Modeling and Characterization of Uncertainty for Optimization of Groundwater Remediation at the Umatilla Chemical Depot

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Abstract

Management of groundwater contamination is a very cost-intensive proposition filled with conflicting objectives and substantial uncertainty. A critical source of this uncertainty in groundwater problems comes from the data for the conductivity values for the aquifer on which the flow and transport of the contaminant is dependent. For a remediation solution to be reliable in practice it is important that it is robust over the error in modeling data. This paper presents our efforts to model the uncertainty for the Umatilla Chemical Depot site at Oregon, a difficult task given that the scarcity of available data precludes use of stochastic hydraulic conductivity generation techniques. The installation's modeling team has divided the site into conductivity zones. We use the results from various pumping tests to establish plausible ranges for the hydraulic conductivity value in each zone. Realizations for each zone are then generated randomly from these ranges. The hydraulic head conditions resulting from each realization are then compared with measured head conditions. To incorporate spatial as well as quantitative differences in the comparison, the first moments of the hydraulic head scenarios are also compared. Unrealistic realizations are eliminated and the remaining realizations are ranked based on the moment values. The ranked realizations will be used for efficient sampling using Latin Hypercube Sampling within the framework of an advanced stochastic multi-objective genetic algorithm to obtain robust, reliable and optimal solutions.

Introduction

Advanced optimization techniques are increasingly being used in conjunction with aquifer simulation models to design more effective remediation systems. Among many others, *Culver and Shoemaker* (1992), *Karatzas and Pinder* (1993), *Ritzel et al* (1994), *Rizzo and Dougherty* (1996), *McKinney and Lin* (1995), *Minsker and Shoemaker* (1998), and *Aly and Peralta* (1999) have implemented various state of the art optimization methods for groundwater management. A major challenge with this approach, 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. The "noise" which exists in certain environments is defined as any factor that hinders the accurate evaluation and assessment of a given trial design. These factors can include the use of approximate fitness functions, the use of noisy data, knowledge uncertainty, modeling and numerical approximations, sampling and human error.

One of our research objectives has been to develop new methods for handling the uncertainty inherent in the management and optimization of a realistic groundwater remediation design, primarily using genetic algorithms to obtain reliable solutions. Approaches using sampling based 'Noisy Genetic Algorithms' have been successfully applied and tested on smaller test cases with single objectives by *Gopalakrishnan and Minsker* (2002). Our current research seeks to extend this work to a much larger and more realistic test case with multiple objectives.

There are various issues involved with such an undertaking. The first and among the more critical is the modeling of the test case and the associated noise. For our work we chose the Umatilla Chemical Depot at Hermiston, Oregon, which has recently been the focus of a demonstration of transport optimization techniques (*Yeh et al.*, 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* (2002) performed a sensitivity analysis by varying the hydraulic conductivities from their expected values, but identifying solutions that would be robust for the range of uncertainties expected was beyond the scope of that project. In this study, we examine the issues involved in extending their work to explicitly incorporate the effect of hydraulic conductivity uncertainty in the modeling based optimization approach to identify more reliable solutions.

The paper has been organized into four main sections. The first section describes the Umatilla site and the remediation technique being used. It further details the simulation models being used to predict the fate and transport of the pollutants at the site. The second section deals with the modeling of uncertainty in the conductivity values. The methodology followed to generate various conductivity realizations is also outlined. The third section discusses the Latin hypercube sampling technique and describes the algorithm used to implement this technique in our case. This is followed by a discussion of future work and some salient conclusions on the method that we suggest for efficient uncertainty modeling and sampling.

Umatilla Case Study

The Umatilla Chemical Depot at Hermiston, Oregon has been chosen as the test case for modeling and optimizing an existing pump-and-treat system. The 19,728 acres military reservation was established in 1941 and operated an onsite explosives washout plant from the 1950s until 1965. During this time around 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). Although regular dredging of the lagoons was undertaken explosives contained in the wash water migrated into the soil and groundwater at the site. Because of the soil and groundwater contamination of the lagoons, the site was placed on EPA's National Priorities List (NPL) 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 of 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 control 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, with the resulting zones shown in Figure 1. 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.
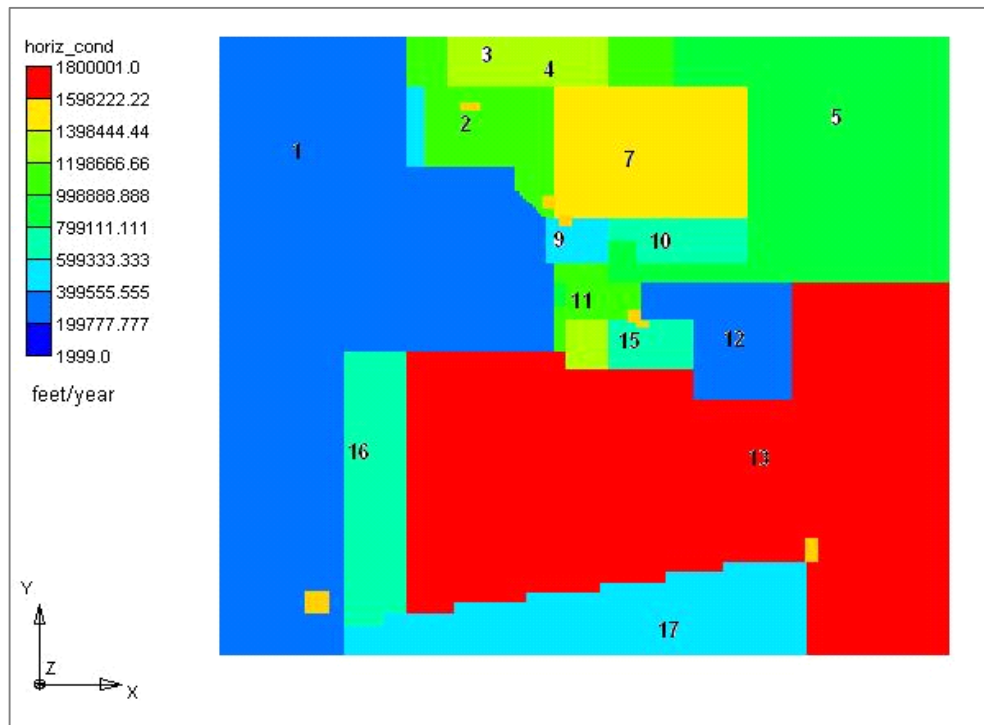

Figure 1: Hydraulic conductivity zones used in the model. Different colors represent different values of hydraulic conductivities.

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. They identified designs with clean up times as low as 4 years and total costs around 1.7 million dollars, a substantial improvement over the existing design, although the existing system was not designed to meet the same objectives.
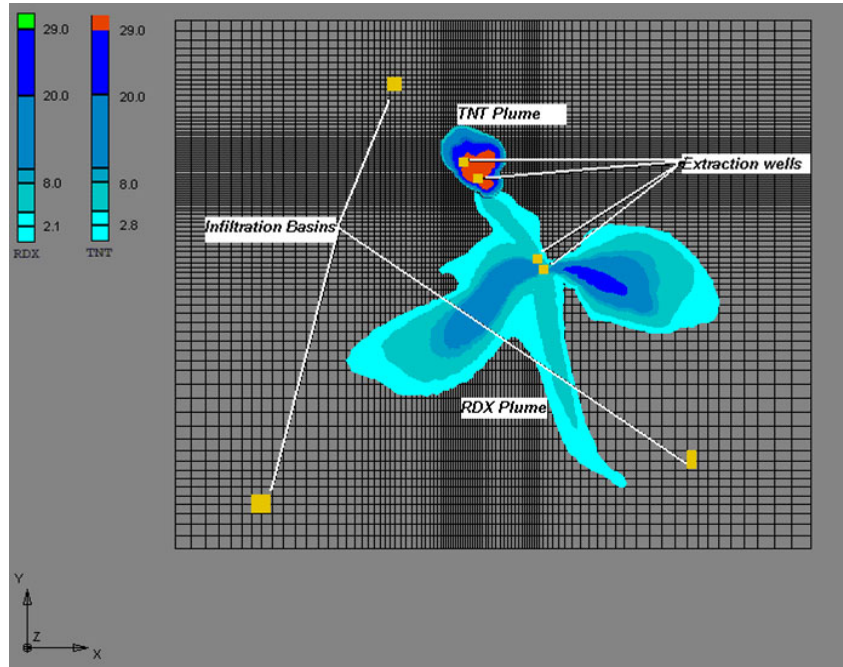
Figure 2: Existing RDX and TNT plume at the site as of October 2000 along with the pumping wells and infiltration basins being used for cleanup, shown on the MODFLOW grid used for simulations

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 3). The feasibility of this approach is dependent on the accuracy of relatively high estimated hydraulic conductivities at the southern end of the site (seen as the red area in Figure 2), which allow the RDX plume to easily be drawn north to wells in the TNT plume. In this study, we examine the effects of uncertainty in the hydraulic conductivity values on the feasibility of this type of solution. We will also examine tradeoffs between cost and clean up efficiency (mass of pollutants remaining in groundwater after remediation) using a multi-objective genetic algorithm approach.

Modeling and Characterization of Noise

Data collection and estimation form the lowest rung of the three tiered approach to simulation/modeling based optimization. The second rung is the simulation model used to predict the fate and transport of the pollutant, which is heavily dependent on the parameters and data selected for modeling. Finally the third rung, i.e. the optimizer, is dependent both on the accuracy of the data and the model used. Noise and uncertainty can be inherent in every step of this process. There can be error in the data collected as well as noise in the state variables and parameters that define the model. Moreover, computational modeling itself introduces approximations that lead to error in the model behavior. Finally, the objectives and decisions being optimized can be uncertain as well, leading to noise at the final level. In this paper we will focus on the first type of noise, namely the noise in state or parametric variables.

In practical cases it is generally impossible to gather sufficient data for completely accurate modeling because the groundwater modeling depends heavily on discrete sampling in specific areas. The results from the sampling are then used to approximate and interpolate these values for the entire region. This process introduces uncertainty at the very first tier of the simulation-optimization approach, which then filters to the other tiers through models that depend upon the first level. Some of the most critical parametric data for a pump and treat groundwater remediation scenario are the hydraulic conductivities in the aquifer. For the Umatilla site, pump test results from 47 monitoring wells (shown in Table 1) were used to identify hydraulic conductivity values for each of the zones shown in Figure 2. Of the 17 zones in figure 2, pumping test data was available for 9 zones. The boundaries of each zone and the values for the 8 zones with no data 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.

Table 1: Conductivity ranges from pumping tests.
Only Zones with sampling results are shown.

Zones	Existing Model Conductivity (ft/day)	Max Cond. (ft/day)	Min Cond. (ft/day)
2	3014	3655	319
5	2466	2673	2466
7	4110	4110	1128
8	600	3445	600
9	1500	5870	974
11	3014	8484	1867
12	1000	6376	1000
13	4932	4932	2617
15	1918	7401	1733

To model the uncertainty in these conductivity values, we generated realizations depicting different conductivity scenarios. Although, sophisticated approaches for generating hydraulic conductivity realizations exist that explicitly consider spatial correlations (for example the nearest neighbor method by *Bartlett*, 1975; or the tuning-bands method used by *Tompson et al*, 1989), the lack of extensive data at this site prevented the use of such approaches. Instead, a simpler approach was taken in which 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. A pictorial depiction of this process is shown in Figure 3, where four conductivity zones are shown with conductivity samples being chosen for zone 9 and 11 from their respective triangular distributions, defined by the conductivity limits ascertained from the field test results. Repeating this process resulted in different hydraulic head realizations for the entire site. A total of 100 realizations were created in this manner.
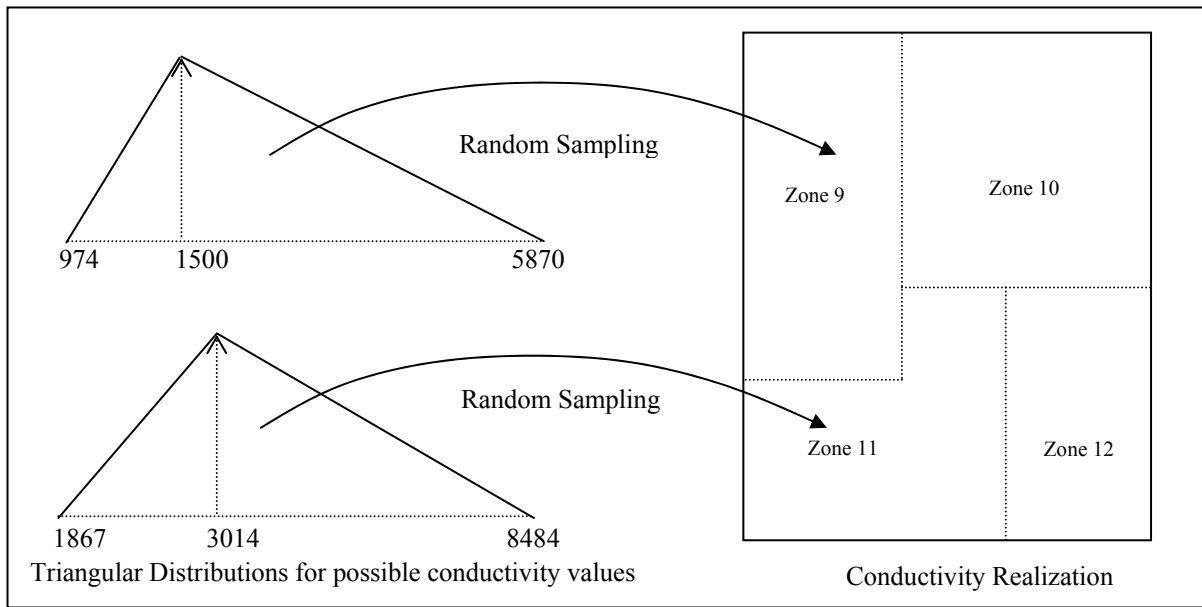
Figure 3: Pictorial depiction of the process to create conductivity realizations through random sampling from triangular distributions.

Of the various realizations generated, it may be possible that some yield hydraulic head scenarios that are very different from the observed average annual hydraulic heads. To eliminate this possibility, each realization was used with the existing well design to run a MODFLOW simulation that predicted the hydraulic heads. These hydraulic head scenarios could then be analyzed to discard realizations that were significantly different from water level observations.

To quantify the difference between the predicted and the observed hydraulic heads, we compared the hydraulic head values in the alluvial aquifer (layer 1) grid. However, we had no quantifiable data for the average hydraulic head values for the site. Thus we used the hydraulic heads predicted from the currently used model, which was seen to have a very close fit with the observed values. Using this as the standard, the cell by cell *absolute difference* between the two hydraulic head grids was taken, giving us an estimate of the quantitative difference between the two scenarios. Next the *first moment* (using ground distance measure from the origin) of this hydraulic head difference matrix was taken. This allowed us to incorporate the spatial differences between the two scenarios along with quantitative ones. The moment of the difference in simulated head values (which we refer to as the *difference moment*) thus generated could now be used to characterize each realization to give an indication of the variability in our sampling pool. The purpose of this exercise was to quantify the difference between a given realization and the standard (existing) conductivity scenario. A pictorial depiction of this process is shown in figure 4 where the existing head scenario and a randomly generated scenario are shown. The result of cell by cell subtraction results in the third grid, from which the first moment is then calculated from the origin.
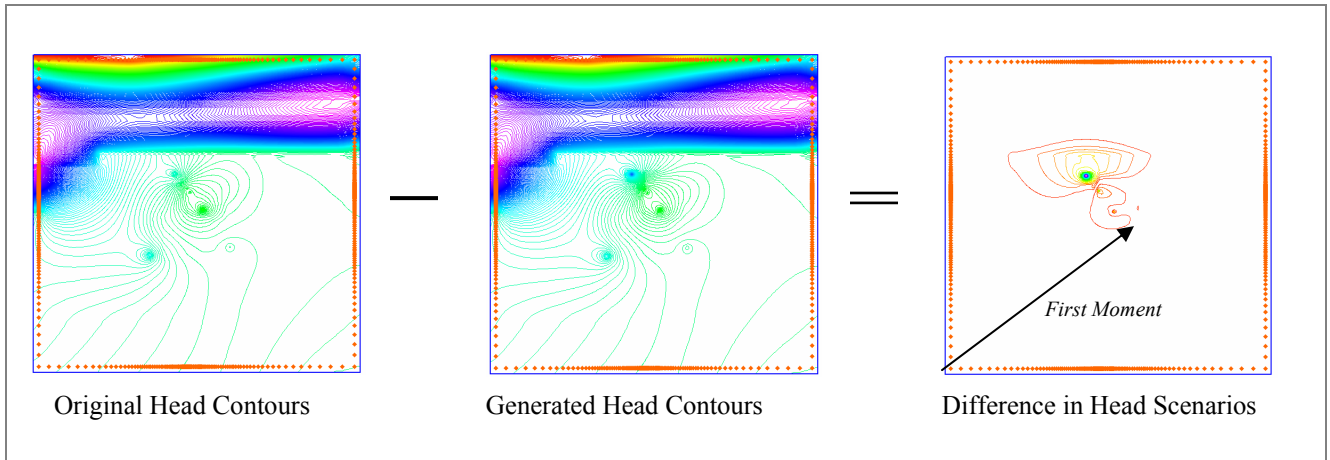
Figure 4: Generation of *Difference Moment* between randomly generated realization and the original scenario.

Ranking based Latin Hypercube Sampling

To incorporate the effect of noise and uncertainty, sampling is carried out from numerous realizations of the hydraulic head scenarios. Sampling can be carried out using the usual method of Monte Carlo sampling, wherein samples are drawn randomly from a pool of all possible realizations. However for this method to be effective and unbiased, the number of realizations has to be adequately large. Since the Umatilla case is very computationally expensive, it is desirable that the sampling be done in a more efficient manner, so that the best results may be achieved using fewer samples. One way of doing this is by using Latin hypercube sampling (LHS) described by *McKay et al*. (1979).

LHS is a stratified sampling technique where the random variable distributions are divided into non-overlapping equal probability intervals. A sample is randomly selected from within each interval for each basic event, which in our case is the choice of a particular realization. In this manner the Latin Hypercube technique ensures that the entire range of each variable is sampled efficiently. To give an example, if the random event is the choice of two numbers from the interval 1 to 10, LHS would divide the entire interval into two sub-intervals (1 to 5, and 5 to 10), and then randomly chose one number from each. Recently *Zhang and Pinder* (2000) demonstrated the utility of this technique for generating random hydraulic conductivity fields, showing that the method gave better results for the same computational cost as Monte Carlo or turning-band methods. Unlike this approach, which used spatial correlation information for the hydraulic conductivity zones, our approach does not take these into consideration due to scarcity of statistical data of the parameter field. To apply this technique to our case, the first step was to quantitatively characterize the uncertainty in the realizations. This was done using the approach described in the previous section to generate the associated conductivity moment and then ranking the realizations based on their difference moments. Figure 5 shows the moments for a set of 100 samples generated and ranked based on the procedure described.

As can be seen the coverage on the variability axis (difference moment axis) becomes sparse for the four highest values of difference moments. These realizations corresponded to excessively large differences between the generated and standard hydraulic head scenario. Thus these realizations were discarded from the pool and the remaining 96 were used for sampling.
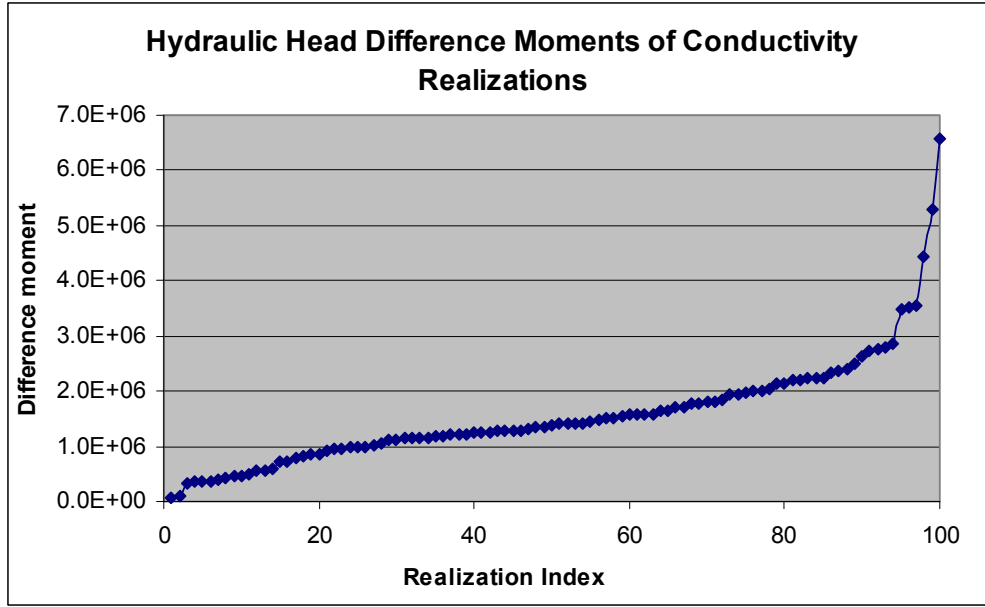
Figure 5: Head Difference (from existing scenario) moments of the hydraulic head scenarios generated using the conductivity realizations.

Depending on the sampling size, the sampling pool was divided based on the difference moments, and then samples were chosen from each sub-pool. For example, if four samples were to be chosen, the range 1 to 96 was divided into the 4 intervals [1, 24), [24, 48), [48, 72), [72, 96], and one number randomly chosen from each interval. The number was rounded off to the next closest integer and the realization corresponding to the index was chosen from the set of all realizations.

Using this methodology for efficient sampling, each candidate design to be evaluated in the optimization algorithm was tested over various conductivity realizations. A multi-objective genetic algorithm was designed such that robust and reliable solutions were preferentially selected to finally give the best combination of optimality and reliability. Results of the genetic algorithm analyses will be presented at the conference.

Summary and Conclusions

This paper outlines a methodology for modeling the uncertainty and noise inherent in a field site model. This is the first phase of our work, after which the above sampling technique will be combined with a state-of-the-art multi-objective genetic algorithm to find the best pump and treat design both in terms of efficiency and reliability. The methodology described has been developed for practical implementation on the particular case, but is also general enough to be used on other such test cases.

As is usually the case with real problems, insufficiency of data and computational complexity are hurdles that practitioners have to face in the real world. Moreover, modeling and characterization of uncertainty is an aspect that is often neglected in optimization, particularly at the field scale. We believe that the approach suggested in this paper is a practical and viable method for combining sparse available data with modeling and sampling techniques to yield more robust solutions.

Acknowledgements

References

Aly, A.H. and Peralta, R.C. (1999) Optimal Design of Aquifer Cleanup Systems under Uncertainty using a Neural Network and Genetic Algorithm, *Water Resource Research*, 35(8), 2523-2532.

Culver, T. B. and Shoemaker, C.A. (1992) Dynamic Optimal Control for Groundwater Remediation with Flexible Management Periods, *Water ResourceResearch* 35(8), 2523-2532.

Karatzas, G. P. and Pinder, G.F. (1993) Groundwater Management using Numerical Simulation and the Other Approximation Method for Global Optimization, *Water Resource Research*, 29(10), 3371-3378.

McKay, M.D., R.J. Bechman, & Conover, W. J. (1979) A Comparison of Three Methods for Selecting Values of Input Variables in the Analysis of Output from a Computer Code. *Technometics*, vol. 21, no. 2, 239-245.

McKinney, D.C. and Lin, M.D. (1994) Genetic Algorithms Solution of Groundwater Management Models, *Water Resource Research*, 31(3), 731-740.

Minsker, B.S. and Shoemaker, C.A. (1998) Quantifying the Effects pf Uncertainty on Optimal Groundwater Bioremediation Policies, *Water Resource Research,* 34(12), 3615-3625.

Peralta, R. C. (2002) Optimal Pumping Strategies For Umatilla Chemical Depot RDX And TNT Plumes, Draft final report presented to Navy Facilities Engineering Command, Systems Simulation/Optimization, Utah State.

Ritzel, B.J., Eheart, J.W. & Ranjithan, S. (1994) "Using Genetic Algorithms to Solve a Multiple Objective Groundwater Remediation Problem," Water Resources Research, 30, (5), 1589-1603.

Rizzo, D.M. and Dougherty, D.E. (1996) Design Optimization for Multiple Management Period Groundwater Remediation, *Water Resource Research*, 32(8), 2549-2561.

Tompson, A.F.B., Ababou, R. & Gelhar, L.W. (1989) Implementation of the Three-Dimensional Turning Bands Random Field Generator, *Water Resource Research*, 25(10), 2227-2243.

Yeh, S.L., Harre, K.J., Becker, D., Yager, K., Greenwald, R., Zhang, Y., Zheng, C., Peralta, R., Minsker, B. (2003): Application of Flow and Transport Optimization Codes to Field-Scale Groundwater Pump and Treat Systems.

Zhang, Y. and G. F. Pinder (2000), "A latin-hypercube method for evaluation of hydraulic conductivity random fields", *Proceedings Computational Methods in Water Resources, Vol 2, 779-784*.

Zheng, C. and Wang, P.P. (1999) *MT3DMS: Documentation and User's Guide*, Report to the US Army Corps of Engineers Waterways Experiment Station, (available at http://hydro.geo.ua.edu).

Zheng, C. and Wang, P.P. (2002) A Field Demonstration of the Simulation-Optimization Approach for Remediation System Design, *Ground Water*.