Research Objective

The main objective of this research is to develop a computer code that will facilitate design of robust risk-based pump and treat groundwater remediation and management systems. The resulting systems will operate under both gradient and concentration constraints. The design is a least cost design. The element of risk in the remediation design considered in this work is that due to the uncertainty in the hydraulic conductivity of the contaminated aquifer in question.

Considerable work has been done in the field of optimal groundwater remediation and management design. Existent design algorithms depend upon the reliability of the groundwater flow and transport models to predict the movement of contamination in a given aquifer. The reliability of these mathematical models is, in turn, dependent upon variables that describe the physical attributes of the aquifer in question. The hydraulic conductivity of the aquifer is the most influential of the state variables that are used to describe groundwater flow and transport. Many models assume the hydraulic conductivity is known with certainty. However, field data shows that the hydraulic conductivity is uncertain

An immediate goal of this research is to successfully apply a new method of optimization to incorporate uncertainty in hydraulic conductivity into the groundwater remediation design subject to gradient and concentration constraints. In doing this, a new method of sampling uncertainty distributions has been formulated and successfully implemented. A new method of solving nonconvex optimization problems has also been successfully developed and applied. This method, called the tunneling method, is an efficient technique for solving optimization problems where multiple interior local minimum values exist in the feasible region (3). The results of this work provide a tool to create cost-effective design-risk-based groundwater-management systems.

Research Progress and Implications

To date, a new method of incorporating uncertainty into the optimization problem has been developed and employed. The method approaches the uncertainty in the hydraulic conductivity by using multiple realizations of different hydraulic conductivity values to represent a given distribution of hydraulic conductivity values (5). The realizations of hydraulic conductivity are selected using a Latin Hypercube strategy and are examined simultaneously. Each realization is considered to be the true realization. The constraint values must be satisfied for this realization. When violations of constraints for the remaining realizations occur, the objective function is penalized. The amount that the objective function is penalized is dependent upon a penalty weight associated with the entire penalty term, as well as a penalty weight associated with the frequency of occurrence of the individual realization. The penalty weight for the entire penalty represents the amount of design risk permitted in the problem. If this term is large, the risk due to the uncertainty in hydraulic conductivity will be avoided. If this value is small, the resulting design will contain a great deal of design risk, however the overall project costs will be lower than in the minimum design-risk case.

The values of hydraulic conductivity associated with each realization are chosen using a new method of Latin-Hypercube selection called equal-area selection. In choosing the values in this manner, the probability of occurrence of each of the representative sample values is equal, and each of the realizations has an equal individual penalty weight. The value of the weight is one divided by the total number of realizations sampled.

In examining an increasing number of realizations determined through equal area selection, convergence of the optimization design is expected to occur. Typically a lognormal distribution is used to represent the uncertainty in hydraulic conductivity; however, this distribution has the property that positive probabilities occur for all positive values of hydraulic conductivity (2). This is not realistic, so we use a beta-distribution to represent the distribution of hydraulic conductivity (1). Convergence of the optimization design subject to gradient constraints alone is observed.

Concentration constraints create non-linear optimization problems. The objective function subject to concentration constraints is nonconvex. Multiple interior local minima occur in this problem. As noted earlier, a new method of solving this type of problem is being applied. This method is called the tunneling method. This method has been shown to be superior to traditional methods when the number of local minima in the problem is large and when the dimensionality of the problem is large. This method also avoids the main disadvantages of traditional methods such as unpredictable performance while approaching the global minimizers and the evaluation of higher-order derivatives (5).

The tunneling method of solving this optimization problem consists of two phases that are cycled through until a global-minimum value is determined. The first phase is a minimization phase where a local minimum value is determined. The second phase is the tunneling phase where a new starting point is determined for the next minimization phase. In the tunneling phase the objective function is transformed into a new function that has the following properties. First, a pole exists at the most recently determined local minimum. Second, the roots of the tunneling phase exist at locations where the original objective function is equal in value to the value determined at the most recently determined local minimum. In creating this tunneling function, a gradient method is used on this function to determine a root of the function. This root will be the new starting point for the next minimization phase. When no roots of the tunneling function are determined to exist, a global minimum is declared.

Planned Activities

The tunneling method has been successfully applied to this problem. However, work is being done to make this code more efficient. While higher-order derivatives are not necessary in the tunneling method, first-order derivatives are necessary where gradient methods are used in both the minimization and the tunneling phases. Because there is no analytic solution to the flow and transport equations, the values of the gradients of the objective functions and the tunneling function can only be determined using perturbation techniques. This problem becomes computationally intense because, for each gradient value, the flow and transport model must be run twice for each realization examined.

At the present time alternative root-finding methods are being examined in the tunneling phase of this algorithm. In particular we are examining the use of Newton's method or a secant method to determine the roots of the tunneling function (4). Further examination of the structure of the computer code is also being revised. Efforts are being made to make the tunneling method more efficient. When the revisions to the tunneling method are complete, work will begin to compare the tunneling method approach to solving this optimization problem to other traditional methods. Methods that will be examined will include genetic algorithms and simulated annealing.

Information Access

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