# Uncertainty Based Multi-Objective Optimization of Groundwater Remediation at the Umatilla Chemical Depot

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*Abstract*

Management of groundwater contamination often involves conflicting objectives and substantial uncertainty. A critical source of this uncertainty in groundwater problems often stems from uncertainty in the hydraulic conductivity values for the aquifer. For a remediation solution to be reliable in practice it is important that it is robust over such potential errors. This paper presents the application of a robust multi-objective optimization method on a field-scale pump-and-treat design problem at the Umatilla Chemical Depot site at Hermiston, Oregon. A simple methodology is used to establish plausible realizations of hydraulic conductivity that are then efficiently sampled within the optimization framework using Latin Hypercube sampling. A noisy multi-objective genetic algorithm, developed and tested earlier on a hypothetical aquifer, is then applied to this field-scale case to come up with a set of robust and Pareto-dominant design solutions for the clean up of contaminants (RDX and TNT) in the groundwater. Interactions between the various trade-offs and the inherent uncertainty at the site are analyzed. Finally it is demonstrated that by using such robust multi-objective optimization schemes, it is possible to increase robustness of the optimal solutions without significant increases in costs.

*Introduction*

Advanced global optimization techniques are increasingly being used in conjunction with aquifer simulation models to design more effective remediation systems.  In the field of groundwater remediation design, *Ritzel et al* (1994), *Karatzas and Pinder* (1996), *McKinney and Lin* (1996), *Rizzo and Dougherty* (1996), *Culver and Shoemaker* (1997), *Minsker and Shoemaker* (1998),, *Zheng and Wang* (1999), *Chan Hilton and Culver* (2000), *Erikson, et al (2002), Maskey et al* (2002), are among the many who have used optimization methods such as nonlinear and linear programming, optimal control, genetic algorithms, simulated annealing and cutting

plane methods. A major challenge with these approaches, as with all groundwater modeling, is that the solutions obtained by this approach are limited by the uncertainty and noise inherent within the simulation model. These 'noisy' factors can include the use of approximate fitness functions, the use of noisy data, knowledge uncertainty, modeling and numerical approximations, sampling and human error. While both the fields of multiobjective and "noisy" (uncertain) optimization have recently been the focus of intensive research in the evolutionary computation field, few researchers have considered combining these two approaches. Some initial work in this area was undertaken by *Hughes* (2001) who used estimates of the uncertainty distribution to deal with noise (uncertainty) within a multiobjective genetic algorithm. Another study was undertaken by *Chan Hilton and Culver* (2000) on groundwater remediation design in problems with uncertain aquifer properties.

Our current research seeks to develop a robust multi-objective optimization framework and apply this to a field-scale case study, the Umatilla Chemical Depot at Hermiston, Oregon. This site has recently been the focus of a demonstration project of transport optimization techniques (ESTCP, 2003). Remediation solutions were developed using simulation models with genetic algorithms, tabu search, and a combination of genetic algorithms and artificial neural networks (*Zheng and Wang*, 2002; *Peralta* 2002). *Peralta* (2003) performed a sensitivity analysis by varying the hydraulic conductivities from their expected values, but identifying solutions that would be robust for the potential range of uncertainties was beyond the scope of that project. This paper focuses on the methodology and application of the noisy multi-objective genetic algorithm (developed and tested on a hypothetical groundwater aquifer) to this test case.

The paper has been organized into four main sections. The first section describes the Umatilla site and the remediation technique being used. The second section briefly describes the modeling of uncertainty in the conductivity values. The third section presents the noisy multi-objective genetic algorithm used on this case. This is followed by results, discussions and conclusions on the lessons learned by incorporating uncertainty with optimality at the Umatilla Chemical depot.

*Umatilla Case Study*

The Umatilla Chemical Depot at Hermiston, Oregon is a 19,728 acre military reservation established in 1941 and operated as an onsite explosives washout plant from the 1950s until 1965. During this time approximately 85 gallons of wash water were discharged into two unlined lagoons at the site. The two major chemicals released were *2,4,6-tri-nitro toluene* (TNT) and *hexahydro-1,3,5-trinitro-1,3,5-triazine* (popularly known as RDX). Because of the soil and groundwater contamination of the lagoons, the site was placed on EPA's National Priorities List in 1984. Various environmental investigation studies, along with human health risk assessments and feasibility studies were conducted for the explosives washout lagoon. A cleanup plan for the groundwater operable unit was selected that consisted of pumping groundwater over an estimated period of 10 to 30 years, treating it with

granular activated carbon (GAC) to remove contaminants, in-situ flushing of subsurface soils beneath the lagoon with the treated water, and reinfiltration of the treated groundwater outside the contaminant plume. This would be combined with monitoring of the remediation process and institutional controls on the contaminated groundwater to prevent its use until cleanup levels are met. The cleanup levels for RDX and TNT were set at 2.1 μg/l and 2.8 μg/l, respectively.

The simulation models used in the test case were MODFLOW (*McDonald and Harbaugh*, 1996) for the prediction of the groundwater flow conditions, and MT3DMS (*Zheng and Wang*, 1999) for the prediction of the transport and reaction of the contaminating species. The entire site was divided into 5 layers, 132 rows, and 125 columns. Of the 5 layers, the last four were in a silt and weathered basalt unit, while the first is an alluvial aquifer. The flow and transport model for this site was developed by a modeling team at the Army Corps of Engineers. Heterogeneities in hydraulic conductivities observed during pump tests were modeled using a zonation approach (for details see USACE, 1996). Using this model, the existing remediation design (shown in Figure 2) has been estimated to require 17 years for cleanup at a total cost of $3.83 million in net present value.
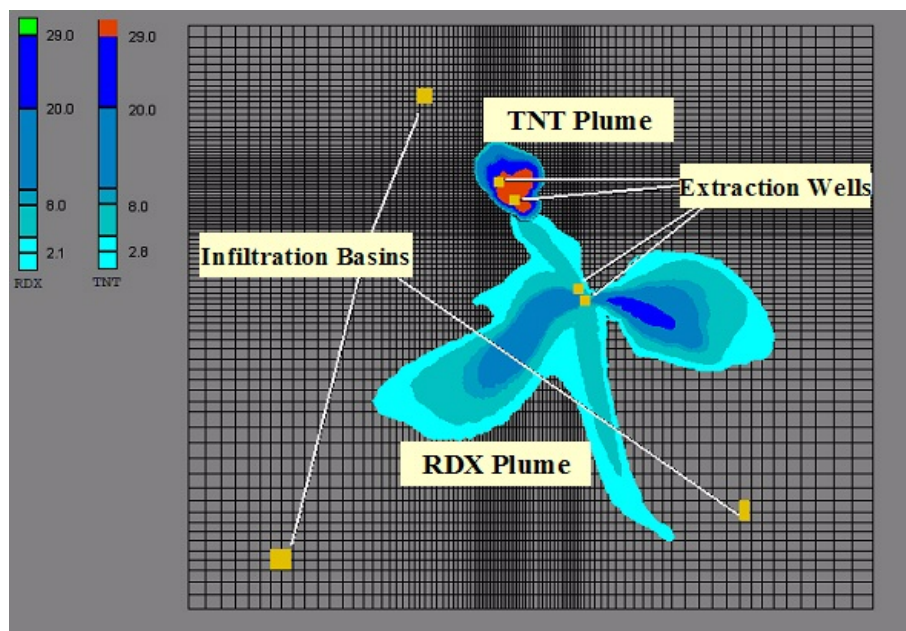


**Figure 1**: Existing RDX and TNT plume at the site as of October 2000 along with the pumping wells and infiltration basins being used for cleanup

Using the simulation-optimization approach, *Zheng and Wang* (2002) and *Peralta* (2002) identified candidate design solutions for the location and pumping rates of the wells and basins for three single-objective formulations. The first two formulations involved minimizing the total remediation cost until clean-up levels were achieved and the third formulation involved minimizing the mass of pollutants remaining in the groundwater after 20 years. Optimal designs were identified with clean up times as

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low as 4 years and a cost of $ 1.66 million. A major finding in their solutions was that the most cost-effective approach to remediation would be to shut down the pumping wells in the RDX plume and focus pumping in the TNT plume (shown in Figure 1). The feasibility of this approach depends on the relatively high estimated hydraulic conductivities at the southern end of the site, which allow the RDX plume to easily be drawn north to wells in the TNT plume. This study examines the effects of uncertainty in the hydraulic conductivity values on the feasibility of this type of solution. There is an obvious tradeoff between the cost of the remediation solution and its efficiency (defined as the mass of pollutants remaining in groundwater after a fixed number of years). Since the mass remaining in the aquifer depends on the conductivities the study also investigates the effect of uncertainty on the tradeoff between cost and efficiency of the remediation strategy.

*Modeling and Characterization of Uncertainty*

In practical cases it is generally impossible to gather sufficient data for accurate modeling because parameters (such as hydraulic conductivities) depend heavily on discrete sampling in specific areas. The results from the sampling are then used to approximate and interpolate parameter values for the entire region. This process introduces uncertainty at the very first step of the simulation-optimization approach. One critical parameter for a pump and treat groundwater remediation scenario is the hydraulic conductivity in the aquifer. For the Umatilla site, the US Army Corps of Engineers used pump test results from 47 monitoring wells to identify hydraulic conductivity ranges for each of the zones shown in Figure 2. The values used in the simulation model were set by calibrating the model to observations of the annual average groundwater elevations for the area using professional expertise and judgment. These values of the conductivities were then used for subsequent simulations of the fate and transport of the contaminant species (see USACE 1996 for more details).

To model the uncertainty in these conductivity values, realizations were generated depicting different conductivity scenarios. Each realization was generated by sampling from the ranges established from the pumping tests in Table 1. The existing values for the conductivities, which result in a close fit between the predicted and measured hydraulic heads, were taken as the most probable value for each zone. Each conductivity value was selected from a triangular distribution, with the upper and lower values given by the minimum and maximum conductivities from the pumping tests and the apex given by the existing model values. Generation of a particular realization entailed sampling for each zone from the corresponding triangular distribution. Repeating this process resulted in different hydraulic head realizations for the entire site. Realizations that gave unrealistic head scenarios were eliminated. A total of 100 realizations were created in this manner.

Each candidate pump-and-treat design solution was tested on several realizations using Latin hypercube sampling (LHS) an efficient stratified sampling technique described by *McKay et al*. (1979). To apply this technique, the first step is to

quantitatively characterize the differences in the realizations. This was done by ranking each realization based on the difference in the predicted heads of the realization and the existing model. Further details about the characterization of uncertainty and the sampling technique can be obtained from *Singh (2003a)*.

### *Noisy Multi-objective Genetic Algorithm*

Most problems in nature have several (possibly conflicting) objectives to be satisfied. The most popular approach to handle multiple objectives is to consider a set of the locally best alternatives, or the solutions that represent the optimal tradeoffs for the solution. These comprise the non-dominated frontier for the problem and the objective now becomes to find the set of solutions that are globally non-dominated (or Pareto Optimal). In other words, the objective is to find solutions to the problem such that there are no feasible solutions that would be better in one criterion without worsening at least one other criterion. This research uses an elitist non-dominant sorting genetic algorithm (NSGA-II) (*Deb et al, 2000*) to find a "population" of non-dominated solutions.

A genetic algorithm (GA) that operates under uncertainty is referred to as a "Noisy GA". When a single-objective GA is solved, sampling is usually used to find the average value the objective, which through the central limit theorem would increasingly tend to the actual mean-average of the distribution of the uncertainty. *Gopalakrishnan et al* (2001) tested this type of approach on a hypothetical groundwater remediation problem and obtained promising results. Most significantly, highly reliable solutions were found with low amounts of sampling (as few as 5 samples per solution). This is critical for the Umatilla case, where a computationally intensive simulation model must be run thousands of times to find the optimal solution.

For the multi-objective case, each objective must be evaluated over multiple realizations and moments are used to decide which solution is most probably dominant over another. Usually only the mean values are compared to decide between two individuals, but since the sample size is limited in this case, this leads to bias in the decision making process. To solve this problem, this study uses a hypothesis test based on a student-t distribution to decide statistically which individual is dominant. If the test is inconclusive, then the two solutions are statistically similar and *the individual with lower standard deviation is preferred*, thus ensuring that more reliable (less uncertain) solutions are given preference in the selection process. See *Singh* (2003b) for details on this approach.

At any time in the GA there may be multiple instances of the same solution (either in the same generation or in previous generations), each being sampled on different realizations. This can be exploited to improve accuracy of the mean and standard deviation estimates. The averaging is extended to consider all identical solutions in the present and past generations (in this case only one previous generation was considered). This form of *extended averaging* over all the samples of identical

individuals leads to a much larger effective sample size for each individual. Moreover, as the GA converges to the optimal Pareto front, the stable solutions in the Pareto front have more and more copies in future generations and are thus sampled more and more. By including all of these samples in the estimates of the objective value, we get more and more reliability as the GA converges.

## *Results*

The final Pareto front for the Umatilla test case is shown below (Figure 3). The red diamonds in Figure 3 show the average total mass remaining above the cleanup limit for a given remediation cost, as predicted by the GA using 5 samples on the final optimal solutions. These solutions were then evaluated using off-line Monte Carlo simulation with all 100 realizations to better estimate the "true" behavior of each solution over all conductivity realizations. The average, $5^{th}$, and $95^{th}$ percentiles from the Monte Carlo simulation are shown by the blue diamonds, green triangles, and pink squares respectively.
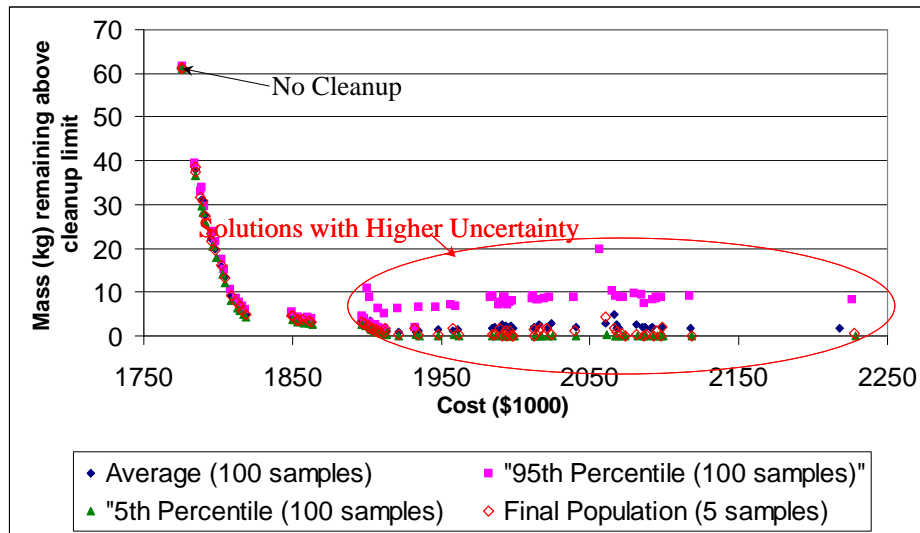


**Figure 3:** Average, $5^{th}$ and $95^{th}$ percentiles for the cost-cleanup tradeoff for the Umatilla Chemical Depot remediation solutions.

Figure 3 shows that there is a significant tradeoff between the cost and the cleanup efficiency, but as the cost increases the improvement in cleanup efficiency decreases. In general, higher costs mean more intensive pumping, and as can be seen there is much greater uncertainty for the more expensive solutions (with lower mass remaining). One of the reasons for higher uncertainty in the low mass solutions is that, as the mass is cleaned up from the site, localized islands of high concentrations remain which correspond to areas with low permeability. The location and amount of this residual mass depends heavily on the conductivities in the field, producing greater variation when these solutions are sampled over the different realizations. Thus even though a particular solution may predict no mass remaining for a given realization, it is not guaranteed to give cleanup for other conductivity scenarios.

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It is also important to investigate what difference considering uncertainty makes to the solution quality. Therefore, the results from the noisy NSGA-II are compared with results from a deterministic version of the same algorithm, which uses only the original hydraulic conductivity realization selected by the Army Corps of Engineers. Figure 4 shows the Pareto optimal front for these two cases (the open blue squares are the deterministic solution). Note that the deterministic NSGA-II does not have a long tail with high costs and low mass. The long tail in the noisy NSGA-II front is due to uncertainty in the mass remaining for a particular solution. This is particularly true for the solutions with low mass remaining. For these solutions, it is not possible to statistically decide among any of the solutions with the given significance level, thus allowing them to remain in the final non-dominated front.
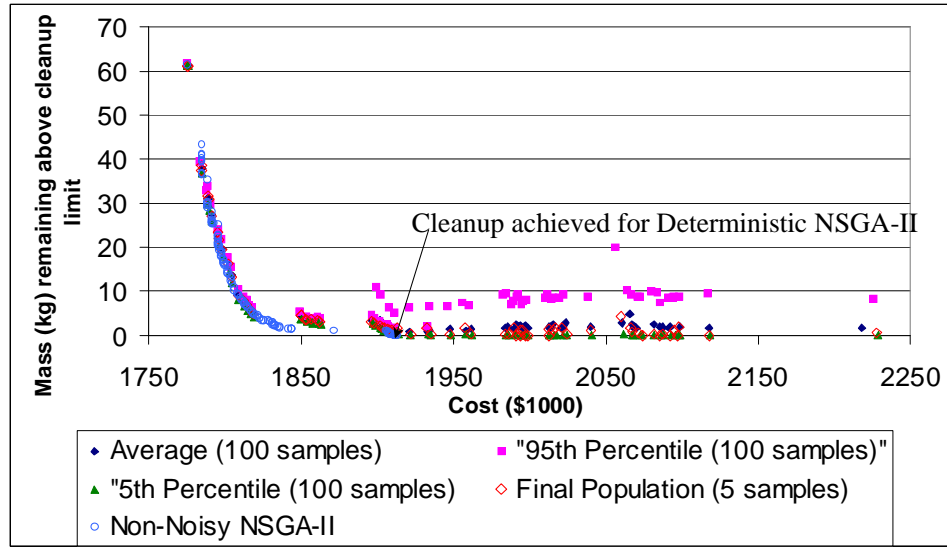


**Figure 4:** Comparison between tradeoff fronts from Noisy NSGA-II and deterministic NSGA-II using the existing conductivity scenario.

Figure 5 compares the solution for which the deterministic NSGA-II predicts total clean up after 5 years for the existing model (shown in Figure 4), with another solution with similar cost and average mass remaining from the noisy NSGA-II (which is close to the cleanup solution shown in Figure 4) . The optimal solution from the deterministic GA was also evaluated using all of the conductivity realizations to estimate the true uncertainty in the solution quality. The cleanup solution for the deterministic NSGA-II was found to have an average cost of $1,913,000 and an average of 0.89 kg of contaminant over the cleanup limit. Thus even though this solution predicts cleanup for the existing model it does not achieve cleanup for other conductivity scenarios. The comparable solution from the noisy NSGA-II had a cost of $1,912,000 and an average mass of 0.98 kg. However, the estimated standard deviation in mass remaining for the deterministic solution was 1.76 kg, while for the noisy solution this was only 0.38 kg. Thus the noisy NSGA-II found a solution with similar cost and cleanup efficiency but much lower (nearly five times lower) variability in the solution quality.

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Figure 5 shows that the two solutions are very similar except for the position of one extraction well and the addition of one extra infiltration basin to the deterministic solution. To find out which of these two changes contributed more to the variability, the extra injection basin was removed and the resulting solution was evaluated using all realizations. The same process was repeated by changing the position of the different extraction well. It was found that the position of the extraction well had a more significant impact on the cleanup efficiency. The main reason for this was that the deterministic NSGA-II was finding a solution with the well installed in a region with much shallower aquifer thickness, while the noisy NSGA-II installed the extraction well in a deeper portion of the aquifer, allowing for more effective pumping.
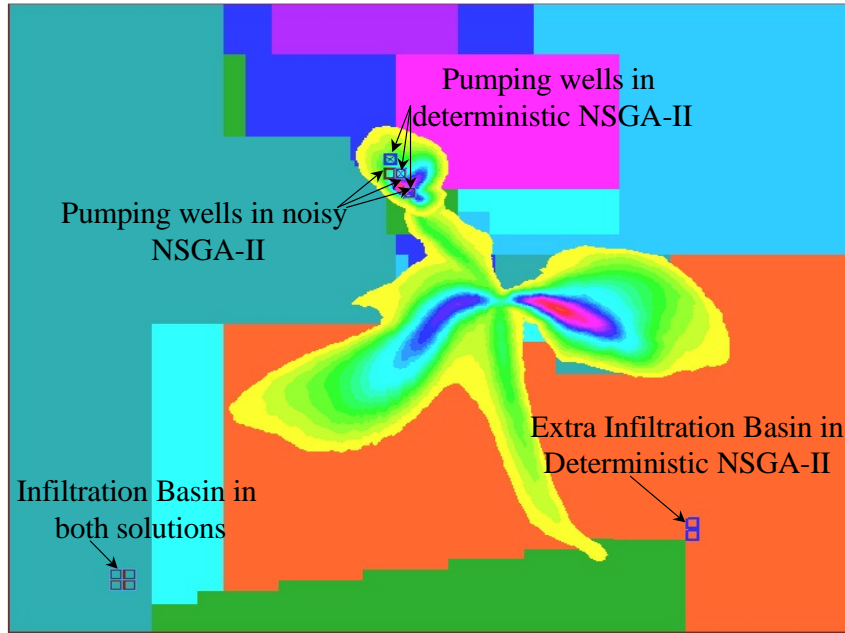


**Figure 5:** Comparison between clean-up solution for the deterministic NSGA-II, with a solution with similar cost and average mass from the noisy NSGA-II.

## *Conclusions*

Including uncertainty and multiple objectives is crucial for most real world problems, as was demonstrated for the Umatilla Chemical Dept field scale case study. For this particular site, the high cost and low residual mass solutions had more uncertainty. The noisy NSGA-II algorithm developed in this study was able to identify solutions that had performance close to cleanup but had much lower uncertainty relative to comparable deterministic NSGA-II solutions. Further investigation of one solution led to the discovery of how critical aquifer thickness was for improving robustness of the optimal solutions. Thus incorporating uncertainty in multi-objective optimization and decision-making gave valuable information about the site and the tradeoffs that exist between the various objectives.

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