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A Simulation and Decision Analysis Approach to Locating DNAPL in Subsurface Sediments

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A Simulation and Decision Analysis Approach to Locating DNAPL in Subsurface Sediments

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Abstract

This report presents a strategy for delineating the location of residual dense non-aqueous phase liquids (DNAPL) that combines probabilistic simulations of DNAPL spill location and volume, geologic texture constraining migration pathways, migration physics through percolation modeling, and a decision analysis model to pick optimal locations for sampling wells. Our strategy is an iterative process of simulating the residual DNAPL location, selecting new locations for data collection, gathering data, and then using the data to condition further simulations of DNAPL migration. As we iterate through this process, data worth analysis is used to determine an appropriate stopping point. We present the results from a preliminary version of our model, showing how the process was used to delineate hypothetical DNAPL spills.

CONTENTS

FIGURES

1 INTRODUCTION

Subsurface contamination in the form of dense non-aqueous phase liquids (DNAPL) poses a significant, yet unresolved, remediation problem. DNAPL such as the chlorinated organic solvents trichloroethene, tetrachlorethene, and carbon tetrachloride have been used for many years as degreasers in many industrial applications across the nation. DNAPL spills are a common problem at Superfund sites and other sites managed by the Department Of Energy, Department of Defense, and private entities.

These toxic compounds have a low solubility in water and tend to travel through the subsurface as a separate organic phase forming a long-term source of dissolved phase groundwater contamination. Dissipation of such a source by dissolution may require hundreds of years, so remediation by either removal or containment of the DNAPL is usually necessary. Recovery of DNAPL from the subsurface is no easy task because (1) delineating the spatial extent of residual DNAPL contamination can be arduous, and (2) existing technologies have a difficult time removing immobilized (residual) and pooled DNAPL. Of these two issues, recovery technologies have received the most attention. However, application of these technologies is impossible without information on the location of the DNAPL. Since the cost of remediation is dependent on the volume of soil that has to be treated, there is a clear incentive to accurately locate the DNAPL.

While many of the techniques needed to delineate free phase and residual DNAPL have already been developed, we know of no approach that combines these techniques in an organized fashion to optimize the process of delineating a DNAPL spill. This paper discusses an approach to delineating DNAPL spills that combines probabilistic modeling of geological features with percolation models of DNAPL flow and a decision theoretic approach to optimizing the location of sampling wells.

In our approach, multiple realizations of DNAPL plume location are provided via Monte Carlo simulation using an invasion percolation model applicable to mesoscale geological sedimentary units. These realizations capture the physics of DNAPL movement through the geologic features controlling DNAPL migration. In this way, uncertainty about the distribution of geologic features and disposal history at the site can be propagated through the modeling to reflect the degree of uncertainty in DNAPL location.

The results of the simulation are summarized by a probability map, which estimates the probability of DNAPL being present at each point on the site. Without further information, the only prudent course of action would be to set up a remediation scheme to cover all points for which the map indicates that there is a non-negligible probability of DNAPL. However, it is possible that additional sampling could reduce the total cost of characterization and remediation by decreasing the volume of soil that must be treated.

The probability map can be used to select potential locations for sampling points. By conditioning the simulation results on the presence or absence of residual or free phase DNAPL at these locations, we construct a decision analysis model which allows us to compute the expected reduction in the total cost of sampling and remediation that could be obtained by sampling at each location. We use this model to select the location of the next sampling point. After the data has been collected, we use the data to condition the simulations and repeat the process. If no new sampling points have positive value, then we stop the sampling process.

The importance of our approach is twofold. First, it may be able to improve the efficiency of the process of delineating DNAPL that acts as a long term source of dissolved phase DNAPL contamination. Second, our approach provides a stopping rule. When the decision analysis model indicates that there are no more economically viable sampling locations, we stop sampling and move on to remediation.

The remainder of this paper is organized as follows: In section 2, we discuss previous work on simulations of geology and DNAPL flow, optimal sampling point location, and hydrogeological decision analysis. In section 3, we describe our methodology and a sample problem. In section 4, we give the results from our sample problem. Our conclusions are presented in section 5.

2 PREVIOUS RESEARCH

Our approach combines simulation of geological properties of a site with simulation of DNAPL flow and the optimization of sampling point locations. Each of these topics has been investigated by other researchers. In this section we review previous research on the simulation of geological properties, DNAPL flow, and the optimal location of sampling points.

2.1 Simulating Geology

Numerous methods can be used to simulate the distribution of geological properties in three-dimensional space. These include geostatistical, geological process-based, geometrical, regionalization, fractal, and other techniques.

Geostatistical methods dominate current thinking on how to simulate the spatial distribution of geological properties. These approaches attempt to describe the bulk behavior of flow over large temporal and spatial scales while accounting for the influence of small-scale perturbations (Thompson and Gelhar, 1990; Dagan, 1982; Gelhar and Axness, 1983; Neuman et al., 1987; Sudicky, 1986). These approaches are computationally tractable and have become highly refined. A major advantage of these techniques is that it is easy to condition the simulation on observed data. However, they generally treat geological systems as a continuum with stationary or near-stationary properties. In many ways this ignores or precludes consideration of the local scale discrete structure to which DNAPL migration is sensitive.

Process-based simulation techniques are an attempt to reproduce the essential physical and chemical mechanisms associated with the development of geologic units. In the case of sedimentary systems, these processes involve sediment erosion, transport, and deposition. These approaches can be applied from centimeters to hundreds of kilometers and have primarily been used to investigate petroleum recovery problems (Cross and Harbaugh, 1989; Tetzlaff, 1989; Koltermann and Gorelock, 1992). They produce relatively realistic distributions of sediments, but generally do not focus on discrete structures at the scale of interest for DNAPL migration. In addition, they require large computational capabilities.

Geometric models do not directly track processes, but instead focus on the resulting geometric arrangement of materials. This reduces the computational burden, but relies on empirical or statistical descriptions of the spatial geometry and arrangement of materials. While early examples of this approach precede process modeling (Bridge and Leeder, 1979; Allen, 1978), this approach has received relatively little attention until recently (Scheibe and Freyberg, 1992; Webb, 1994).

Other mechanisms exist, such as regionalization (Bohling et al., 1990; Harff and Davis, 1990; Harff et al., 1990), that depend on multivariate statistical methods for mapping boundaries within large data sets. While these are explicitly discrete, they require large data sets from the field and are not explicitly used as a method of simulating multiple realizations of geology. Fractal simulation approaches (Turcotte, 1986; Wheatcraft and Tyler, 1988) are similar to stochastic simulation in applying a mathematical construct to the total field of geological properties. So far they have met with little success, but are still being pursued (Ghilardi et al., 1993).

2.2 Simulating DNAPL Migration

A critical component of our approach is the modeling of DNAPL movement to its final locations within a given geologic realization. In this paper we consider the use of a percolation type model for macro scale DNAPL migration. Percolation models are considerably faster than standard two or three phase flow codes and therefore allow incorporation of more geologic detail. We expect that detail with respect to textural changes within and across geologic units will be vital in the prediction of non-wetting, dense fluid migration.

Under many conditions, DNAPL movement through the saturated zone will be controlled by gravitational and capillary forces. This presumes that flows are sufficiently slow that viscous forces are small with respect to gravity and capillarity. For such conditions, laboratory studies suggest that for non-wetting DNAPL, pore scale behavior leads to capillary fingering in horizontal homogeneous micromodels (Lenormand and Zarcone, 1985) and an interplay of gravity fingering and capillary fingering in non-horizontal systems (Wilson et al., 1990). For both of these situations, forms of percolation theory can be used to model the immiscible displacement process at the pore scale.

Standard percolation (SP) was introduced by Broadbent and Hammersly (1957). While this theory has proven to be quite useful for modeling phase changes and critical phenomena, it is of limited use for modeling incompressible, two-phase, immiscible fluid displacements in porous networks (e.g., porous media). To more adequately represent fluid-fluid displacements in porous networks, Wilkenson and Willemsen (1983) introduced invasion percolation (IP), which incorporates phase accessibility rules to assure that connectivity within phases is considered in the pore filling criteria. IP has been applied to immiscible flow in porous media by a number of researchers (Ferrand and Celia, 1992), and has been shown to effectively model displacements in two-dimensional pore networks in micromodels where a non-wetting fluid invades a wetting fluid (Wilkinson and Willemsen, 1983).

2.3 Selecting Sample Locations

Boreholes are a primary tool in the delineation of DNAPL spills. It is critical to our approach that we intelligently select the locations of these sampling points.

Early work concerns the optimal location of boreholes for the determination of hydrogeological parameters such as transmissivity. In this approach, kriging and other geostatistical techniques are used to obtain estimates of the unknown parameter at points between the sampling points. Optimization techniques are then used to select well locations that minimize the uncertainty in the kriged estimates of the unknown parameter. Papers in this line of research include Olea, 1984; Hughes and Lettenmaier, 1981; Bogárdi et al., 1985; Spruill and Candela, 1990; McBratney et al., 1981; McBratney and Webster, 1981; Jones et al., 1979; Carrera et al., 1984; and Christakos and Killam, 1993.

In many cases we are not so much interested in hydrogeological parameters as in the resulting groundwater flow and transport of contaminants. A second line of research has developed in which geostatistical models of hydrogeological parameters are used in conjunction with differential equation models of flow and transport. Well locations are selected to minimize a measure of the uncertainty in a derived quantity, such as the head or concentration of a contaminant. For example, Wagner (1995) minimizes the trace of the covariance matrix of the parameters being estimated. Other research in this line includes Andricevic and Foufoula-Georgiou, 1991; Loaiciga, 1989; McKinney and Loucks, 1992; and Tuciarelli and Pinder, 1991.

We often need more information about the distribution of the contaminant concentration than just the mean and variance. For example, in designing a remediation scheme for a contaminant plume, we need to delineate the region in which there is any significant probability of the concentration exceeding a safe level. In a third approach, Monte Carlo simulations of the transmissivity field are used with flow and transport models to obtain information about the distribution of the head or contaminant concentration. This approach is very computationally intensive because of the large number of simulation runs required. For example, Meyer and Brill (1988) describe a procedure for locating wells in a groundwater monitoring network to optimize the probability of detecting a contaminant plume. Monte Carlo simulations are used to determine the probability of the plume being present at a number of fixed locations; then a subset of the locations that maximizes the probability of detecting the plume is selected. This model was expanded to include a second objective of minimizing the area of a plume at the time of detection by Cieniawski et al. (1995). Hudak and Loaiciga (1992) describe a procedure for selecting well locations that maximize the coverage of a contaminant plume.

Decision analysis techniques can also be used to optimize the location of sampling points. A recent collection of papers discusses the application of decision analysis techniques to a variety of hydrogeological problems (Freeze et al., 1992). James and Freeze (1993) used decision analysis techniques in predicting aquitard continuity. James and Gorelick (1994) have used decision analysis techniques to select sampling locations to delineate a dissolved phase contaminant plume. In this approach, Monte Carlo simulations of the contaminant plume are used to estimate probabilities of contamination at various locations and the maximum likely width of the contaminant plume. Data worth analysis is performed by estimating the expected reduction in the total cost of remediation and sampling that could be obtained by gathering additional samples. When the expected reduction in total cost is negative, characterization stops and remediation begins. A similar approach was used to delineate a gas phase plume by Peterson et al. (1993).

3. METHODOLOGY

Figure 1 gives an overview of our approach to delineating a DNAPL spill. The process is essentially a loop in which we start by simulating the DNAPL plume and condition the simulations to match previous observations. We then use the simulation results to construct a probability map of the DNAPL plume. Based on this probability map, we construct a decision analysis model which is used to determine which (if any) of the possible sampling points has a positive expected value in reducing the total cost of sampling and remediation. If additional data is required, we gather the data and use it to condition the simulations in the next iteration of the loop. If none of the potential sampling locations have positive expected value, we stop sampling and begin the remediation process.

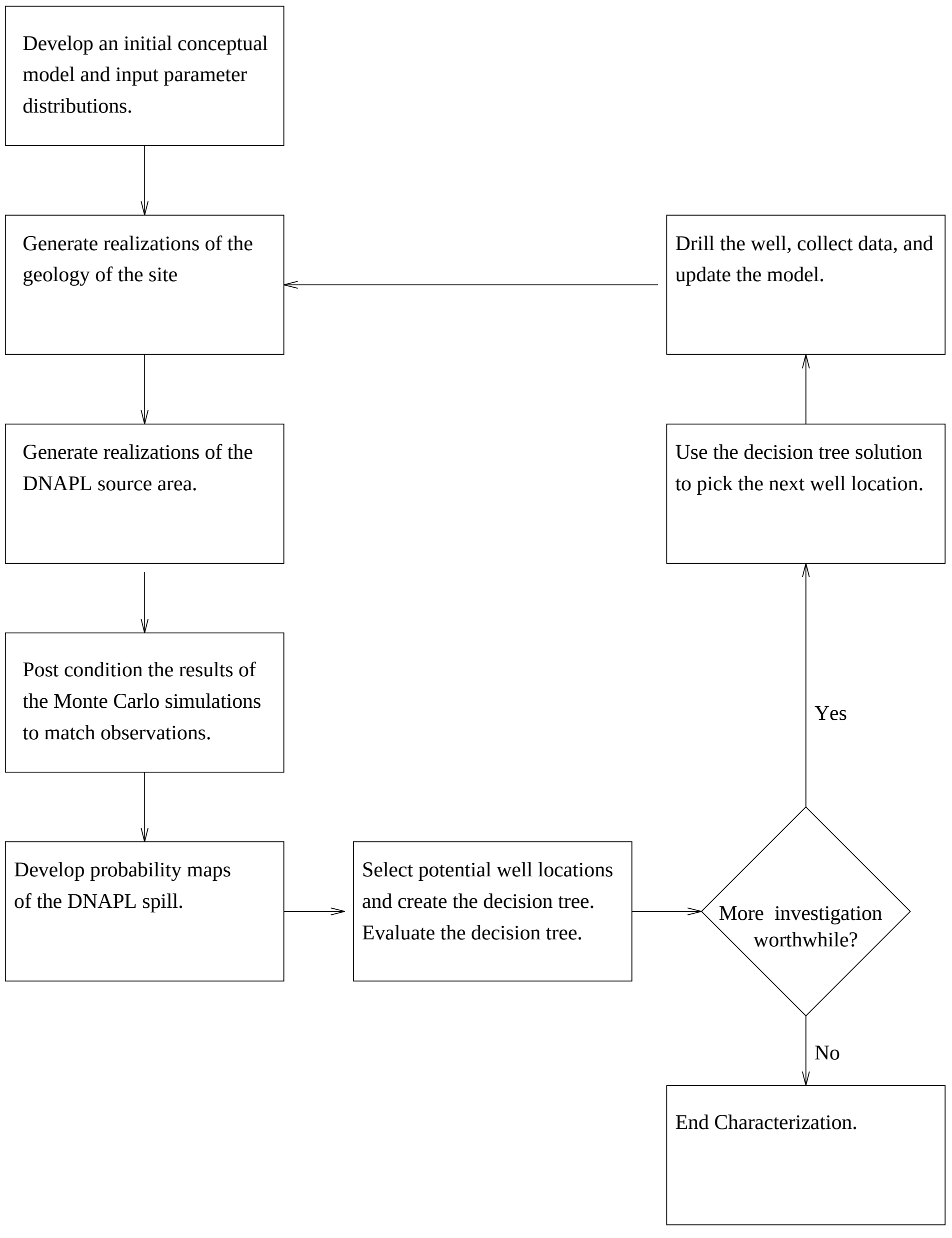

Figure 1: Flowchart for the Decision Making Process.

The process begins with an initial model based on any observations that may have been made during initial evaluation of the site. In order to begin the simulation phase, we need an initial conceptual model of the geology of the site, information about the type of DNAPL that was spilled, locations where the DNAPL was spilled, and the amounts of DNAPL that were spilled. Since it is unlikely that we will have the exact information, we will normally treat these parameters as random inputs to the simulation models. The distributions of these random inputs will, in most cases, have to be determined by subjective expert judgment.

Due to the high level of sensitivity of DNAPL migration to geological texture, any simulation approach used to trace DNAPL movement must accommodate discrete geological structure in a way that is relatively realistic. While there are numerous mechanisms for estimating the spatial arrangement of properties, few focus on accurately representing the curvilinear geometry that exists in most geological systems. Geometrical models explicitly accommodate these discrete structures. Consequently, it was decided that a geometrically-based model would be preferable for the first implementation of our approach. For this initial attempt to integrate our work, a computer code, BCS-3D (Webb, 1994), was used to produce estimates of the three-dimensional internal geometry of sediment units for braided-stream deposits.

BCS-3D uses a random-walk approach, which is a modification of previous attempts to simulate braided-stream geomorphic patterns (Howard et al., 1970; Krumbein and Orme, 1972; Rachocki, 1981; Webb, 1994), to describe the formation of braided-channel networks. The concept of hydraulic geometry (Church, 1972) is incorporated to translate a two-dimensional topological network to a three-dimensional topographic surface. A series of these surfaces is stacked vertically with some offset to produce a three-dimensional description of internal sedimentary architecture. Individual elements in the architecture are associated with specific sediment units based on a description of flow energy in the form of the Froude number (Harms et al., 1982). The simulations are derived from runs calibrated to a composite set of measurements from two field studies in systems with similar physical characteristics; the Ohau River in New Zealand (Mosley, 1982), and the Squamish River in British Columbia, Canada (Brierley, 1989). A more complete description of model development and calibration is given in Webb (1994).

We have chosen to use percolation models of DNAPL flow in this study for a variety of reasons; primarily because we expect the percolation model to more accurately reflect the physics of DNAPL flow at scales of interest than conventional multiphase flow codes (Glass et al., 1995). This allows us to incorporate more geological detail into our models. Another important reason is the massive computational effort required to use multiphase flow codes in a Monte Carlo framework.

In analyzing the results of these simulations, we have chosen to work with two-dimensional, "top view" projections of the three-dimensional simulations.

For the example problem discussed in this paper, in which the aquifer is shallow and of constant depth, this simplification of the problem is appropriate. In other situations, this simplification of the problem might not be appropriate. Although we could theoretically do all of our analysis in three full dimensions, the storage requirements would be completely impractical. For example, it would require approximately 15 gigabytes of storage to store the results of the 136,000 simulations of our example problem.

Once we have generated a large number of simulations of the DNAPL spill, we can use the simulation results to construct a "probability map," which shows our estimate of the probability that DNAPL is present in different parts of the site. For each point, we estimate the probability as the fraction of simulation runs in which the DNAPL reached that point. Similar probability maps have been used by Rautman and Istok (1996) and Istok and Rautman (1996).

In considering a probability map, it is important to remember that the probability map shows estimates of the probability of free phase or residual DNAPL at each location. Depending on the number of realizations used, there can be significant statistical uncertainty in these estimates. In particular, estimates of the 0% probability contour are extremely sensitive to the number of simulation replications used in computing the probability map. As we add more replications of the simulation, the 0% contour will steadily expand. For this reason, we have chosen not to use the 0% contour in our decision making. Instead, we select a fixed low probability, such as 0.5%, and use it in our decision analysis. Reliable estimates of such a contour can be obtained with a limited number of simulation replications.

Information from sampling wells can be incorporated into the probability map in a straightforward way. We condition the probability map by only considering those simulation replications which match all available observations of the DNAPL spill. In this paper, we assume that it is possible to determine precisely whether or not residual DNAPL is present at a given location. In conditioning simulations, we only take into account such DNAPL hits and misses. This simple scheme suffers from one major problem. As we gather more data, the number of replications that satisfy all of the conditions is sharply reduced. Thus, we may have to start with hundreds of thousands of replications of the simulation in order to obtain as many as one thousand replications that match a set of observations. More efficient approaches have been developed to condition some types of geostatistical simulations. However, to the best of our knowledge, no techniques have been developed to condition simulations of DNAPL flow on DNAPL hits and misses.

It would also be possible to condition the simulations on other observations, such as geological features in core samples. Since the BCS-3D model is incapable of conditional simulation, we have not explored this possibility.

We have assumed that the objective of a sampling scheme is to delineate the free phase and residual DNAPL with an acceptable degree of precision and in such a way as to minimize the total costs of delineation and remediation. In order to construct an optimal sampling scheme, we must have adequate models of the costs of sampling and the costs of remediation. In particular, these models should be able to forecast the cost of drilling sampling wells and the cost of remediation based on a probability map. A more sophisticated model would also incorporate human health risk and regulatory compliance. Clearly, these models will depend heavily on the particular characteristics of an individual site. However, we feel that it should be possible to construct adequate models of this type.

In solving our example problem, we have adopted a simple cost model. We chose the rule of remediating all areas of the probability map inside the 0.5% contour. The 0.5% contour was chosen as a surrogate for more sophisticated health risk or regularity compliance rules. Remediation costs are estimated at $1,000 per square meter, and monitoring wells, installed and sampled, cost $20,000 each.

In determining exactly where to gather sample information, many possible strategies exist. For example, we could simply ask a human expert to evaluate the probability map and determine where to sample next. Another very simple strategy is to set up a grid over the entire site and drill at each grid point.

In this paper, we consider a strategy based on decision analysis techniques (Clemen, 1991; Freeze et al., 1992; James and Gorelock, 1994). In determining the value of sampling at a location X, we start by using the probability map to estimate the probability of encountering DNAPL at location X. We next condition on a "hit" at location X and compute the resulting probability map. We also condition on a "miss" at location X. In either case, the additional information is likely to result in a conditional probability map with a reduced cost of remediation. Mathematically,

$$E[C_t]|\text{sample at X}=C_s+P(\text{hit})E[C_r|\text{hit at X}]+P(\text{miss})E[C_r|\text{miss at X}]$$

Here C_t is total cost, C_s is the cost of sampling, and C_r is the cost of remediation. For our example problem, C_r=(Area with P(DNAPL) > 0.5%)($1,000 per square meter).

We need to decide whether the expected reduction in remediation cost outweighs the cost of gathering the additional data. If $E[C_t]$|sample at X] is less than $E[C_t]$|no sample], then on average, it will be worthwhile to sample at location X. This difference in expected costs is the expected value of sample information (EVSI) (Clemen, 1991). When several sampling locations have positive EVSI, we select the location with the largest positive EVSI. When we reach a point where none of the potential sampling locations has positive EVSI, we should stop delineating the free phase and residual DNAPL and begin remediation.

The selection of potential sampling locations is an important issue. We could compute the EVSI at all possible sampling locations, or only at a more manageable subset of potential sampling locations. The process of computing the expected value of sample information at a point requires the computation of a conditional probability map, which is done by selecting all simulation realizations that match the condition at the proposed sampling location. This is somewhat time consuming. For the computational results reported in this paper, we have limited our sampling locations to 361 points on a five meter grid spacing.

4. RESULTS

In order to demonstrate the decision-making process described in the previous section, we performed a simulation experiment. This experiment is based on a hypothetical spill in a shallow aquifer. Our hypothetical DNAPL spill consists of between perchloroethen (PCE), an organic solvent. The spill volume is uniformly distributed between 3,785 liters (1,000 gallons) and 11,355 liters (3,000 gallons). The spill location is at a random point uniformly distributed with a twenty meter by twenty meter square at the center of the site. The site has a 4.5-meter-thick aquifer with geology that is assumed to consist of braided-stream deposits. The deposits are oriented primarily in the north-south direction. The site has a negligible vadose zone.

The geology and DNAPL flow simulations were performed on a 100 by 100 by 90 grid, in which each grid cell represented a 1 meter (horizontal) by 1 meter (horizontal) by 5 cm (vertical) section of the site.

We first generated two realizations of the spill to be used as example "target spills." A total of 136,458 simulation replications were generated in the time available, each consisting of a unique geology and DNAPL spill. For each target spill, we used the procedure described in the previous section to delineate the DNAPL. We also asked a human expert to delineate the same spill.

4.1 The First Example

Figure 2 shows the geology for our first example. Figure 3 shows the hypothetical DNAPL spill. Figure 4 shows a two-dimensional "overhead" view of the hypothetical DNAPL spill.

We first used the procedure described in section 3 to delineate the spill. Figure 5 shows the initial probability map. Figure 6 shows the probability map after 29 wells.

This probability map is based on 11,442 realizations that matched the observations at each of the 29 sampling locations.

The procedure terminated after 29 wells with a 0.5% probability contour that covered 1,733 square meters. The total cost of sampling wells and the remediation scheme comes to $2.3 million. The actual area of the hypothetical spill was 268 square meters. Figure 7 shows the hypothetical spill and the 0.5% contour. Note that hypothetical spill is completely contained within the 0.5% contour.

We next asked a human expert to delineate the spill. For each well location selected by the expert, the expert was given information on whether or not there was DNAPL present and at what depth the DNAPL was found. Figure 8 shows the results of the human expert's work. The solid lines enclose the area that the expert designated for remediation. The expert used a total of 39 wells, and designated an area of 588 square meters for remediation. The total cost for sampling and remediation came to $1.4 million. Figure 9 shows the hypothetical DNAPL spill and the area delineated by the human expert. Unfortunately, the human expert was overly confident—the hypothetical spill extends beyond this boundary at several points.

4.2 The Second Example

Figure 10 shows the geology for our second example. Figure 11 shows the hypo-thetical DNAPL spill. Figure 12 shows a two-dimensional "overhead" view of the hypothetical DNAPL spill.

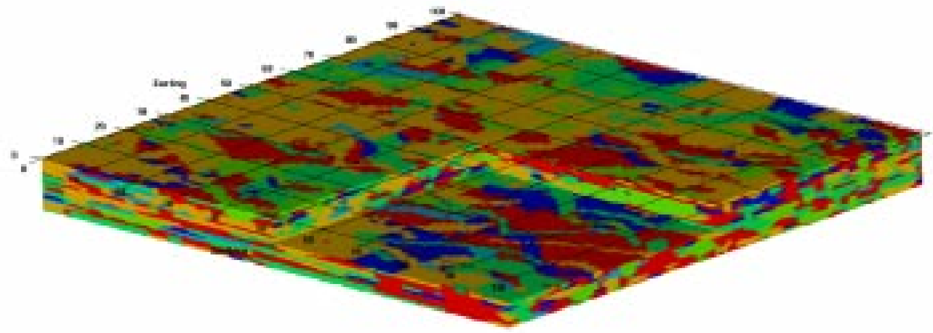

Figure 2: Example 1, Geology.

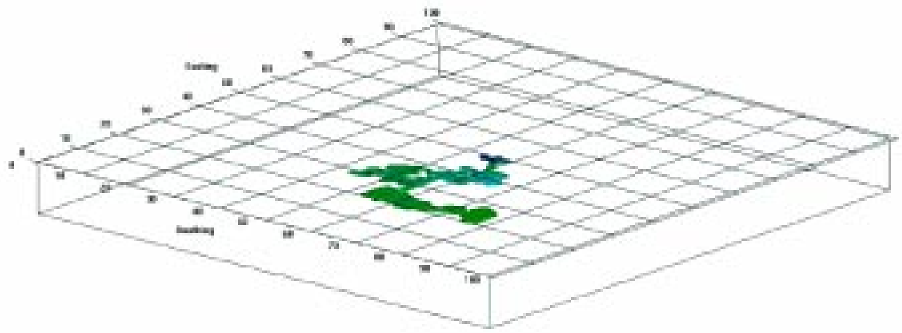

Figure 3: Example 1, DNAPL spill.

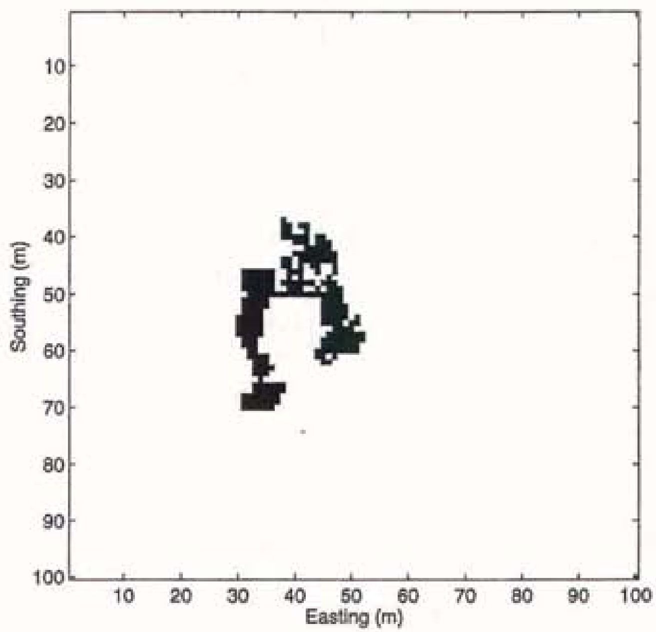

Figure 4: Example 1, DNAPL spill.

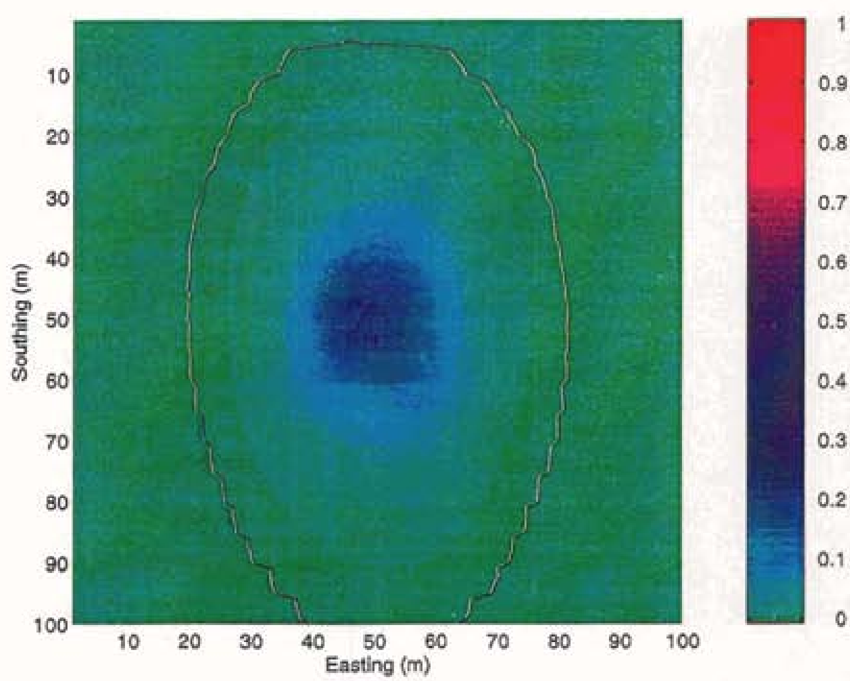

Figure 5: Example 1, Initial Probability Map, showing probability of DNAPL occurrence. The contour line is drawn at p=0.5%.

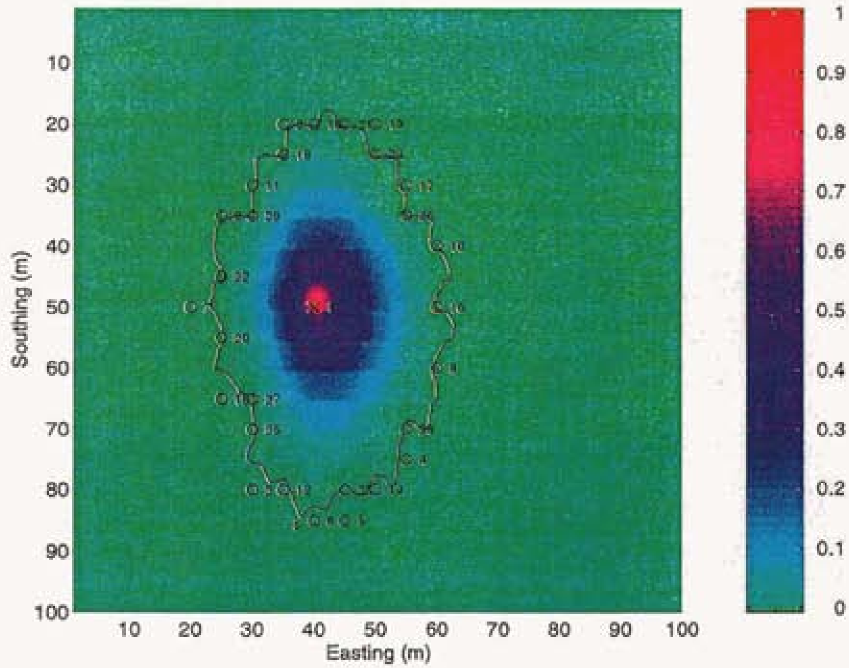

Figure 6: Example 1, Final Probability Map, showing probability of DNAPL occurrence. The contour line is drawn at p=0.5%. "x" indicates a DNAPL hit. "o" indicates a DNAPL miss. Numbers refer to sample ID.

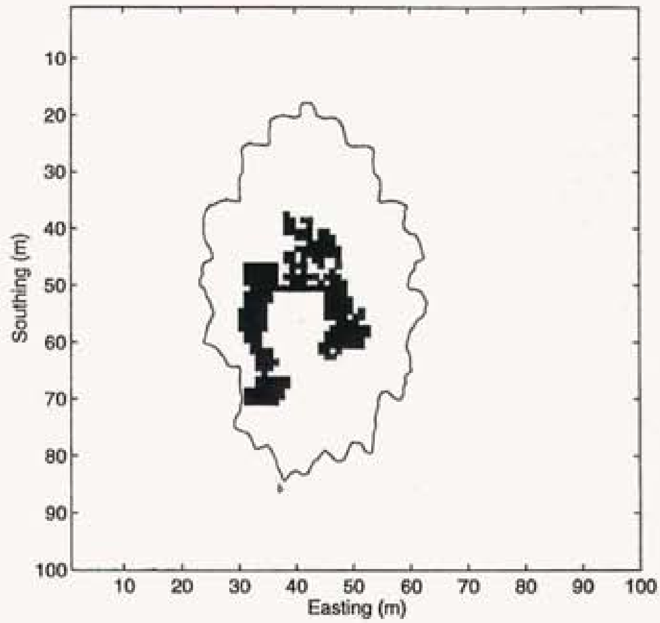

Figure 7: Example 1, Actual DNAPL spill in relation to the p=0.5% contour.

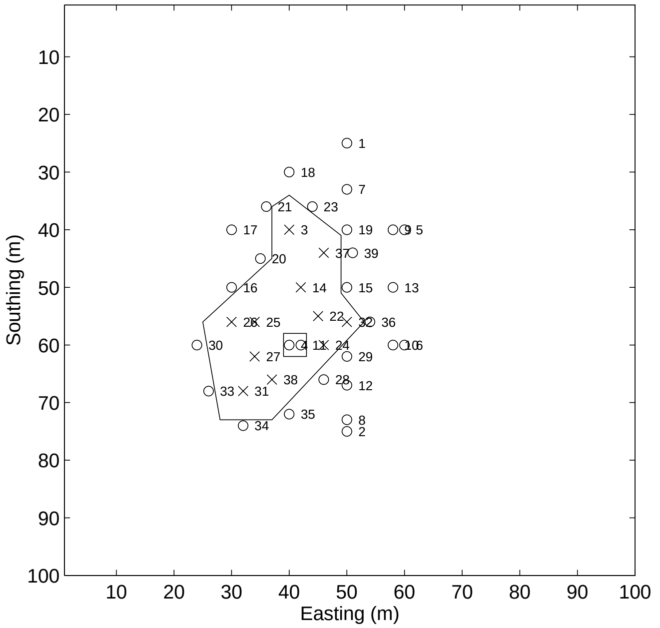

Figure 8: Example 1, Human Expert. “x” indicates a DNAPL hit. “o” indicates a DNAPL miss. Numbers refer to sample ID.

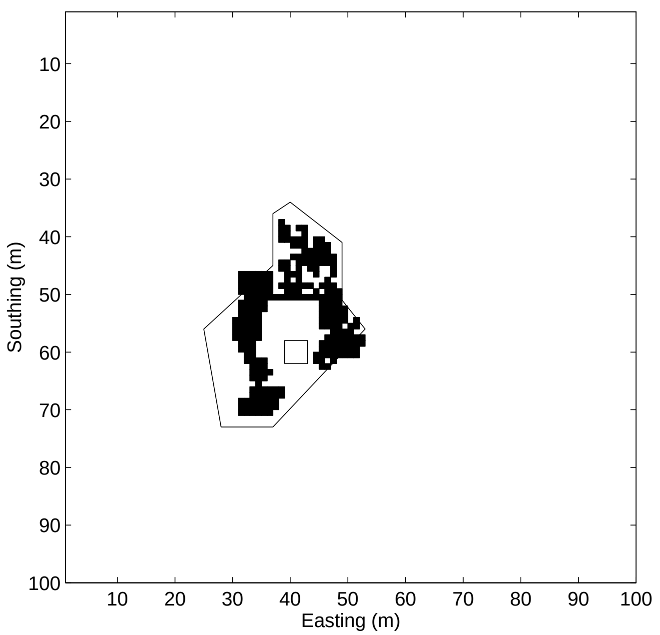

Figure 9: Example 1, Actual DNAPL spill in relation to the area delineated by the human expert.

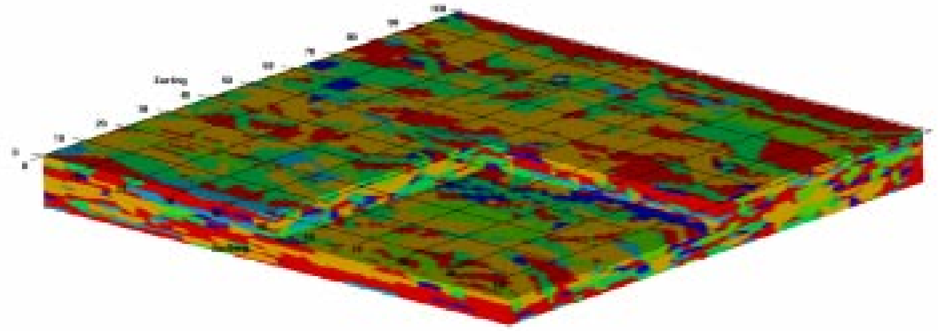

Figure 10: Example 2, Geology.

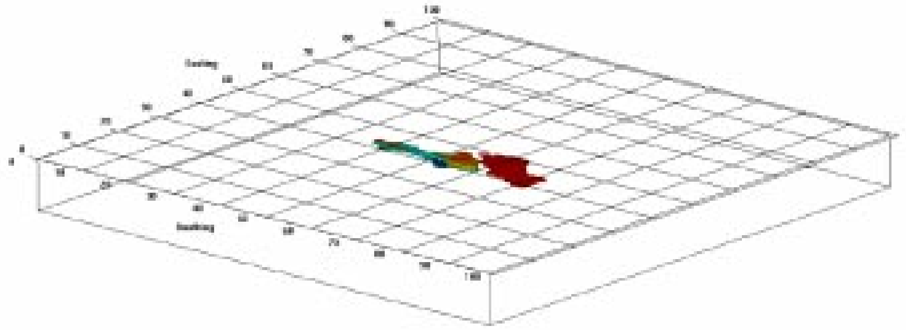

Figure 11: Example 2, DNAPL spill.

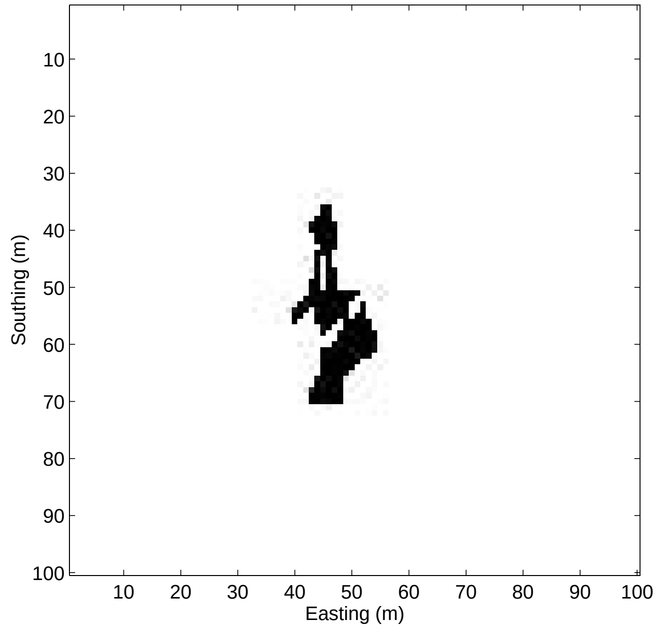

Figure 12: Example 2, DNAPL spill.

Again, we used the procedure described in section 3 to delineate the spill. Figure 13 shows the initial probability map. Figure 14 shows the probability map after 25 wells. Unfortunately, after 25 wells, our initial pool of over 130,000 realizations had been reduced to only 64 realizations. Thus, we had to terminate the procedure early because of the lack of suitable simulation realizations. After 25 wells, the 0.5% probability contour covered 2,197 square meters. The total cost of sampling wells and the remediation scheme comes to $2.7 million. The actual area of the hypothetical spill was 202 square meters. Figure 15 shows the hypothetical spill and the 0.5% contour. Note that hypothetical spill is completely contained within the 0.5% contour.

We next asked our human expert to delineate the spill. For each well location selected by the expert, the expert was given information on whether or not there was DNAPL present and at what depth the DNAPL was found. For this example, the human expert was also given conditional probability maps after each well. Figure 16 shows the results of the human expert's work. The solid lines enclose the area that the expert designated for remediation. The expert used a total of 25 wells, and designated an area of 807 square meters for remediation. The total cost of sampling and remediation came to $1.3 million. Figure 18 shows the hypothetical DNAPL spill and the area delineated by the expert. This time, the hypothetical spill was entirely contained within the area designated for remediation by the expert. However, as the probability map in Figure 17 shows, there were other simulation realizations that matched the human experts observations and went beyond the area designated for remediation. In fact, the 0.5% contour on this map includes an area of 3,109 square meters. Thus, if the human expert had used the same 0.5% contour to designate the area to be remediated, the expert's solution would have cost $3.6 million.

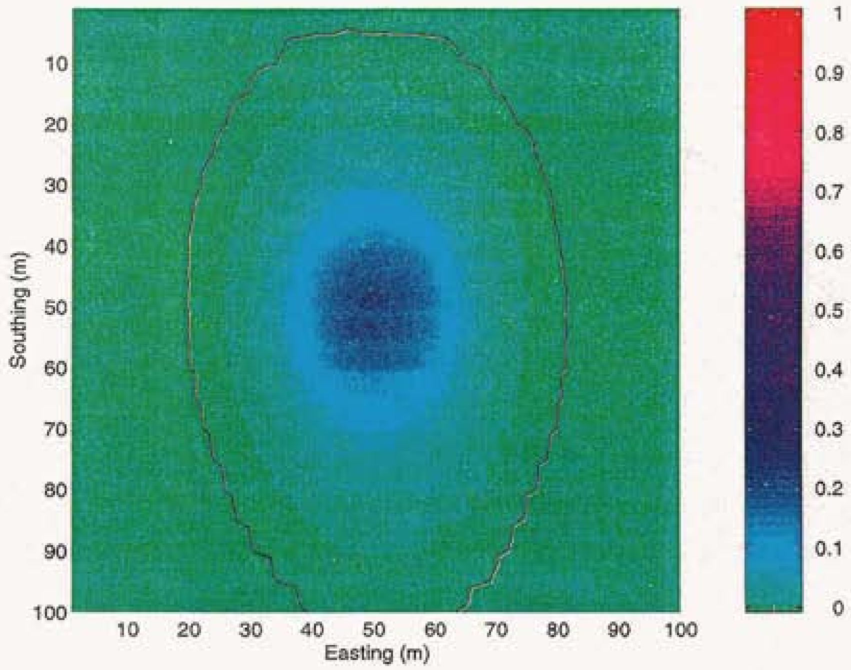

Figure 13: Example 2, Initial Probability Map, showing probability of DNAPL occurrence. The contour line is draw at p=0.5%.

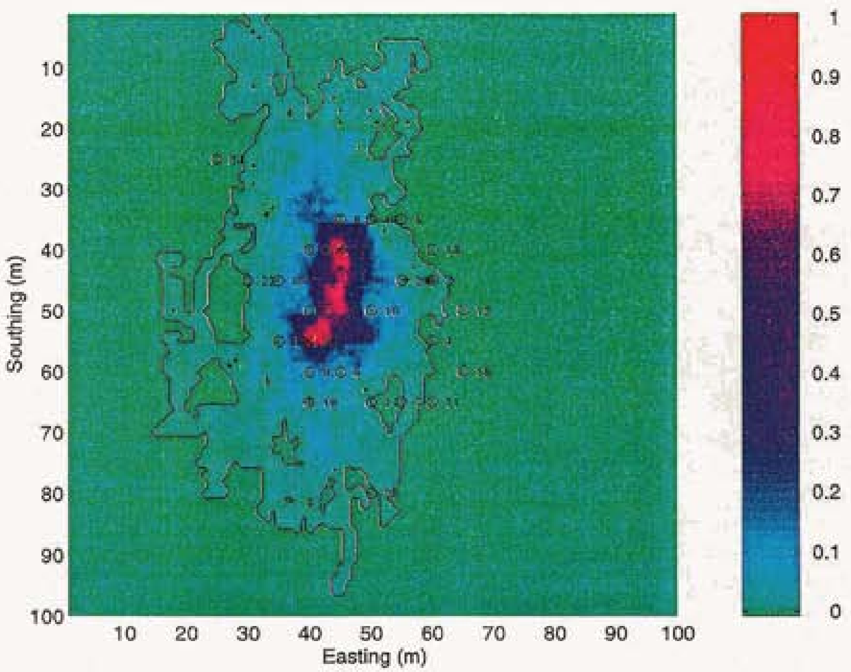

Figure 14: Example 2, Final Probability Map, showing probability of DNAPL occurrence. The contour line is drawn at p=0.5%. "x" indicates a DNAPL hit. "o" indicates a DNAPL miss. Numbers refer to sample ID.

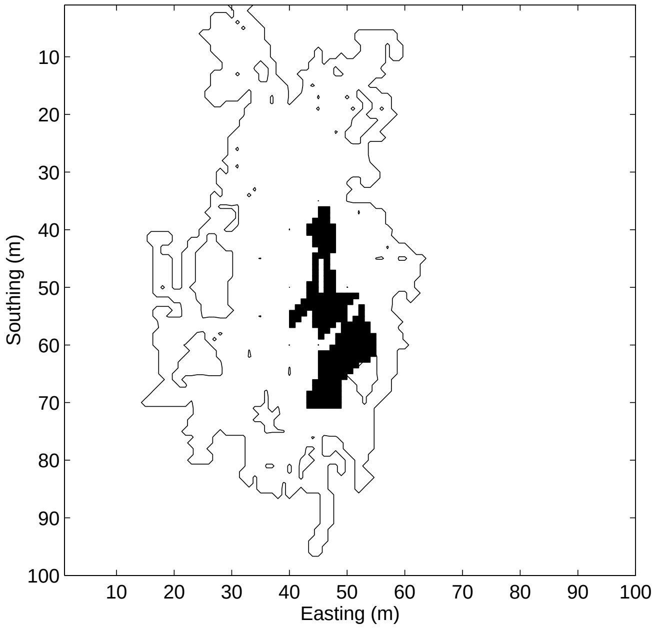

Figure 15: Example 2, Actual DNAPL spill in relation to the p=0.5% contour.

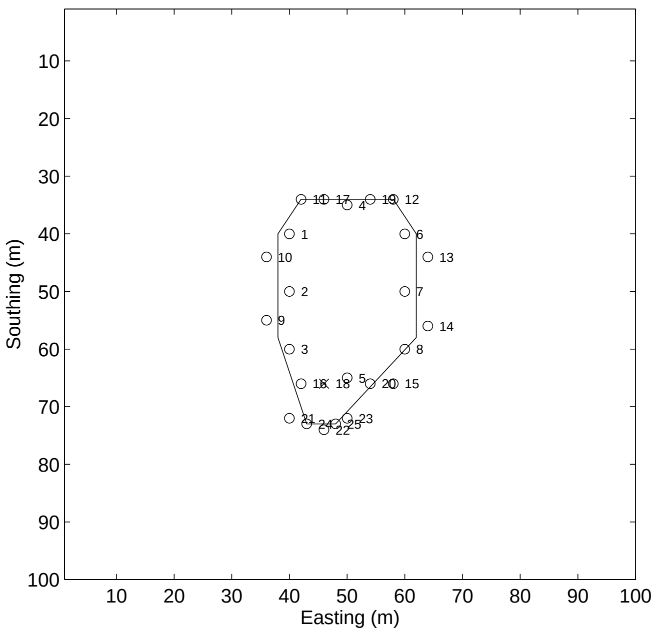

Figure 16: Example 2, Human Expert. "x" indicates a DNAPL hit. "o" indicates a DNAPL miss. Numbers refer to sample ID

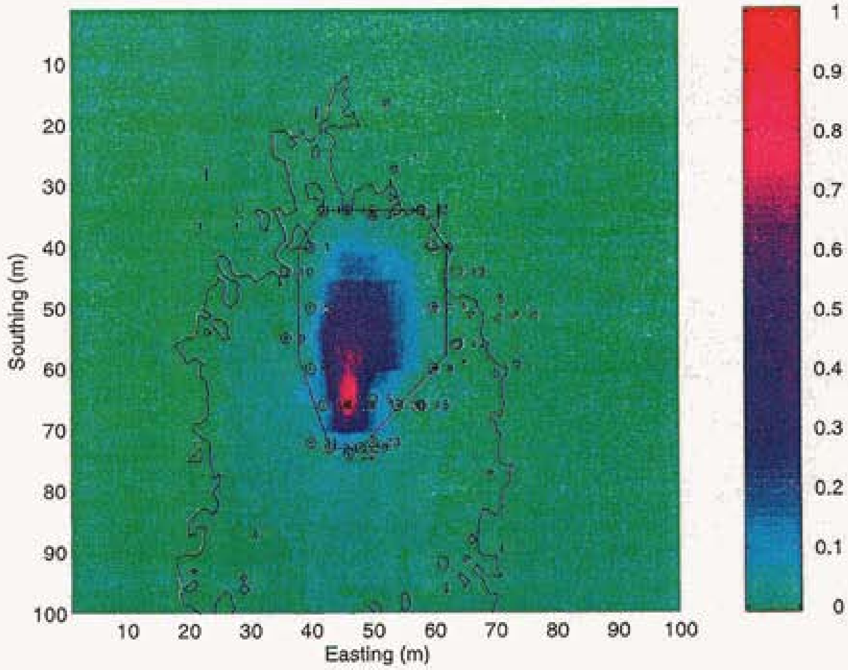

Figure 17: Example 2, Human Expert, Final Probability Map, showing probability of DNAPL occurrence. The contour line is drawn at p=0.5%. "x" indicates a DNAPL hit. "o" indicates a DNAPL miss. Numbers refer to sample ID.

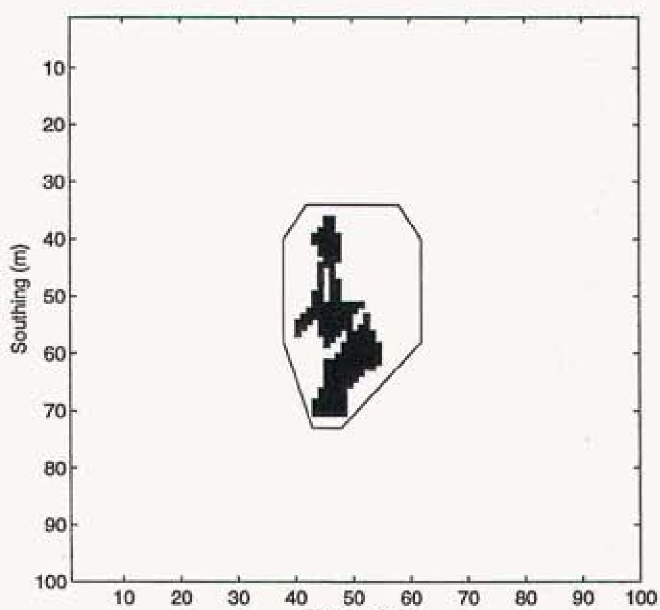

Figure 18: Example 2, Actual DNAPL spill in relation to the area delineated by the human expert.

5 DISCUSSION AND CONCLUSIONS

This paper describes an iterative procedure for delineating a DNAPL spill that combines information from sampling wells and from simulations of a site's geology with a percolation model of DNAPL flow. We have implemented this procedure on a Cray T-3D and used it to delineate a hypothetical DNAPL spill.

The results of this computational experiment indicate that the decision-analysis approach can be used to reduce the total cost of sampling and remediation for DNAPL spills. Our results are similar to those of James and Gorelick (1994) in that the decision analysis strategy is effective in reducing total cost. However, we have found that our problem is more difficult than the problem studied by James and Gorelick. It typically takes more than 25 sampling wells for either a human expert or our automated approach to delineate a hypothetical DNAPL spill, whereas James and Gorelick (1994) were able to delineate their dissolved phase contaminant plume with as few as six wells. This is partly because the DNAPL flow studied in this paper is much more complicated than the dissolved phase contaminant plume considered by James and Gorelick (1994). Another important difference is that our problem involves the delineation of a two-dimensional spill instead of the determination of the width of a required capture zone.

An important advantage of our approach is that it provides an objective criterion for selecting the area to be treated by a remediation scheme for free phase and residual DNAPL. Although we would like to use a more sophisticated measure that combines elements of cost, health risk, and other factors, the use of a fixed probability contour does provide a reasonable surrogate for these objectives. In contrast, a human expert can select an area for remediation, but cannot provide decision makers with a quantitative indication of the likelihood that this area includes the entire DNAPL spill. It is easy for a human expert to become overconfident and specify an area for remediation that might not contain the entire DNAPL spill.

It should be noted that it is possible to have an expert select well locations and combine this with the use of a fixed probability contour to select the area to be remediated. In our second example, we provided the human expert with probability maps after each well. The 0.5% probability contour that resulted from the expert's sampling turned out to be somewhat larger than the contour that resulted from our automated procedure.

The use of a massively parallel processor was critical in achieving our results—it would have taken over 50,000 hours of simulation on our Sun workstation to obtain the 136,458 simulation realizations used in this study. With the aid of the Cray T3-D, we were able to compute these simulation runs in a few days. However, even this very large number of realizations was inadequate—the simple scheme of throwing out realizations that don't match observations is clearly an impractical way to condition the simulation on large numbers of observations. Further work is needed on ways to generate conditional simulations of DNAPL flow.

There are a number of other ways in which this research could be extended. The geological simulation used in this study is applicable only to situations in which the geology consists of braided stream deposits. There is a need to extend this approach to other geological situations. We have focused on the problem of delineating free phase and residual DNAPL. There is also a need to delineate dissolve phase DNAPL. This would involve the use of conventional models for the transport of dissolve phase contaminants. Finally, the specific cost model used in our study would clearly need to be adjusted for use in any real situation.

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