Project ID: **60069**

Project Title: **Least-Cost Groundwater Remediation Design Using Uncertain Hydrogeological Information**

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RESEARCH OBJECTIVE:

The research conducted by at the Research Center for Groundwater Remediation Design at the University of Vermont funded by the Department of Energy continues to focus on the implementation of a new method of including uncertainty into the optimal design of groundwater remediation systems. The uncertain parameter is the hydraulic conductivity of an aquifer. The optimization method utilized for this project is called robust optimization. The uncertainty of the hydraulic conductivity is described by a probability density function, PDF.

RESEARCH PROGRESS AND IMPLICATIONS:

The first year of this project involved the implementation of this method to a groundwater plume containment problem to determine a risk adverse remediation design. Through this study a new method of sampling a PDF was developed. Also, a new PDF, the beta-distribution function, was considered to describe the uncertainty of the hydraulic conductivity. The last year of investigations has been an expansion of the results from the first year of investigation. The robust optimization problem has been extended to include contaminant concentration restrictions. No research group has attempted this because solving the transport equation is computationally intense due to the nonlinearity of the equation. Research this past year also includes validation of the use of the beta-distribution function to describe the uncertainty in the hydraulic conductivity. While the goals of this research project have remained the same this past research year, the research we have completed in the field of optimization design has been substantial in development of a useful risk adverse remediation design algorithm.

This optimization has been extended to include added complexity in the optimization problem. The algorithm now provides a risk adverse least-cost design for a remediation system that will contain a plume of contaminated groundwater as well as decreases the concentration of contaminant in the groundwater at specified observation locations. This is done by imposing both gradient and concentration constraints on the optimization problem. Uncertainty in the hydraulic conductivity of the contaminated aquifer is addressed by using multi-scenario approach to optimization called robust optimization. Each scenario is representative of a possible hydraulic conductivity field. The hydraulic conductivity values that characterize each scenario are calculated using the equal area method developed in the first part of this study. The nonlinear robust optimization problem is solved using the outer approximation approach. By using equal area selection and outer approximation, it has been possible to develop a robust optimization algorithm that will determine a risk adverse remediation system that satisfies both groundwater flow gradient constraints and concentration limitations.

Validating the use of the beta-distribution function to describe the variation of hydraulic conductivity is performed using an extensive data set of hydraulic conductivity values measured in the Dakota Sandstone. Kenneth Belitz and John Bredehoeft of the U.S. Geological Survey provided this data set to our research group. The complete data set consists of drill0-stem test data and water-well pump test data taken in Nebraska, Wyoming, Kansas, Colorado and South Dakota. Because the locations of the drill stem data were more localized and the data more reliable than the water-pump data, the drill stem data was analyzed for this study.

The model used for the analysis of the robust optimization problem that includes the gradient constraints and the concentration constraints is the same model used in the initial study. The present optimization algorithm allows the model user to indicate the maximum allowable gradient between specified nodes and the maximum allowable resultant concentration at specified observation locations. The robust optimization problem analyzes multiple scenarios by adding penalty values to the objective function when constraint violations occur for each scenario. The model user controls the weight of the penalty term. It is possible to change the type of distribution used to describe the variation of the hydraulic conductivity and in some cases, the method of sampling of that distribution. With all of these capabilities, this model is becoming a functional model for practical remediation design. There are, however, important questions that one must address before using this model for their remediation scheme.

The value of the penalty weight in the robust optimization problem affects the optimal solution of the problem significantly. In the robust optimization problem the degree of uncertainty within a model is transformed into a cost value by way of the penalty term. If the penalty weight is large, then the violations have a higher value and the solution of the robust optimization problem is more risk adverse. The penalty weight can be thought of as an additional cost one will be fined if a contaminated plume is not contained or the contaminant concentrations are not lowered within a certain amount of time.

This optimization problem was run with both gradient and contamination constraints. The results were compared to results where only gradient constraints were imposed upon the problem. These problems produced very similar results. The reason these solutions are similar is because concentration constraints are often orders of magnitude smaller than the gradient constraint. One penalty weight is used for all constraint violations. For this reason, the penalty terms associated with concentration constraint violations will often be orders of magnitude smaller than the penalty terms associated with gradient constraint violations.

Two types of probability density functions have been used to describe the variability of the hydraulic conductivity within the modeled aquifer, the beta-distribution function and the lognormal distribution function. The analysis done using the entire lognormal distribution function to describe the variation in the hydraulic conductivity indicates that as the number of scenarios increases, the optimal solution increases steadily. Using the beta-distribution function, the optimal solutions also increase steadily. At this point convergence has not been determined in either analysis. More analyses are underway to examine the differences encountered when using these distribution functions in the problem where gradient and contamination constraints are imposed on the model.

The validation of using the beta-distribution function to describe the hydraulic conductivity data set began by applying an accepted parameter estimation technique to the acquired Dakota Sandstone data to determine the best fitting beta-distribution function to this data. The data is greatly skewed towards low values of hydraulic conductivy, and for this reason, the beta-distribution that was found to best fit this data was a beta-distribution function of the J form. While the J form of the beta-distribution function has a limited range of values, the probability value increases to infinity as the hydraulic conductivity value approaches zero and it is zero at the maximum value of the hydraulic conductivity provided. Using the J form of the beta-distribution function in conjunction with the equal area method of selection to determine the values associated with each scenario can be problematic. As the number of scenarios increases, the value with the highest frequency of occurrence approaches zero, i.e. the cluster of hydraulic conductivity values gets closer to zero. This is not realistic because it is assumed that the aquifer has positive hydraulic conductivity, not zero.

An alternative approach to using the beta-distribution function to describe the Dakota Sandstone data involves a transformation of the data. Because the data is greatly skewed towards small hydraulic conductivity values relative to the total range of values represented in the data set, the natural logarithm of each of the data points was taken to determine a new data set that is less skewed. The beta-distribution function that best fit this transformed data set was then determined using an accepted parameter estimation method. The equal area method was applied to this beta-distribution function and the delimiting values were then transformed back to the original data space using the inverse function of the natural logarithm. These values represent the scenario values that were used at each step to represent the natural variability of the hydraulic conductivity. The statistical properties of the original data are not altered when the transformations are applied to the data. For this reason, the statistical integrity of the results is not sacrificed when using this method. When using this transformation method in conjunction with the equal area method, as the number of scenarios increases, the value of hydraulic conductivity with the highest frequency in the representative sampling approaches the observed value of hydraulic conductivity with the highest frequency. Further, the beta distribution function determined in the transformed data space has a limited range of values and so the values determined using equal area selection also have limited range. The scenario values have the limited range desired for the robust optimization problem.

PLANNED ACTIVITIES

This research is at a critical point. The work we have completed this year has provided us with a powerful algorithm from which we can perform many analyses. Using concentration constraints in the risk-based analysis will continue. We will examine more extensively the affects of using different distribution functions to describe the variability of hydraulic conductivity in these new models. Because these problems are computationally intense, these analyses will take some time.

The algorithm will be revised. Revision within the algorithm will include using two different penalty weights, one for the gradient constraint violations and one for the concentration constraint violations. This will allow different penalty weights to be assigned to the different types of constraints. Revisions will also be made to increase the efficiency of the outer approximation solver for the non-linear optimization problem. We will also include a new option when applying the beta-distribution function to describe the uncertainty in the hydraulic conductivity. This option will allow the model user to either apply the beta-distribution to original data, or to the data transformed by taking the natural logarithm of the data. The results from these applications will be compared.

Once the algorithm is satisfactorily revised, analyses will continue with more complex models. A larger number of possible well locations will be examined. We will also investigate how the location of the observation points affects the robust optimization solution. Results of these exercises will display some of the powerful uses of this risk adverse optimization algorithm to designing a least-cost remediation system.

OPTIONAL ADDITIONAL INFORMATION

The graduate student working on this project is Ms. Karen Ricciardi, a doctoral student in the Department of Mathematics and Statistics at the University of Vermont.