In Situ Bioremediation of Perchlorate-Contaminated Groundwater using a Multi-Objective Parallel Evolutionary Algorithm

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Abstract - **Combining horizontal flow treatment wells (HFTWs) with *in situ* biodegradation is an innovative approach with the potential to remediate perchlorate-contaminated groundwater. A model has been developed that combines the groundwater flow induced by HFTWs with biodegradation processes that result from using the HFTWs to mix electron donor into perchlorate-contaminated groundwater. The model can be used to select engineering design parameters that optimize performance under given site conditions. In particular, one desires to design a system that 1) maximizes perchlorate destruction, 2) minimizes treatment expense, and 3) attains regulatory limits on downgradient contaminant concentrations. Unfortunately, for a relatively complex technology like *in situ* bioremediation, system optimization is not straightforward. In this study, a general multi-objective parallel evolutionary algorithm call GENMOP is developed and used to stochastically determine design parameter values (flow rate, well spacing, concentration of injected electron donor, and injection schedule) in order to maximize perchlorate destruction while minimizing cost. Results indicate that the relationship between perchlorate mass removal and operating cost is positively correlated and nonlinear. For equivalent operating times and costs, the solutions show that the technology achieves higher perchlorate mass removals for a site having both higher hydraulic conductivity as well as higher initial perchlorate concentrations.**

1.0 Introduction

Perchlorate is an oxyanion that the aerospace industry has used since the 1940's as a constituent in solid rocket fuel (EPA, 1999; Herman and Frankenberger, 1998). Due to the absence of legal restrictions, a lack of knowledge of perchlorate health effects, and a deficient understanding of the processes affecting perchlorate fate and transport, significant quantities of ammonium perchlorate were released into the environment over the years (Urbansky, 1998), resulting in perchlorate groundwater contamination problems that we face today. Perchlorate contamination from these past practices now affects the drinking water of 15 million U.S. citizens (EPA, 1999).

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The chief health problem caused by perchlorate is due to its potential to interfere with hormone production in humans. The thyroid gland normally uptakes iodide from the bloodstream to make hormones; however, the presence of perchlorate in the bloodstream causes the thyroid gland to uptake perchlorate instead of iodide, thereby disrupting hormone production. Animal studies also show perchlorate's potential to interfere with muscle movement (Urbansky,1998).

Unfortunately, perchlorate is mobile and persistent in the natural environment. The perchlorate problem is exacerbated because remediation of perchlorate-contaminated water is difficult. Conventional methods of remediating perchlorate-contaminated groundwater involve so called "pump-and-treat" technologies. That is, groundwater is pumped to the surface for treatment. Pumping the contaminated water to the surface involves additional costs, risks, and regulatory requirements. In addition, many aboveground treatment technologies, like ion exchange and reverse osmosis, merely concentrate the contaminant, but do not destroy it. For these reasons, researchers have been investigating technologies that can be applied to destroy the contaminant in place below ground (or *in situ*). One such technology, *in situ* bioremediation, makes use of indigenous microorganisms. Fortunately, it has been shown that perchlorate can be used as an electron acceptor by certain microorganisms, which appear to be ubiquitous (Wu *et al.*, 2001). *In situ* perchlorate bioremediation involves mixing an electron donor (like ethanol or acetate) into perchlorate-contaminated water, which is then injected into the subsurface where these microorganisms biochemically reduce the perchlorate to innocuous byproducts. A system to mix electron donor into perchlorate-contaminated groundwater, without having to pump contaminated water aboveground, is illustrated in Figure 1. This system which is known as a horizontal flow treatment well (HFTW) system (Stoppel and Goltz, 2002; Parr, 2002; Knarr, 2003), consists of two treatment wells, each with two screened intervals. One well pumps contaminated water in an upflow direction, the other in a downflow direction. After electron donor is added to the water, it is injected into the aquifer (through the upper screen of the upflow well and the lower screen of the downflow well) where bioactive zones form. In the bioactive zones, indigenous microorganisms consume the electron donor, in the process destroying the perchlorate, which serves as an electron acceptor. Note that a field

demonstration of this approach is planned to begin in late 2003.

In order to apply the technology in the field, project managers need to understand how contaminated site conditions and technology design parameters impact technology performance. One way to gain this understanding is to use a technology model to select

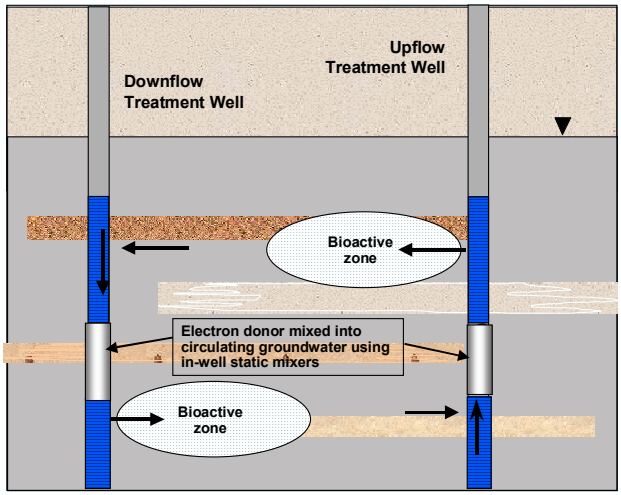

Figure 1. Cross-sectional view of horizontal flow treatment well (HFTW) system used to induce *in situ* bioremediation of perchlorate-contaminated groundwater.

engineering design parameters that optimize performance under given site conditions. In particular, a project manager desires to design a system that 1) maximizes perchlorate destruction, 2) minimizes treatment expense, and 3) attains regulatory limits on downgradient contaminant concentrations. Unfortunately, for a relatively complex technology like *in situ* bioremediation, with a number of engineering design parameters to determine, as well as multiple objectives, system optimization is not straightforward.

In this study, a multi-objective evolutionary algorithm (MOEA) is used to determine design parameter values (water flow rate through the treatment wells, treatment well spacing, concentration of injected electron donor, and injection schedule) that optimize the first two objectives; to maximize perchlorate destruction while minimizing cost. Multi-objective optimization is briefly addressed in Section 2, then the HFTW problem is formulated in Section 3. A generic MOEA is developed in Section 4 with the experimental design defined in Section 5 and results discussed in Section 6.

2.0 Multiple Objective Optimization

A multi-objective optimization problem (MOP) consists of decision variables, two or more objective functions, and constraints. These three components of an MOP are decision variables., objective function: and constraints. Standard MOP and multi-objective evolutionary algorithm (MOEA) definitions and nomenclature can be found in (Coello Coello et al., 2002). Such symbolic formulation includes feasible regions in objective space, feasible solutions, solution dominance and non-dominance, true and approximate Pareto optimal solutions P*/ P_{known} and Pareto front PF*/ PF_{known}, fitness sharing, niche count, sharing function, mating restrictions, ranking and the required evolutionary algorithm characteristics. The goal of a Pareto-based MOEA is convergence of PF_{known} towards PF*. MOEAs operate on a population of candidate solutions (chromosomes) as opposed to a single solution; therefore, the strength of an MOEA is its ability to uncover *multiple* nondominated solutions (P_{known}).

Various MOEAs have been proposed including the original Multi-Objective Genetic Algorithm (MOGA) by Fonseca and Fleming (1993) which used ranking and fitness sharing. Horn *et al*. (1994) developed the niched Pareto genetic algorithm (NPGA), which uses Pareto domination tournaments and fitness sharing chromosome selection. Srinivas and Deb (1994) introduced the nondominated sorting genetic algorithm (NSGA), so-named because it is based on a nondominated sorting procedure. Deb *et al*. (2002) developed the non-dominated sorting genetic algorithm-II (NSGA-II) to rectify flaws of the original NSGA. Many other variations also exist (Coello Coello, Van Veldhuizen, Lamont, 2002). For this application we develop our own parallel MOEA that incorporates appropriate constructs.

3.0 Formulation of HFTW MOP

A technology model was developed that incorporated the important processes that affected the fate and transport of perchlorate undergoing *in situ* bioremediation induced by using an HFTW system to add electron donor into perchlorate-contaminated groundwater (Parr, 2002). The model simulated the steady-state groundwater flow field resulting from operation of the HFTWs, and then used this flow field to determine dissolved perchlorate transport, competing electron acceptors (oxygen and nitrate), and electron donor (acetate) over time. Acetate was assumed to be added at the treatment wells at a specified concentration and schedule, and initial and boundary concentrations were specified for the other compounds. Microorganisms were assumed to be immobile, with the rate of microbial growth described by dual-Monod kinetics; that is, the growth of the microorganisms depended upon consumption of the electron donor in the presence of one or more of the electron acceptors. Similarly, consumption of the electron donor (acetate) and acceptors (oxygen, nitrate, and perchlorate) was described by Monod kinetics. In particular, the rate of consumption of perchlorate was directly related to the concentration of microorganisms and electron donor, and was slowed by the presence of the competing electron acceptors (oxygen and nitrate). The model includes ten nonlinear differential equations with various aquifer, kinetic parameters and constraints (Parr, 2002; Knarr 2003). These equations were numerically solved using a self-adaptive, partial

implicit finite difference technique coded in FORTRAN over a rectangular grid (Knarr, 2003).

Having developed a technology model, we can formulate an HTFW multi-objective problem. Over a given time of technology operation, we desire to 1) destroy as much perchlorate as possible and simultaneously 2) keep operating costs of the remediation technology low. These objectives can be represented as f_1 and f_2, respectively. Decision variable characteristics must be identified so that a site engineer could manipulate them in order to pursue these objectives. Such characteristics are:

Q = pump rate (m^3/day) for each well in the HFTW
d = spacing between the two treatment wells (meters)
$\boldsymbol{C_{in}}$ = injected concentration of acetate (mg/L)
p = acetate injection pulse duration (in 32^{nds} of a day)

We now want to mathematically express the objectives f_1 and f_2 as functions of the decision variables. However, objective f_1 (mass perchlorate destroyed) cannot be explicitly written as a function of the decision variables. Looking at the technology model, we can see that f_1 is a function of the decision variables, but determining f_1 for a given set of decision variable values requires numerical evaluation of the set of partial differential equations that comprise the technology model. Therefore, objective f_1 is generally represented as Mass perchlorate destroyed = $f_1(Q, d, C_{in}, p)$. The relationship between f_2 (total operating cost) and $[Q, d, C_{in}, p]$ can be explicitly formulated. To simplify our comparison of operating costs for different implementations of the remediation technology, operating cost differences are assumed to be due only to differences in a) the cost of electron donor and b) the cost of operating the pumps. That is, we implicitly assume that capital costs, as well as other recurring costs (*e.g.* maintenance) for different technology implementations are equal.

Cost of electron donor depends upon how much electron donor is injected over the duration of the remediation period *t*, and we can write this cost as:

Material cost = $2 * Q * t * C_{in} * p/32 * 1000\ L/m^3 * Price_{donor}$

with the following parameter values:
number of treatment wells = 2
treatment period (days) = t
maximum pulse duration (32 pulse units = 1 day) = 32
conversion factor = 1000 L/m^3
$Price_{donor}$ = price of electron donor injected ($/mg donor)

The remediation technology also incurs the cost of operating the pumps in the two HFTWs. Assuming continuous pump operation, the pump cost equation becomes:

Pump cost = $2 * Q * t * E * Price_{elec}$

With the following parameter values:
number of treatment wells = 2
E = energy required to overcome headloss (kW-hr per m^3)
$Price_{elec}$ = price of electricity ($/kW-hr)

Objective f_2 can explicitly be defined as a function of decision variables noting that Operating cost = Material cost + Pump cost:

$$\mathbf{f_2(Q, C_{in}, p)} = 2 * Q * t * C_{in} * p/32 * 1000\ L/m^3 * Price_{donor} + 2 * Q * t * E * Price_{elec}$$

$$\mathbf{f_2(Q, C_{in}, p)} = 2 * Q * t * (C_{in} * p/32 * 1000\ L/m^3 * Price_{donor} + E * Price_{elec})$$

Finally, we must recognize the constraints that our problem domain imposes. The technology model imposes lower and upper bounds on each of the decision variables which we can designate as Q_{min}, Q_{max}, d_{min}, d_{max}, $C_{in,min}$, $C_{in,max}$, p_{min}, and p_{max}. With our objectives, decision variables, and constraints identified, a multi-objective problem can be formulated; i.e., search for all vectors $\mathbf{x} = [Q, d, C_{in}, p]$ that:

maximize $f_1(\mathbf{x})$ = *mass perchlorate destroyed* and
minimize $f_2(\mathbf{x}) = 2 * Q * t * (C_{in} * p/32 * Price_{donor} + E * Price_{elec})$

subject to the following constraints:

$Q_{min} \le Q \le Q_{max}$; real-valued
$d_{min} \le d \le d_{max}$; integer-valued
$C_{in,min} \le C_{in} \le C_{in,max}$; real-valued
$p_{min} \le p \le p_{max}$; real-valued.

The specific objective is to find sets of engineering parameters $[Q, d, C_{in}, p]$ *that yield an optimal trade-off relationship between technology effectiveness (with respect to perchlorate mass removal) and cost***.** Ideally, the solution set $[Q, d, C_{in}, p]$ should be further constrained to values that yield downgradient perchlorate concentrations that fall below some maximum level. The rationale for this constraint is that regulations typically prescribe a maximum contaminant level downgradient from the source. However, the ability of the technology to yield sufficiently low perchlorate levels is largely uncertain and thus, this additional constraint would risk over-constraining the problem and yielding no solutions. Therefore, instead of formulating downgradient perchlorate concentration as an objective or constraint, we simply monitor downgradient perchlorate concentration to gain an understanding of how different technology implementations affect the relative magnitude of this important parameter.

There are some important considerations in selecting a suitable search algorithm to solve this problem: 1) Objectives f_1 and f_2 have common decision variables $[Q, C_{in}, p]$, but the mathematical relationship between f_1 and f_2 is unknown. In other words there is no analytical expression for the theoretical Pareto Front (PF*). 2) An explicit relationship between f_1 and $[Q, d, C_{in}, p]$ is unavailable. 3) Because a discrete plot of the Pareto front is the only representation achievable, the plot must adequately span the extremities of the Pareto front. 4) Due to the relatively long computation time in evaluating a decision variable set with the technology model, an efficient stochastic search algorithm is essential.

4.0 Specific MOEA Development

In developing an appropriate MOGA to solve the proposed HFTW problem, the following characteristics are necessary: Pareto-based, real-valued crossover and mutation operators, fitness sharing, and parallel

computation. Parallelization is a practical necessity due to the intensive computation requirements of the FORTRAN technology model. Thus, this MOEA design is an evolution of our parallel generational genetic algorithm software developed for an aggregated-objective groundwater remediation problem (Garrett, 1999). It also uses a "framing" parallel model in this object-oriented software structure. Note that Garrett's software incorporated the arithmetic crossover and mutation operators defined by GENOCOP III (Michalewicz, 1994). It should be mentioned that Garrett's work with an aggregated fitness function reflected results that were very similar to the suggestions of consulting experts. The new MOEA extensions include integration of ranking and fitness sharing into Garrett's (1999) genetic algorithm computer code as well as generic Pareto-based computation and interfacing to the different flow and transport application model. The ranking selection method of course emphasizes favorable Pareto solutions and fitness sharing forms niches for the HFTW MOP. Based upon its structure, this new real-valued MOEA is given the name GENeral Multi-Objective Program (**GENMOP**).

Since the GENMOP chromosome generally consists of genes representing the decision variable, the specific chromosome for our two-well HFTW system contains the associated engineering parameters. Chromosomes also have auxiliary genes devoted to objective function values, Pareto-ranking, and downgradient perchlorate concentration, but these auxiliary genes are not involved in crossover or mutation. Decision variables are real-valued except for well-spacing, which is integer-valued.

The GENMOP relies on the following user-specified parameters: 1) Initial population size ($|Pop_0|$): 2) Mating pool size ($|MP|$): 3) Number of generations (N): 4) Niche radius (σ_{share}): 5) Mutation probability (p_m). Aspects of the multi-objective groundwater remediation application developed by Erickson et al. (2002) which used the NSGA were also studied in regard to explicit parameter values. Many aspects of existing MOEA packages [Coello, Coello et al, 2002] such NPGA2, NSGA-II, PAES-II, SPEA2 were also evaluated for possible inclusion.

The GENMOP starts by randomly generating an initial chromosome population Pop_0 of size $|Pop_0|$ in which all chromosomes comply with decision variable constraints. The created chromosomes are stored in a set called Pop_{cum},because it is a cumulative collection of chromosomes; the algorithm continually appends the new chromosomes to Pop_{cum}. After Pop_{cum} is created, objective function values are evaluated for each chromosome. The objective function values are Pareto-rank for each chromosome in Pop_{cum}. A particular chromosome $\mathbf{x}$ receives a rank that equals the number of chromosomes that dominate chromosome $\mathbf{x}$. Hence, all nondominated solutions have rank = 0, and low rank corresponds to high fitness. This Pareto-ranking method mimics the method of Fonseca and Fleming (1993).

Once chromosomes are Pareto-ranked, the generation subroutine is initiated, which begins by selecting chromosomes to be copied to a reservoir called a mating pool (*MP*) where they await crossover and mutation. The user-specified parameter $|MP|$ limits the number of chromosomes in *MP*. Two properties that drive selection are the Pareto rank and the "crowding" in objective/fitness space. As long as space in *MP* is sufficient, GENMOP copies all rank-zero chromosomes to *MP*, then all rank-1's, then all rank-2's, etc. Simply put, when space is sufficient, Pareto rank drives selection. This method ensures that better, low-ranking chromosomes receive selection priority.

However, as low-ranking chromosomes are progressively copied, space in *MP* depletes. Eventually the algorithm encounters chromosomes of some rank k whose quantity exceeds remaining space. Because all k-rank chromosomes have equal rank, and therefore fitness, the algorithm resolves the dilemma of which chromosomes to select by picking chromosomes that are least crowded in objective space. The purpose of this selection strategy is to develop chromosomes that map to relatively uninhabited sections of the Pareto front, which for the decision maker means more diverse tradeoff options. The metric for assessing crowding in objective space is the niche count. This technique is called *equivalence class sharing*, which was originally described by Horn *et al*. (1994).

Let $\mathbf{x}_i$ be some k-rank chromosome such that I = 1, 2, 3…[number of rank k chromosomes], and assume that the number of k-rank chromosomes exceeds remaining space in the mating pool. Also, let chromosome $\mathbf{x}_j$ be any chromosome in Pop_{cum} where j = 1, 2, 3…[size of Pop_{cum}]. The GENMOP searches Pop_{cum} for the most current maximum and minimum values of both objective functions f_1 and f_2. These maximum and minimum values are subsequently used to normalize objective function values for every $\mathbf{x}_i \in$ {rank k chromosomes} and $\mathbf{x}_j \in Pop_{cum}$ as follows:

$$f_1'_i = (f_{1i} - f_{1min}) / (f_{1max} - f_{1min})$$
$$f_2'_i = (f_{2i} - f_{2min}) / (f_{2max} - f_{2min})$$
$$f_1'_j = (f_{1j} - f_{1min}) / (f_{1max} - f_{1min})$$
$$f_2'_j = (f_{2j} - f_{2min}) / (f_{2max} - f_{2min})$$

where

$f_1'_i$ = dimensionless value of f_1 based on $\mathbf{x}_i \in$ {rank k chromosomes}
$f_2'_i$ = dimensionless value of f_2 based on $\mathbf{x}_i \in$ {rank k}
$f_1'_j$ = dimensionless value of f_1 based on $\mathbf{x}_j \in Pop_{cum}$
$f_1'_j$ = dimensionless value of f_2 based on $\mathbf{x}_j \in Pop_{cum}$
f_{1i} = value of f_1 based on $\mathbf{x}_i \in$ {rank k chrom.}

f_{2i} = value of f_2 based on $\mathbf{x}_i \in$ {rank k}
f_{1j} = value of f_1 based on $\mathbf{x}_j \in Pop_{cu}$
f_{2j} = value of f_2 based on $\mathbf{x}_j \in Pop_{cum}$
f_{1min} = minimum value of f_1 within Pop_{cum}

f_{1max} = maximum value of f_1 within Pop_{cum}
f_{2min} = minimum value of f_2 within Pop_{cum}
f_{2max} = maximum value of f_2 within Pop_{cum}

This normalization makes both objective function values dimensionless, which is helpful due to the incommensurable units of both objective functions (mass and dollars). The distance d_{ij} between points $(f_1'_i, f_2'_i)$ and $(f_1'_j, f_2'_j)$ in dimensionless objective space is calculated as:

$$d_{ij} = [\ (f_1'_i - f_1'_j)^2 + (f_2'_i - f_2'_j)^2\ ]^{½}$$

Distance d_{ij} and the niche radius σ_{share} are then used to compute the sharing function:

$$Sh(d_{ij}) = 1 - d_{ij} / \sigma_{share} \qquad \text{for } d_{ij} \le \sigma_{share}$$
$$= 0 \qquad \text{for } d_{ij} > \sigma_{share}$$

The parameter σ_{share} basically defines the radius of a circle around point $(f_1'_i, f_2'_i)$; points inside the circle contribute to crowding, and points outside the circle do not. $Sh(d_{ij})$ is a metric for assessing the proximity or crowding between point $(f_1'_i, f_2'_i)$ and some other point $(f_1'_j, f_2'_j)$. If $(f_1'_j, f_2'_j)$ lies within the circle surrounding $(f_1'_i, f_2'_i)$ (i.e. $d_{ij} \le \sigma_{share}$), then the sharing function assumes a value such that $0 \le Sh(d_{ij}) \le 1$. The closer the two points are to each other, the higher the value of the sharing function; the maximum value $Sh(d_{ij}) = 1$ indicates the two points overlap. If point $(f_1'_j, f_2'_j)$ lies outside the circle surrounding $(f_1'_i, f_2'_i)$ (i.e. $d_{ij} > \sigma_{share}$), then crowding is negligible ($Sh(d_{ij}) = 0$).

The niche count m_i for chromosome $\mathbf{x}_i \in$ {rank k chromosomes} is computed according to:

$$m_i = \Sigma_{\mathbf{x}j \in Popcum}\ Sh(d_{ij})$$

Because m_i is a summation of sharing function values, it provides an overall measure of how "crowded" chromosome $\mathbf{x}_i$ is in objective space. A high niche count implies a high degree of crowding, and vice versa. After calculating the niche count m_i for each $\mathbf{x}_i \in$ {rank k chromosomes}, the remaining slots in *MP* are filled with chromosomes having the lowest m_i values.

GENMOP preferentially selects chromosomes with low niche counts to improve chances of generating points in less-occupied regions of the Pareto front. Chromosomes in *MP* proceed to crossover and mutation. The process relies on several crossover/mutation operators, which Garrett (1999) employed based upon (Michaelwicz, 1996). Mating restriction does not appear to be a critical component of any MOGA, and no sound theory justifies its inclusion (Veldhuizen and Lamont, 2000). Therefore mating restriction with crossover was not incorporated.

All chromosomes in *MP* participate in crossover. That is, for i = 1 to |*MP*|, chromosome $\mathbf{x}_i$ crosses over with $\mathbf{x}_r$, where $\mathbf{x}_r$ is randomly chosen from *MP* (pool crossover operates differently). The GENMOP employs the following crossover operators:

<u>*Whole arithmetical crossover*</u>: linearly combines all corresponding genes of $\mathbf{x}_i$ and $\mathbf{x}_r$, to create new chromosomes $\mathbf{x}'_1$ and $\mathbf{x}'_2$; crossover applies to the "whole" chromosome (i.e. all genes of $\mathbf{x}_i$ and $\mathbf{x}_r$)). The algorithm randomly retains $\mathbf{x}'_1$and discards $\mathbf{x}'_2$.

<u>*Simple crossover*</u>: randomly selects a gene and swaps it between $\mathbf{x}_i$ and $\mathbf{x}_r$ to make $\mathbf{x}'_1$ and $\mathbf{x}'_2$. The algorithm randomly retains $\mathbf{x}'_1$and discards $\mathbf{x}'_2$.

<u>*Heuristic crossover*</u>: uses chromosomes $\mathbf{x}_i$ and $\mathbf{x}_r$ to make a single offspring $\mathbf{x}'_1$ such that $\mathbf{x}'_1 = R\cdot(\ \mathbf{x}_r - \mathbf{x}_i) + \mathbf{x}_r$. The value R is a uniform random number between 0 and 1, and the rank of $\mathbf{x}_r$ is the same or less than the rank of $\mathbf{x}_i$

<u>*Pool crossover*</u>: randomly copies alleles from chromosomes in *MP* and assembles the alleles to make $\mathbf{x}'_1$.

GENMOP selects a particular crossover operator based upon an adaptive probability distribution. At the first generation, all crossover operators have equal probability of selection. For all following generations, the selection probability for a particular operator "adapts" or adjusts based upon the attributes of the new chromosome $\mathbf{x}'_1$. If $\mathbf{x}'_1$ dominates $\mathbf{x}_i$, then the crossover operator was successful in increasing fitness, and its selection probability consequently increases in the next generation. Conversely, if $\mathbf{x}_i$ dominates $\mathbf{x}'_1$, then crossover was unsuccessful, and its probability of selection decreases. If neither chromosome dominates the other, the operator's selection probability stays the same.

Crossover creates new chromosomes that are then susceptible to mutation. Mutation is controlled by the user-specified mutation probability (p_m). For each new chromosome, a random number (r: $0 < r < 1$) is selected from a uniform distribution. If $r < p_m$, then one of 3 mutation operators affects the new chromosome; otherwise, mutation does not occur. The process randomly selects which mutation operator based on the same adaptive probability distribution described. Crossover and mutation ultimately create a new chromosome population Pop_{new}, whose size equals the mating pool size |*MP*|.

GENMOP evaluates all members of Pop_{new} and appends them to Pop_{cum}. Thus, Pop_{cum} keeps all chromosomes from past generations and inherits new ones. Pop_{cum} is a set of accumulated chromosomes, and its cardinality is prescribed by $|Pop_{cum}| = N\cdot|MP| + |Pop_0|$. Each chromosome is ranked in Pop_{cum}, and the generation cycle restarts with selection.

5.0 Design of Experiments

A total of four runs for models of two physical-sites (Nevada, California) were executed using the GENMOP to produce an estimated Pareto set (P_{known}) and Pareto front (PF_{known}). Note that one of the research objectives is to perform the optimization search under various contaminated-site conditions. Key parameters that establish these different conditions between the two sites are hydraulic conductivity (ease with which water flows through the geologic formation), regional hydraulic gradient (driving force for regional groundwater flow) and initial contamination source concentration. Runs 1 and 3 simulate treatment periods of 300 days and 600 days, respectively, using data for Site 4, Nevada (Parr, 2002):

Aquifer Characteristics (Nevada)

Hydraulic Conductivity = 7.6 m/day
Hydraulic Gradient = 0.01

Source Characteristics (Nevada)

Oxygen Concentration = 2.8 mg/L
Nitrate Concentration = 60 mg/L
Perchlorate Concentration = 330 mg/L

Runs 2 and 4 simulate treatment periods of 300 days and 600 days, respectively, using data for Site 2, California (Parr, 2002):

Aquifer Characteristics (California)

Hydraulic Conductivity = 2.59 m/day
Hydraulic Gradient = 0.001

Source Characteristics (California)

Oxygen Concentration = 0.55 mg/L
Nitrate Concentration = 0.5 mg/L
Perchlorate Concentration = 160 mg/L

Site 4 in Nevada has approximately triple the hydraulic conductivity, ten times the hydraulic gradient, and double the source concentration of Site 2 in California. Site 4 also has larger initial concentrations of competing electron acceptors (oxygen and nitrate) than Site 2.

The Parr (2002) technology model is a set of partial differential equations representing flow and transport, biological reactions, and biomass growth in a subsurface system with microorganisms utilizing an electron donor (acetate) to reduce three electron acceptors (ClO_4^-, oxygen, and nitrate). The flow and transport model involves four separate, 3-dimensional advection/dispersion partial differential equations that represent transport of the electron donor (acetate CH_3COO^-) and three electron acceptors (oxygen, nitrate, and ClO_4^-), respectively. The biological treatment submodel consists of five differential equations that represent production/consumption rates due to microbial redox reactions; these terms are formulated based on a dual-Monod, multi-electron acceptor biodegradation submodel. The biomass grow is represented by a single differential equation. The following lists some of the parameters used in solving the model equations and GENMOP for all four runs:

Decision variable constraints

Q_{min} = 10 m^3/day Q_{max} = 150 m^3/day
d_{min} = 3 m d_{max} = 165 m
$C_{in,min}$ = 0 mg/L $C_{in,\,max}$ = 1,000 mg/L
p_{min} = 0 p_{max} = 32

Cost coefficients

$Price_{donor}$ = $\$2.666\times10^{-6}$ per mg donor
$Price_{elec}$ = \$0.067 per kW-hr

Aquifer parameters

Porosity = 0.30
Retardation factor for acetate (CH_3COO^-) = 1.48

GENMOP parameters

$|Pop_0|$ = 50 $|MP|$ = 10
N = 100 σ_{share} = 0.4 p_m = 0.01

The Q_{max} is an appropriate real-world value that would not result in excessive groundwater drawdown due to pumping at the sites. Values for d_{min} and d_{max} are based upon the dimensions of the site model. The value for $Price_{donor}$ is based upon an estimated bulk cost of \$286.20 per 55-gallons of a 50/50 mixture of acetic acid (CH_3COOH) and water. Realistic values for the other parameters that describe the kinetics of biodegradation and microbial growth were chosen based on laboratory studies (Parr, 2002; Knarr, 2003). These values were held constant for all model simulations. MOGA parameter values are based on our experience.

The GENMOP software (using Redhat LINUX version 7.3 and MPI version 1.2.7.1) executes the technology model, computes the cost formula for each new chromosome, and provides the Pareto computation. The objected-oriented C++ coded algorithm uses the Message-Passing Interface (MPI) to enable parallel computation among 32 Aspen dual-processor machines, each with 1-GB memory and two 1-GHz Pentium III processors that separately evaluate the technology model for each chromosome. In addition to decision variable and objective function values, the maximum perchlorate concentration is stored at a specified distance downgradient of the HFTW system. The purpose of including this output is to assess the ability of the treatment technology to meet downgradient regulatory requirements.

6.0 Technology Model with GENMOP Results

The Two perchlorate-contaminated sites in Nevada and California, are of course modeled using the HFTW technology model. The Nevada site had relatively high perchlorate concentrations and large groundwater flows compared to the California site. For each site, two sets of runs were performed; the first set of runs simulated treatment system operation for 300 days and the second set simulated 600 days of operation. For each set of runs, engineered parameter values were varied over realistic ranges, and the GENMOP determined the Pareto optimal set of parameter values for the given run conditions.

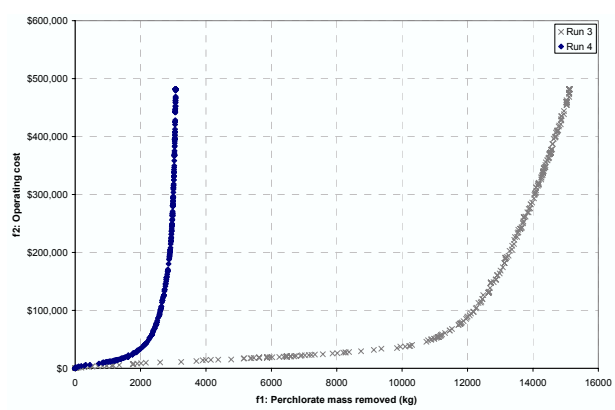

Figure 2. Pareto fronts for Nevada (Run 3) and California (Run 4) sites - (600 day simulations)

Figure 2 compares the generated Pareto fronts for the Nevada and California sites. Note that for the same cost, much more perchlorate mass can be removed at the Nevada site, where groundwater flows more readily (due to the high hydraulic conductivity at the site) and contaminant concentrations are higher than at the California site. We also see that for both sites, the incremental cost of perchlorate removal increases nonlinearly as mass removed increases.

Figure 3 plots perchlorate concentration downgradient of the treatment wells versus perchlorate mass removed for both dominated and nondominated solutions at the Nevada site. Recall that downgradient perchlorate concentration was not one of the objective functions or constraints, although it is an important parameter, as regulations typically would specify the allowable downgradient concentration. Figure 3 shows that as might be expected, downgradient concentration decreases as more perchlorte mass is removed by the treatment system. It should also be observed that the very low concentrations corresponding to high cost solutions, that is, pumping rates and the quantities of electron donor that must be added are high.

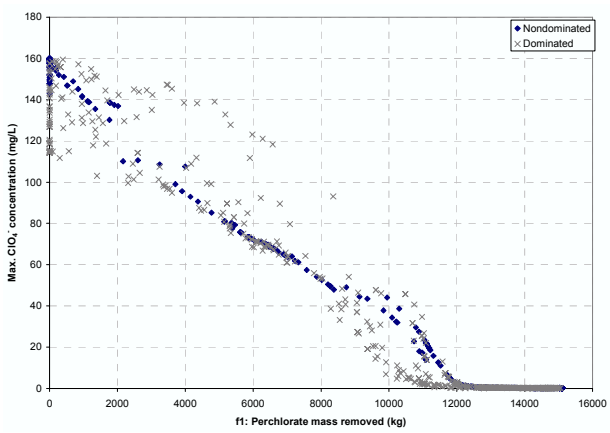

Figure 3. Maximum perchlorate concentration downgradient of the treatment wells versus perchlorate mass removed at the Nevada Site (600 day simulations)

Interestingly, Figure 4, which plots perchlorate concentration downgradient of the treatment wells versus perchlorate mass removed at the California site, behaves differently and presents some unexpected results. Here we see that there are a number of solutions that simultaneously have low mass removed and low downgradient concentrations. These solutions correspond to low cost solutions; that is, pumping rates and the quantities of electron donor that must be added are low. The reason for this apparent contradiction (low cost, low mass removal solutions that results in low downgradient concentrations) is that in these solutions, the treatment wells are located very close to each other and due to the low hydraulic conductivity and gradient at the site, regional groundwater flow velocities are small. Due to this small separation between the treatment wells and slow regional groundwater flow, water pumped by the HFTWs recycles through the bioactive zones many times and very low concentrations are attained, although very little mass is being treated.

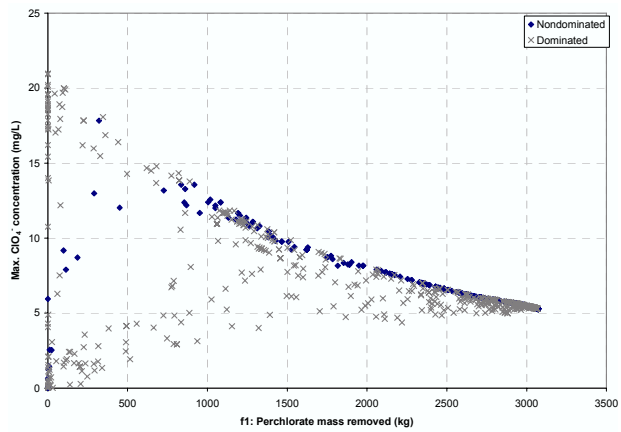

Figure 4. Maximum perchlorate concentration downgradient of the treatment wells versus perchlorate mass removed at the California Site (600 day simulations)

Otherwise, the California site and Nevada site results are similar, with downgradient concentrations decreasing as perchlorate mass removed increases, though due to the difficulty with which water flows at the California site, the magnitude of mass removed and the downgradient concentrations that may be attained are less than at the Nevada site.

7.0 Conclusions

The general multi-objective genetic algorithm developed in this study, GENMOP, is shown to be useful for determining technology design parameters for *in situ* bioremediation of perchlorate to minimize cost (defined as operating cost) and maximize technology performance (defined as perchlorate mass removal). As implied the technology model is quite complex resulting in a complicated computational structure. Nevertheless, GENMOP determined various sets of engineering design parameters $[Q, d, C_{in}, p]$ that provided a decision maker with combinations of cost and mass removal that are close to "Pareto optimal", that is to say, nondominated by other potential solutions. This set of solutions allows a decision maker to select a system design based on the weighting of the relative importance of performance versus cost.

One disadvantage of GENMOP is the need for relatively extensive computer resources (time and CPU power) to evaluate the technology model. Also, the selection of program parameters ($|Pop_0|$, $|MP|$, N, σ_{share}, p_m) was based on the experience and judgment of local

experts. It is unclear whether selection of a different set of parameters would generate different results. However as anticipated, the Pareto fronts generated indicate that the incremental operating cost increases as the technology removes more perchlorate mass.

Also observed is that the bioremediation technology's ability to remove perchlorate mass is not well correlated with its ability to achieve diminished downgradient perchlorate concentrations, especially for a contaminated site with relatively low groundwater flow. In other words, mass removal and diminished downgradient concentration are not redundant objectives. Therefore, decision makers must separately consider and weight each of these remediation goals when deciding on design parameters. It appears important to include downgradient perchlorate concentration as either an additional objective or a constraint when implementing a multi-objective optimization scheme.

Using the detailed techniques discussed, GENMOP can be employed in other highly dimensional MOPs that have very complex real-world real-valued models. GENMOP improvements can continue to solve these types of MOPs. Regarding more elaborate MOEA parallelization efficiencies, we are considering the concepts in Van Veldhuizen, Zydallis, and Lamont, 2003.

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