two scenarios of cost financing were assessed: annualized and present worth cost. The annualized cost scenario assumed that a bond for the complete remediation costs was purchased at the beginning of

Table 4
Parameters used in NPGA.

Parameter	Symbol	Value	Units
Tournament size		2	–
Niche radius		0.5	–
Probability of crossover		0.9	%
Probability of mutation		0.001	%
Treatment goal	M	1	%

the remediation period as in

$$J_{Ann} = J\frac{(1+i)^{n_t}-1}{i(1+i)^{n_t}} \tag{12}$$

where i is the interest rate. The present worth cost scenario assumes that operating capital was used to pay for each operating cost period and capital investment was available for the initial purchase and installation of equipment as in

$$J_{PW} = J_{cap} + \sum_{l=1}^{n_t}\left[(1+i)^{-n_t}J_{op}\right]t_l \tag{13}$$

where

$$J_{cap} = a_1 N_w \tag{14}$$

$$J_{op} = \sum_{k=1}^{N_w}\left(a_2 Q_k H_k + a_3 Q_k \frac{C_{k,l}}{K_{AB}C_{k,l}^{1/n}}\right) \tag{15}$$

In both scenarios, we use an interest rate of $i = 5\%$.

4 Results and Discussion

Figure 3 shows the cost-time tradeoff curve obtained with the multi-objective optimization run and the single-objective optimization runs used for benchmarking. The results are presented as costs and remediation normalized to the minimum and maximum values. The minimum values for both cost and time are 0. The maximum remediation time is 5,000 days; the maximum costs corresponds to the cost obtained for the single objective optimal solution for T = 1,000 days (without penalty, see paragraph after next).

The multi-objective results match the single objective runs well, providing a confidence in the multi-objective procedure. However, the multi-objective results do not cover the full extent of the points for higher remediation times found with the single-objective runs. The lack of points in the higher remediation time region for the multi-objective procedure indicates that niching apparently is not sufficient to extend the tradeoff curve into this region. Towards the lower remediation times ($T \leq$ 1,000 days), there are no feasible solutions with respect to the cleanup goal. We have provided the point for T = 1,000 days, where the indicated cost does not include the penalty for not meeting the cleanup goal, as a reference point.

Within the feasible region, the trade-off curve exhibits a weak relationship between cost and remediation time. The lack of dependence of cost on time can be explained by examining the breakdown of the costs as a function of remediation time, as indicated in Figure 4. The results in Figure 4 show that the treatment cost component overwhelms the well installation and pumping operation costs, and that the treatment cost is relatively constant. Since we base the treatment cost on an equilibrium GAC-contaminant relationship (see equation (1)), the treatment cost is directly related to the total mass of contaminant removed and sent to the treatment system. In our framework, the total mass of contaminant removed is fixed as a constraint $(1 - M)$; resulting in relatively constant treatment costs and relatively constant total costs. We note that the slight variation of treatment cost is due to the fact that some of the optimal solutions slightly exceed the remediation goal of $M = 1\%$

The results in Figure 4 can be compared to other works where the relationship between cost and remediation time has been examined [5] [4]. In [5], cost vs. time relationships are presented for a range of mass removal rates. The mass removal rates correspond to $1 - M$, or the global mass of contaminant removed from the aquifer, normalized by the initial contaminant mass. For low mass removal rates (30–50%), cost strongly increases with remediation time. However, for higher mass removal rates (60–90%), the cost does not vary significantly with time, which is in agreement with our results ($1 - M$=99%). The results of [4] also indicated minimal sensitivity of cost to time, for longer remediation times. However, for shorter times (¡ 3 years) and for the case where drawdown constraints are imposed, strong, but opposing, relationships were found.

Although the results in Figure 4 indicate that cost does not vary significantly with time, since the contaminant mass removed is relatively constant, the volume of water extracted from the aquifer depends on remediation time. Figure 5 shows the contaminant concentration in the extraction well as a function of

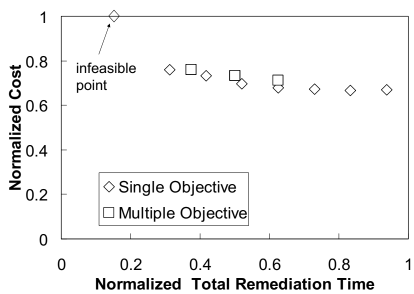


Fig. 3. Optimization results for single and multi-objective cases

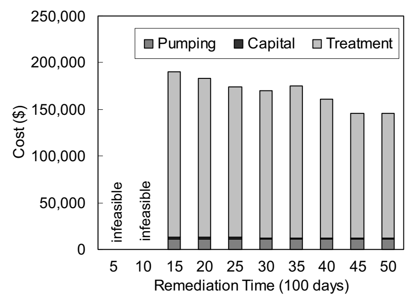


Fig. 4. Cost breakdown for single objective optimization results

cumulative volume of water removed for a few total remediation times. These results indicate that the longer remediation times result in lower volumes of water removed. This result occurs because the pumping rate required to meet the remediation goal for a given remediation time varies in a sub-linear manner with respect to remediation time.

The results in Figure 5 may have be significant in a management sense, since it is generally desirable to reduce the volume of extracted water. Furthermore, the results in Figure 5 indicate that higher concentrations are delivered to the treatment system for the longer remediation times (and correspondingly lower pumping rates). In general, for real GAC systems, GAC usage is more efficient when the concentrations delivered to the GAC treatment system are higher. The results shown in the present work do not support the implication that treatment costs should be lower for longer remediation times (and correspondingly lower pumping rates), due to the fact that we base the treatment cost on an equilibrium GAC-contaminant relationship.

If we compare the results for the three different cost objective functions (i.e., results obtained with equations (1), (12), and (13)) for a given remediation time, the value of the decision variables obtained for a given remediation time remain constant. This trend indicates that optimal design of the remediation is insensitive to the financial management scheme. However, the fact that the financial scenario (”conventional” vs. annualized vs. present worth cost) does not impact the optimal value of the decision variable does not imply that the tradeoff curves will not vary among the different financial scenarios.

The results for the present worth financial scenarios, shown in Figure 6, indicate a slight relationship for cost vs. time, where cost decreases as time increases, for the longer remediation times. This trend indicates that spreading the operational costs over a longer time period results in lower costs, as would be expected from the inverse relationship between cost and the number of time periods (see equation (13)). However, this trend needs to be confirmed, since the multi-objective run for the present worth scenario did not produce points for the highest remediation times.

For the annualized cost scenarios, neither the multi-objective nor the single-objective optimization runs produced consistent results, as shown in Figure 6. This performance is due to the complex relationship between time and cost for annualized costs, as indicated in equation (12). Adjustment of the heuristic parameters used to control the NPGA, especially the niche radius, may produce better results.

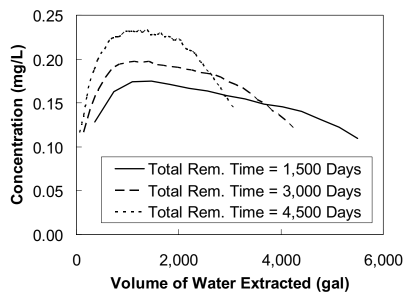


Fig. 5. Concentration vs. volume of water extracted for different remediation times

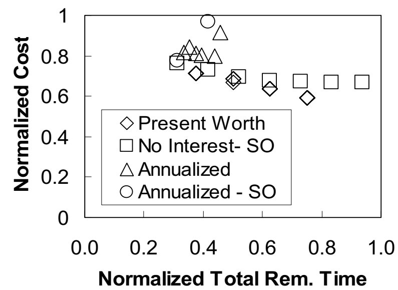


Fig. 6. Optimization results for cases with annulaized and present worth cost scenarios. SO indicates runs conducted with single-objective optimization

5 Conclusions

This work has demonstrated the development and application of multi- objective optimization to assess tradeoffs between groundwater remediation costs and the time required to complete the remediation. Results obtained with a true multi-objective optimization algorithm (NPGA) agreed with results obtained with a single-objective optimization algorithm, where remediation time was fixed as a constraint. For the physical and chemical models and parameters applied in this work, we found that remediation costs were not sensitive to remediation time, when the financing of the remediation costs were not considered. If we were to relax the cleanup goal constraint; however, it appears that costs will sharply increase for shorter remediation times. We also find that when a present worth financial management scenario is considered for estimating costs, remediation costs decrease as the remediation time increases. Results for annualized financing scenarios were inconclusive.

This work has produced many avenues for future research. First, the multi-objective optimization results did not cover the full range of Pareto-optimal points. The components of the optimization algorithm that impact the spread of the Pareto front (e.g. niching and tournament selection) need to be reassessed to overcome this limitation. Second, we realize that the insensitivity of cost with respect to time is at least partly due to the function adopted for the treatment costs. We will experiment with a more realistic cost function, i.e. a function that accounts for the kinetics of GAC-contaminant interactions. Third, we will explore how the aquifer physical and chemical parameters impact the nature of the cost-time tradeoff curves. Fourth, we will adjust the optimization framework so that tradeoff curves are produced where the decision variables can change with time.

Finally, although we have applied the multi-objective optimization approach to a relatively simple design problem (single, fixed-extraction well, pump-and-treat design), we suggest that our approach can be applied to more complex pump-and-treat problems and to other remediation technologies.

Acknowledgements

This research was supported by NSF grant BES-0083112 and USEPA grant CR826614-01-0.

Thanks to Reed Maxwell, Lawrence Livermore National Laboratory; Mark Erickson, AMEC Earth & Environmental, Inc.; and Jeff Horn, Northern Michigan University; for use of source code and help.

References

[1] A. S. Mayer, C. T. Kelley and C. T. Miller, Adv. Water Resour., 25 (2002), 1233.
[2] M. Erickson, A. S. Mayer and J. Horn, Adv. Water Resour., 25 (2002), 51.
[3] E. R. LaBolle G. E. Fogg and A. F. B. Tompson, Water Resour. Res., 32 (1996), 583.
[4] D. Ahlfeld and E. Hill, Ground Water, 34 (1996), 341.
[5] J. Bear and Y. Sun, J. Contam. Hydrol., 29 (1998), 225.
[6] J. Horn, *The nature of niching: genetic algorithms and the evolution of optimal, cooperative populations*, PhD thesis, University of Illinois at Champaign, Urbana, Illinois, (1997).
[7] R. M. Maxwell, *Understanduing the effects of uncertainty and variability on groundwater-driven health risk assessment*, PhD thesis, University of California, Berkeley, California, (1998).