Chapter 1
A Simulation and Decision Analysis Approach to Locating DNAPLS in Subsurface Sediments*

Brian Borchers† Stephen H. Conrad‡ Roger Cox‡ Robert J. Glass Jr.‡
Erik K. Webb‡

Abstract

We present a strategy for delineating DNAPL spills that combines probabilistic simulations of DNAPL spills with a decision analysis model to pick optimal locations for sampling wells. Our strategy is an iterative process of simulating the DNAPL spill, selecting new locations for sampling wells, gathering data, and then using the data to condition further simulations. 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 a simulated DNAPL spill.

Subsurface contamination in the form of dense non–aqueous phase liquids poses a significant and yet unresolved remediation problem. DNAPLs such as the chlorinated organic solvents TCE, PCE, TCA, and carbon tetrachloride have been used for many years as de–greasers and in many industrial applications across the nation. DNAPL spills are a common problem at Superfund sites and other sites managed by the DOE, DOD, and private entities.

While many of the techniques needed to delineate DNAPL spills 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. We present a strategy for delineating DNAPL spills that combines probabilistic simulations of DNAPL spills with a decision analysis model to pick optimal locations for sampling wells. In this paper, we describe our approach and present the results of a preliminary version of our model.

Procedure

Our strategy is an iterative process of simulating the DNAPL spill, selecting new sampling well locations, gathering data, and then using the data to condition further simulations. As we iterate through this process, data worth analysis is used to determine an appropriate stopping point. A flowchart of this procedure is shown in figure 1.

A computer code, BCS–3D [12], is used to produce realizations 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 patterns [8, 10, 11], to describe the formation of braided–channel networks. The concept of hydraulic geometry [1] is incorporated to translate a two-dimensional topological network

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†Department of Mathematics, New Mexico Tech, Socorro, NM 87801.

‡Sandia National Laboratories, Albuquerque, NM.

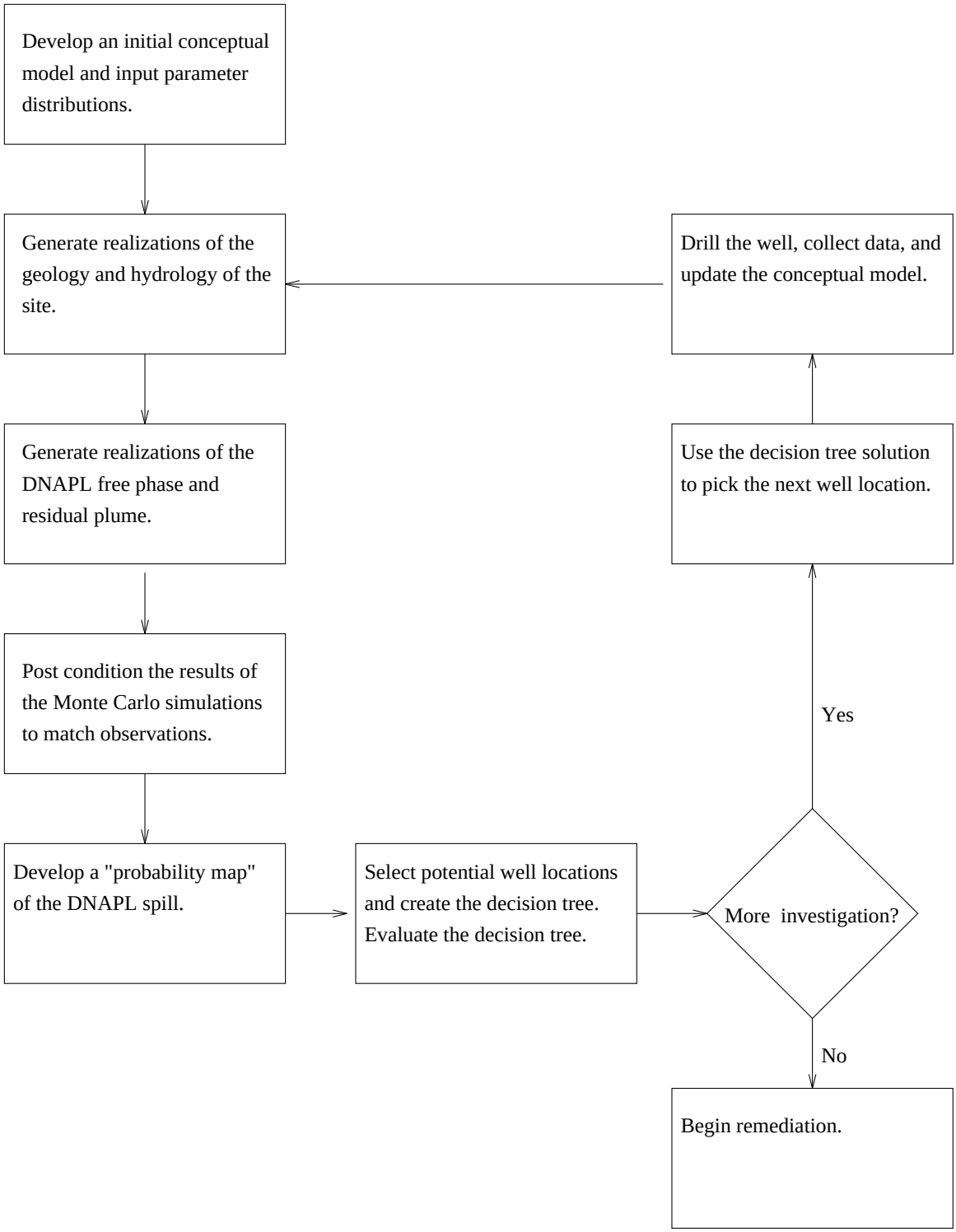

FIG. 1. *The Decision Making Process.*

to a three-dimensional topographic surface. This approach was selected because of its ability to realistically simulate the geologic structure of our sample problem. However, other approaches to simulating the geology might be more appropriate for other sites.

An up–scaled invasion percolation model [7] is used to simulate DNAPL flow. Wilkenson and Willemsen (1983) introduced invasion percolation (IP) models of fluid flow in porous media. IP has been applied to immiscible flow in porous media by a number of researchers [2] and has been shown to effectively model displacements in two-dimensional pore networks in micromodels where a non–wetting fluid invades a wetting fluid [13]. For wetting fluid invasion, macroscopic fronts typically form and IP must be modified to reflect interfacial smoothing induced by pore geometry [4, 5, 6]. Our model upscales the invasion percolation approach to larger blocks, with dimensions on the order of tens of centimeters.

We have chosen to use a percolation model of DNAPL flow in this study for a variety of reasons. Our primary reason is that we expect the percolation model to more accurately reflect the physics of DNAPL flow than conventional multiphase flow codes [7]. Another important reason is that our percolation model is much faster than the multi–phase flow codes traditionally used to simulate DNAPL flow.

We use BCS–3D and the invasion percolation model to generate a large number (thousands to tens of thousands) of realizations of the site geology and DNAPL free phase and residual plume. This process can easily be done in parallel on a network of workstations or a massively parallel processor. The realizations can be post conditioned by removing any realization that is not in agreement with data that has been gathered. We then combine the remaining realizations into a "probability map", which shows our estimate of the probability that DNAPL is present at each point on the map.

In picking well locations, we make use of a decision tree model that incorporates probabilities of DNAPL "hits" and "misses" that have been obtained from the simulations. The model also incorporates the expected cost of drilling sampling wells and the cost (per unit area) of remediation. We then pick the well location that leads to the greatest expected decrease in the total cost of sampling and remediation. If the expected decrease in the total cost is less than the cost of gathering additional information, we stop the characterization process and begin remediation. This is similar to the data worth analysis described in [3, 9].

Results

Our hypothetical DNAPL spill consists of 10,000 gallons of an organic solvent. The spill location was at an unknown point somewhere within a ten meter square at the center of the site. The site has a five meter thick aquifer with geology that is assumed to consist of braided deposits.

We first generated one realization of the site geology and DNAPL spill. A map of the plume is shown in figure 2a. We treated this plume as the "real" spill. We then generated 4,000 simulated DNAPL spills. The initial probability map for our test case is shown in figure 2b. On this map, the darker regions represent areas where there is a high probability that the DNAPL is present, while lighter regions represent a low probability of DNAPL presence.

We then began an iterative process of selecting sampling well locations, obtaining information from the "real" plume, and conditioning future simulations on the information from sampling wells. Figure 2c shows the probability map after three iterations. Two sampling wells have hit the DNAPL, while one well missed the plume. We have substantially reduced the uncertainty in the extent of the DNAPL plume.

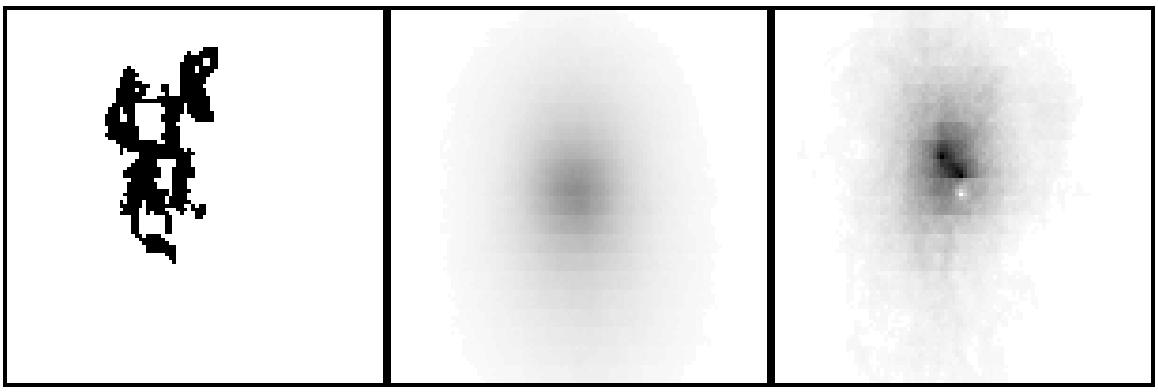

FIG. 2. *A hypothetical DNAPL spill*

Conclusions and Future Work

We have developed 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. Our approach optimizes the collection of additional data so as to minimize the total cost of delineating and remediating the spill. This procedure has been implemented in software and tested on a small example. We are in the process of validating the up–scaled invasion percolation model with laboratory experiments. We are also in the process of porting the simulation codes to an Intel Paragon MPP so that we may efficiently generate tens of thousands of realizations. Finally, we are preparing to validate the procedure with a study of an actual spill at a DOE site in Paducah, Kentucky.

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