Evaluating Subsurface Uncertainty Using Modified Geostatistical Techniques

by:

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ABSTRACT

There is a great deal of uncertainty about the distribution of geologic and hydrologic properties in the subsurface and the migration routes and extent of contaminants at most hazardous waste sites. This is because site data is limited. This research develops four geostatistical techniques which facilitate the assessment of and/or the reduction in the level of uncertainty associated with describing the subsurface. First, jackknifing and Latin-Hypercube sampling are used to define the uncertainty in the experimental semivariogram. Second, directional differences in the spatial variation of a semivariogram often cannot adequately be described using anisotropy factors; the kriging process is modified to accommodate three unique, orthogonal, semivariogram models. Third, the conditional simulation process is modified to use indicator classes rather than the threshold level between indicators. Fourth, zones at a site are modeled using individual and merged model semivariograms.

Using these methods is complex; consequently, a software package, UNCERT, was developed to integrate data collection, data evaluation, site interpretation, ground water flow and contaminant transport modeling, and data and model visualization. This software user interface makes the use of these modified geostatistical methods a practical endeavor.

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CHAPTER 1

INTRODUCTION

When designing a remediation plan for a hazardous waste site where the ground water is contaminated, there are several questions of concern about the contaminant: where is it, where is it going, how long will it take to get there, and what can be done to contain or remove it. To answer these questions, one critical question is, what are the subsurface hydrologic flow conditions. Unfortunately, as important as this question is, a precise answer is difficult to obtain. This is largely because we can only sample a small volume of the site; on the order of one 1/100,000th of the site. Exploratory drilling is expensive and can create new migration routes between contaminated and uncontaminated aquifers or zones, outcrops are generally very limited, and the distribution of the materials that control the hydrologic conditions vary widely. Because of the complexity of the hydrogeologic flow system, and the scarcity of data, there is usually substantial uncertainty in the subsurface description.

To describe some of this uncertainty, this research project develops several geostatistical techniques with the purpose of better defining or reducing uncertainty. A software package is also developed to aid modelers with the data analysis, geostatistics and ground water flow and contaminant transport modeling. The geostatistical techniques developed here are:

- Jackknifing the semivariogram and Latin-Hypercube sampling. These methods are useful for defining the uncertainty associated with the semivariogram model definition and applying that uncertainty in conditional indicator simulation.

- Directional semivariogram models. With traditional kriging techniques, the model semivariogram is defined and oriented in the direction with the longest spatial continuity, thus the longest model range. The spatial correlation, not oriented parallel to the principal axis, is defined by anisotropy factors describing the minor perpendicular axes. This approach is computationally efficient, but it is limiting. The method developed in this research allows the modeler to describe and krige each orthogonal axis independently.

- Class discrete indicator simulation. Traditional discrete indicator simulation techniques are based on the cumulative probability that a cell is less than a cut-off level or threshold. When non-continuous, discrete data are evaluated, this approach can be non-intuitive. A method where the probability that a discrete indicator class occurs at a cell location is developed here. For the semivariogram analysis, this method is more intuitive; for the simulation process, sensitivities due to indicator ordering are easier to test; and though order relation violations are more common, the remedy is mathematically more appropriate.

- Zonal Kriging. One of the basic assumptions in kriging is the assumption of stationarity (Journel and Huijbregts, 1978). This implies that the spatial variation across the site is approximately constant. For many sites this may be reasonable, but for others, this assumption will lead to significant errors. The zonal kriging method developed in this research project allows the model to be divided into unique and transitional regions.

A collection of program modules was developed to make these techniques practically useful for ground water modelers (as well as researchers from other disciplines). The software package is called UNCERT, for its task is to facilitate uncertainty assessment of ground water problems. It is composed of a number of individual modules: array, block, contour, distcomp, grid, histo, modmain, mt3dmain, sisim, surface, vario, and variofit. These cover a variety of statistical, geostatistical, ground water flow and contaminant transport models, and visualization applications. These run in any UNIX, X-windows/motif environment. All the major applications and tools utilize a user friendly, graphical user interface. Help manuals are also available for each package on-line using HTML (Hypertext Markup Language).

Each of these methods or tools is presented in an individual chapter. These chapters can be read as “stand-alone” documents, though they are all related to geostatistics and reducing uncertainty. Chapter 2 describes Jackknifing and Latin-Hypercube Sampling; Chapter 3, directional semivariogram analysis; Chapter 4, class versus threshold based indicator simulation; and Chapter 5, Zonal Kriging. In the final chapter, Chapter 6, there is a brief description of the UNCERT software package which contains the software described in Chapters 2 through 5, and many other statistical, geostatistical, visualization, and ground water modeling tools. A more complete description of the UNCERT package can be found on the tape (along with the source code) in Appendix A, or on the World Wide Web at http://uncert.mines.edu/.