A Stochastic Method for Characterizing Ground-Water Contamination

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Abstract
It is becoming widely recognized that field-scale ground-water contaminant plumes are irregular and difficult to predict. Factors which complicate the characterization of such plumes include geological variability, data limitations, and uncertainties about the source of contamination. This paper describes a new approach to site characterization which accounts for variability and uncertainty in a systematic way. The site characterization procedure extracts more information from limited data by combining field measurements with predictions from a stochastic ground-water model. The model provides prior estimates of the mean and standard deviation of solute concentration throughout a contaminated site. These estimates are updated whenever new measurements of hydraulic conductivity, head, and/or concentration become available. The updated concentration standard deviation estimates may be used to guide the placement of sampling wells and to evaluate the accuracy of the site characterization. If updating and data collection are carried out sequentially, over a series of discrete sampling rounds, the sampling network can evolve in response to new information. A case study described in the paper illustrates how the characterization procedure can be applied to a typical field site.

1. Introduction
Recent field studies indicate that real-world contaminant plumes are highly irregular and difficult to predict (Mackay et al., 1986; LeBlanc et al., 1991; Garabedian et al., 1991). Figure 1 shows the complex structure of some typical solute plumes observed in a tracer test carried out at Otis Air Force Base on Cape Cod (LeBlanc et al., 1991). In another field experiment described by Sudicky et al. (1983), the tracer plume split into separate parts which drifted off in different directions, contradicting the predictions of nearly any conventional model of contaminant transport. Such results suggest that small-scale hydrogeological variability is more significant than has been generally assumed. The problem of predicting solute movement is further complicated by chemical reactions and sorption, which have been observed to modify field-scale transport in unexpected ways (Mackay and Cherry, 1989). Nonaqueous phase liquid contaminants and fractured geological media present additional problems which are important but are beyond the scope of this paper.

Several factors make it difficult to characterize the field-scale transport of soluble contaminants. First, the subsurface environment is very heterogeneous—geological properties vary dramatically over space and recharge can vary over both space and time. Second, hydrogeological properties and contaminant concentrations are expensive to measure and can, for the most part, only be observed at scattered wells or boreholes. Third, it is frequently difficult to determine the location and composition of the source (or sources) of contamination. All of these problems are familiar to the site managers and consultants responsible for site assessments and cleanup programs (see, for example, Freeze and Cherry, 1989). Uncertainties about the way contaminants move in the natural environment translate into problems for both risk assessment and remediation. If we do not detect contamination because our sampling network is poorly designed, we may greatly underestimate the risk to human health. If we are unable to accurately locate a subsurface contaminant plume, it is less likely that cleanup efforts will be successful.

This paper describes a new approach to site characterization which addresses some of the problems listed above. Our approach attempts to provide improved descriptions of subsurface conditions by combining field measurements with model predictions (Graham and McLaughlin, 1989a, b; 1991). Although field measurements convey important local information, they are usually too limited to provide a good synoptic picture of subsurface conditions. Conversely, models tell us much about the physical and chemical processes which control solute movement but they generally do not account for the heterogeneity encountered at real field sites. When models and measurements are combined, we can obtain a physically reasonable site description which makes the most of each source of information. This description can take many forms, including multidimensional contour maps of solute concentration and estimates of contaminant fluxes across site boundaries.

Of course, contour maps and flux estimates constructed from a limited amount of data are uncertain, no
Fig. 1. Contoured concentrations (in ppm) of solute plumes observed during tracer tests at Otis Air Force Base, Cape Cod, Massachusetts (from LeBlanc et al., 1991). (a) Areal distribution of maximum concentrations; and (b) Vertical concentration distribution in a centerline section at 174 days after injection.

matter how they are derived. Our approach enables us to evaluate the uncertainty of these estimates. Estimation uncertainty depends on the heterogeneity of the subsurface environment as well as the quantity and quality of data available. Better predictions are obtained at a relatively uniform site where field measurements are plentiful than at a heterogeneous site where measurements are limited. The uncertainty assessments provided by our site characterization procedure can be conveyed in a number of different ways. One of the most informative is to plot uncertainty contours (expressed in terms of the estimation error standard deviation) throughout the site. The resulting maps indicate where predictions are most suspect and where additional field measurements will be most beneficial. They may
be used to guide field monitoring programs, to assess risks, and to plan remediation activities.

We begin by summarizing our approach to site characterization. Next we illustrate this approach with results obtained at a coal tar disposal site in upstate New York. The field study provides valuable information about the strengths and limitations of our characterization procedure. We conclude with a discussion of ways in which the procedure could be improved and applied in the future.

2. A Systematic Approach to Site Characterization

Although the concept of combining measurements and model predictions sounds reasonable, it may not be obvious just how this should be done in practice. We adopt a statistical approach which is based on Bayesian estimation theory (Schweppe, 1973). This theory treats data collection as a way of reducing the uncertainty associated with idealized models of the natural world. In order to apply Bayesian concepts to site characterization, we need to identify the sources of uncertainty which have the greatest influence on solute transport. At most sites these include spatial variations in hydraulic conductivity, spatial variations in chemical retardation and reaction parameters, spatial and temporal variations in recharge, and uncertainty about the source of contamination. We can use mathematical models to determine how uncertainties in these “input variables” translate into uncertainties in “dependent variables” such as hydraulic head and solute concentration. Uncertainty is quantified in terms of statistical quantities such as means, variances, and correlation scales.

Our statistical analysis of ground-water flow and transport provides a concise description of the subsurface environment at a heterogeneous field site. This “prior” description can be improved (or updated) when field measurements become available. Measurement updating works best when it is carried out sequentially, over several discrete stages. In this case, the updated description from one stage becomes the prior description for the next. Sequential updating allows the sampling network to evolve over time in response to new information. The updated statistics obtained after several successive sampling rounds may be used both to characterize existing subsurface contamina- tion and to predict the likely distribution of contamination in the future.

The following paragraphs discuss each part of our characterization procedure in more detail. Additional information is provided in a series of recent papers by Graham and McLaughlin (1989a, b; 1991) and Li and McLaughlin (1991).

2.1 Describing Natural Heterogeneity

The types of natural heterogeneity observed in the real world are rarely simple, as is illustrated in the log hydraulic conductivity plot reproduced in Figure 2. This shaded contour plot was constructed from permeameter measurements of 650 small (approximately 10 cm diameter by 10 cm long) cores removed from a vertical section of highly cemented Caliche soil in southern New Mexico. The section spanned an area of only 20 m by 6 m, but the conductivity measurements range over four orders of magnitude. Moreover, these values do not reveal any obvious spatial structure, such as horizontal layering. The spatial correlation scales are only a few meters in the horizontal and about 50 cm in the vertical.

Complex patterns of heterogeneity such as the one shown in Figure 2 can be represented probabilistically if the variable in question is assumed to be a spatial (or temporal) function drawn at random from an infinite population of physically plausible alternatives. Instead of trying to identify the particular function found at a given site, we can work with the statistical properties of the underlying population. The statistical description can be made more precise if the variable of interest is observed at a number of discrete sampling points. In this case the population membership can be restricted to functions which are able to reproduce measured values (within sampling error).

It is possible to obtain limited amounts of information on hydraulic conductivity variability from soil samples or hydraulic tests. This information can serve as a guide for selecting an initial set of hydraulic conductivity statistics (e.g., a constant mean and a stationary spatial covariance or spectral density function). The statistics of other uncertain input variables (e.g., recharge, retardation and biodegradation rates, and source composition) are more difficult to estimate from commonly available field data and must usu-

Hydraulic Conductivity in cm/day

- below 25
- 25 to 100
- 100 to 250
- 250 to 500
- 500 to 1000
- above 1000

Fig. 2. Contoured log_{10} hydraulic conductivity values obtained from soil samples collected at an experimental site near Las Cruces, New Mexico (data from Wierenga et al., 1989; conductivity units are cm/day).
the measurement does not provide much information about the estimation point and the updated estimated will be close to the prior. On the other hand, if the correlation is high, the measurement is more informative and the updated estimate will be close to the measured value. Intermediate correlations give estimates which are somewhere between prior and measured values.

The same procedure can be used to update estimates of one variable with measurements of another. So, for example, hydraulic conductivity and velocity estimates at one location could both be updated with head observations taken at another location. The general expressions for the updated means and covariances obtained from a single measurement are:

\[ \tilde{u}(x) = \bar{u}(x) + W(x,x_m) \left[ v^*(x_m) - \bar{v}(x_m) \right] \]  

\[ \text{Cov}[u(x),v(y)|v^*(x_m)] = \text{Cov}[u(x),v(y)] - W(x,x_m)\text{Cov}[v(x_m),v(y)] \]

where the weighting function \( W(x,x_m) \) is given by:

\[ W(x,x_m) = \frac{\text{Cov}[u(x),v(x_m)]}{\text{Cov}[v^*(x_m),v^*(x_m)]} \]

Here \( \bar{u}(x) \) and \( \bar{u}(x) \) represent prior and updated means of the variable \( u(x) \) estimated at location \( x \) while \( \bar{v}(x_m) \) and \( v^*(x_m) \) represent prior and measured values of another variable \( v(x) \) observed at location \( x_m \). The symbols \( \text{Cov}[u(x),v(y)] \) and \( \text{Cov}[u(x),v(y)|v^*(x_m)] \) represent prior and updated covariances between \( u(x) \) and \( v(y) \), where \( x \) and \( y \) are two generic locations and \( \text{Cov}[u(x),v(y)|v^*(x_m)] \) is read "the covariance of \( u(x) \) and \( v(y) \), given the measurement \( v^*(x_m) \)." Note that the uncertainty in an estimated concentration value (as measured by its variance) decreases when it is updated with new measurements. This is confirmed by (6) if \( v(y) \) is set equal to \( u(x) \). The degree of uncertainty reduction obtained at any given time and location depends on the configuration of the measurement locations and on the heterogeneity of the site. More extensive discussions of Bayesian updating are provided in Schweppe (1973), Maybeck (1979), Bencala and Seinfeld (1979), and Graham and McLaughlin (1989a, b).

2.4 Designing a Sequential Monitoring and Characterization Program

The uncertainty reduction achieved during Bayesian updating is a convenient measure of the information provided by a field sampling program. Consequently, programs that yield more uncertainty reduction for a given expenditure are generally preferred. This concept can be used to guide the sampling design decisions that must be made during a site characterization. If the characterization is carried out sequentially, over a series of discrete sampling rounds, a map of the most recently obtained concentration variance (or standard deviation) may be used to identify the areas where uncertainty is greatest at any given round. These areas are the most promising locations for new sampling wells. When measurements are collected at the new wells, the variance map may be updated and the next set of sampling locations selected. A sampling design based on progressively updated variances can adapt to new field information if the perturbation equation used to derive prior statistics is continually relinearized about the best available mean estimates. This type of adaptive design strategy allocates limited sampling resources more efficiently than an approach which selects all well locations at the beginning of the site characterization, before field data become available (Graham and McLaughlin, 1989b).

2.5 Summary

We can now summarize the site characterization procedure outlined in the previous paragraphs. First, we introduce a probabilistic description of natural heterogeneity at the field site. Second, we derive prior statistics which concisely describe how geological properties, hydrologic variables, and contaminant concentrations are related. Third, we develop a procedure for updating our statistical description of the site whenever field data become available. Finally, we carry out a sequential program of data collection and updating, progressively developing a better and better characterization of subsurface conditions. These concepts are illustrated in the field application described in the next section.

3. Application to a Coal Tar Disposal Site

3.1 Description of the Field Site

During 1989 and 1990 we applied the site characterization procedure described above to a coal tar disposal site in upstate New York. Figure 4 shows a plan view of the site with the modeled area superimposed. The unconfined ground-water aquifer at this rural site is composed of unconsolidated glacial materials. The shallow water table lies approximately 3 meters below the ground surface, which slopes down to a seepage face at the eastern end of the site. The general direction of ground-water flow is from west to east. Discharge from the seepage face flows into small tributaries (seeps) of the Hudson River. The site is contaminated with coal tar by-products leaching from several shallow deposits buried in the early 1960s. The dissolved contaminants range from single ring aromatics such as toluene to aromatic compounds with more than 20 benzene rings. Here we focus on naphthalene, primarily because of its relatively high solubility and low volatility (Hyman, 1990). Estimates of ground-water travel times indicate that the naphthalene plume has reached a steady-state, with inflow from the source balanced by outflow into the seeps.

The study site shown in Figure 4 has been used for a number of different research investigations sponsored by the Electric Power Research Institute (EPRI) and other organizations. As a result there has been considerable interest in characterizing subsurface contamination at the site. Shortly before our project began, EPRI funded an extensive site investigation which included hydrologic, soil, and ground-water sampling. Much of the field work was carried out by personnel from META Environmental, Inc. and Atlantic Environmental, Inc. NET Atlantic, Cambridge Division, was responsible for analyzing the soil and ground-water samples.
We became involved in the coal tar field study just after the first major round of sampling was completed. At this time a number of piezometers had been installed throughout the site, and several clusters of screened monitoring wells had been placed along transects crossing the plume centerline. Our objective in joining the site characterization effort was to test the sampling and modeling concepts developed in our earlier theoretical work and to help the field investigators with their reconnaissance efforts. By the time the field study was completed, 100 piezometers, 18 multilevel samplers, and 45 monitoring wells were installed. In addition, 18 estimates of hydraulic conductivity were obtained from laboratory analyses and slug tests.

The initial site characterization plan was to obtain all ground-water samples from clusters of screened monitoring wells. However, the first round of samples revealed significant vertical variations in both soil and ground-water naphthalene concentrations. This prompted us to install several multilevel samplers in an effort to obtain better vertical resolution of the contaminant plume. Some of the sampling issues involved in this decision are illustrated in Figure 5. Screened monitoring wells produce flow-weighted concentrations averaged over the length of the screen. If the well screen extends much above or below the main body of the plume, the resulting average concentration measurement can be misleadingly low. By contrast, multilevel samplers draw ground water through small sampling ports which, for all practical purposes, provide point observations of local ground-water concentrations. The simple multilevel samplers installed at our study site are limited by their reliance on peristaltic pumps, which function only to a depth of about 10 meters below the water table. Also, most multilevel sampler designs are suitable only for use in coarse soils which readily collapse around the sampling device. Nevertheless, these samplers can provide very useful high resolution information when they are properly installed.

Fig. 5. Hypothetical vertical section through a solute plume showing some of the sampling issues involved in characterizing vertical variability.

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information about regional water-level variations did not reveal much about soil contamination since they lay well outside the area affected by the plume. Conversely, informative soil sampling locations tended to be too clustered to provide a good synoptic picture of large-scale flow features. Our experience suggests that such conflicts are best resolved through negotiation since it is difficult to rank professional priorities in an objective way. The computer-generated information provided by our site characterization procedure played an important role in our discussions of sampling alternatives. In fact, we were quite encouraged by the willingness of other members of the team to include our model-based predictions in the decision process. Everyone seemed to agree on the need for more systematic and efficient approaches to the site characterization problem.

3.2 Field Sampling Results

The locations of the piezometers, multilevel samplers, and well clusters used in the coal tar site characterization are indicated on Figure 4. As mentioned earlier, these were installed over several sampling rounds spaced a few months apart. It is instructive to compare concentration measurements obtained from different sampling devices located near one another. Figures 8 and 9 show vertical profiles of naphthalene concentration as measured in soil samples, screened well water samples, and multilevel sampler water samples. Each set of profiles is aligned with a chart of stratigraphic data taken from well logs. It is apparent that there is considerable vertical variability at the site, with the plume spanning a depth of only about 10 feet. Moreover, there does not seem to be a simple relationship between the

Fig. 6. Multilevel sampler design used in the case study (port detail shown in inset).

The multilevel samplers used at the coal tar site were based on a design used by the United States Geological Survey in an extensive tracer test located in Cape Cod, Massachusetts (Garabedian, 1987; LeBlanc et al., 1991). A diagram of a complete sampler with a detail of a typical sampling port is shown in Figure 6. Initially, two versions of the multilevel sampler were tried at the site—one using flexible polyvinyl chloride (PVC) tubing and one using less flexible aluminum tubing. Although PVC is less expensive and somewhat easier to work with, comparisons of measurements from nearby PVC and aluminum samplers suggested that naphthalene sorbs on PVC tubing, causing the resulting concentration measurements to be biased downward. This is illustrated in Figure 7, which compares naphthalene concentrations in nearby PVC and aluminum samplers installed during the early stages of the site investigation. In order to minimize the effects of sorption, we used only aluminum samplers in subsequent sampling rounds. Further details on the design and operation of the multilevel samplers may be found in Hyman (1990) and in Hyman and McLaughlin (1991).

There were three major sampling rounds at the coal tar site after the initial reconnaissance. Sampling locations for each round were selected by consensus, with the agreement of all parties involved. A typical example illustrates some of the conflicts which arose during the design discussions. Many of the boreholes drilled at the site were used both for piezometer installation (for hydrologic characterization) and for soil sampling (for chemical characterization). In some cases, borehole locations that appeared to offer useful

Fig. 7. Comparison of observed naphthalene concentrations (in ppm) from metal (aluminum) and plastic (polyvinyl chloride) multilevel samplers.
naphthalene concentrations observed in nearby soil and water samples. Sometimes soil concentrations are high when water levels are low and sometimes the reverse is true. Although naphthalene is clearly sorbed on soil at the site, the mechanisms controlling the magnitude of the sorption effect are not obvious from the concentration data.

A different view of the naphthalene data is obtained by examining a vertical cross section shown in Figure 10. This section is taken more or less down the center of the plume, along a broken line running from the source to the seeps. Figure 10 suggests that the plume drops somewhat, especially near the seeps, and possibly splits into two parts above and below a clay lens between Station 19 and MLS-12. Also, the thickness and concentration profiles of the plume seem to change significantly along the cross section. The available data indicate that the actual naphthalene concentrations are considerably more variable than would be predicted by a transport model based on uniform geologic properties.
3.3 Site Characterization Results

The data summarized above provide the field information needed to test our site characterization procedure. We focus here on a two-dimensional characterization which examines the horizontal extent of naphthalene contamination at the site. This characterization is based on the two-dimensional vertically averaged model of (1) through (4), with all updates derived from vertically averaged well and multilevel sampler measurements. Three-dimensional extensions are discussed in the final section of this paper.

The model parameters used to derive prior dependent variable statistics for the site characterization procedure are summarized in Table 1. The prior hydraulic conductivity mean is assumed to be spatially uniform and fluctuations about this mean are assumed to conform to the spatial spectral density function given in the table. This spectral density specifies the relative amount of log conductivity variability found at different spatial scales. The values for all prior hydraulic conductivity statistics were estimated from available soil permeability and pump tests. The mean head profile was assumed to be a linear function of location. The coefficients used to describe the mean head were estimated from water-level observations collected during the initial site survey. The mean naphthalene concentration in the source area was assigned a bell-shaped distribution over space, with the peak value set equal to the highest observed concentration in the source area. The second moment of this spatial distribution was selected to reflect, in an approximate way, uncertainties about the exact location of the buried coal tar deposit. Other inputs listed in Table 1 were assigned values believed to be typical for the soils found at the coal tar site.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum naphthalene concentration in the source area:</td>
<td>2.50 ppm</td>
</tr>
<tr>
<td>Source radius (4 standard deviations of Gaussian spatial distribution):</td>
<td>40 m</td>
</tr>
<tr>
<td>Source concentration standard deviation:</td>
<td>0.2 ppm</td>
</tr>
<tr>
<td>Transverse local dispersivity:</td>
<td>0.2 m</td>
</tr>
<tr>
<td>Log hydraulic conductivity correlation scale:</td>
<td>15 m</td>
</tr>
<tr>
<td>Geometric mean of hydraulic conductivity:</td>
<td>3.14 m/day</td>
</tr>
<tr>
<td>Log hydraulic conductivity standard deviation:</td>
<td>1.0 (unitless)</td>
</tr>
<tr>
<td>Effective porosity:</td>
<td>0.347 (unitless)</td>
</tr>
<tr>
<td>Prior mean head function (in feet):</td>
<td></td>
</tr>
</tbody>
</table>

\[ h(x, y) = 288.7 + 0.01x \]

where \( x \) is the longitudinal coordinate relative to an origin located at the center of the source area.

\[ S_{00}(k_1, k_2) = \frac{2a_0^2 a^2 (k_1^2 + k_2^2)}{\pi (k_1^2 + k_2^2 + \lambda^2)^3} \]

where \( k_1 \) and \( k_2 \) are the longitudinal and transverse components of the wave number vector (m\(^{-1}\)), \( a = \pi/(4A) \), and \( \lambda \) = correlation scale = 15 m.
log hydraulic conductivity and source values used in the
stochastic model are adjusted to make the predicted head
and concentration distributions more compatible with the
observed values of these variables. The adjustment process is
guided by covariances and cross-variances derived from the
model's governing equations. The site characterization
procedure does not attempt to fit the observed values per-
fected since it recognizes that these values may be in error
(measurement error is included in the Bayesian updating
algorithm). The final updated plume represents a compro-
mise between information provided by the prior model and
information provided by the field measurements. In areas
where measurements are unavailable, the prior estimate
persists through updating. In areas near reliable measure-
ments, the prior estimate is essentially forgotten after
updating.

Figure 12 illustrates the concentration standard deviation
(or uncertainty) associated with each of the mean
plumes plotted in Figure 11. The prior standard deviation
profile shown in (a) exhibits two peaks located on either side
of the estimated plume centerline. These peaks reflect the
high uncertainty of estimates computed where concentra-
tion gradients are steep. Uncertainty is much lower along the
centerline where gradients are small. Similar results are
reported in Graham and McLaughlin (1989a, b, 1991).

When the prior mean is updated with head observations, the
concentration uncertainty decreases somewhat and the
uncertainty profile becomes more irregular, as indicated in
(b). However, the general shape of the concentration stan-
dard deviation profile looks much like the prior. The uncer-
tainty reduces much more when concentration measure-
ments are added.
ments are added, as indicated in (c). This indicates that the updated naphthalene plume plotted in Figure II(c) is a much better estimate of conditions at the site than the simple prior estimate used to start the characterization procedure.

The areas in Figure II(c) with the highest concentration uncertainties are most likely to benefit most from additional sampling and would, therefore, be prime candidates for new wells. The desirability of continuing a given site characterization program depends, of course, on the program's goals and on the availability of sampling resources. Since the uncertainty level indicated in Figure II(c) was sufficient to meet the needs of our case study, no further sampling was warranted. In other situations it might be advisable to continue the site investigation.

Our selection of measurement locations was influenced by several considerations, including the derived prior concentration statistics, access limitations at the wooded site, and the need to satisfy a number of different scientific objectives. No attempt was made to "optimize" the sampling network by, for example, searching for the set of well locations that minimizes some aggregate measure of concentration uncertainty. This decision reflected our feeling that a strict optimization would not provide the flexibility needed to meet the project's objectives. Also, an optimal design based on a two-dimensional model cannot be expected to consider three-dimensional effects that are clearly important at the site. Nevertheless, optimal design is a subject that deserves further consideration in the future, particularly when a fully three-dimensional procedure becomes available.

The performance of our site characterization procedure can be evaluated by comparing differences between predicted and measured concentrations. These differences should be consistent with the characterization algorithm's own estimate of concentration uncertainty. At the coal tar site, the prediction errors were generally higher than expected, especially near the edges of the contaminant plume. After some experimentation we became convinced that this result reflects the influence of recharge variability. Available water-level data suggest that recharge varied significantly over the time period of interest. Studies by Rehfeldt (1988), Nafl et al. (1989), and Goode and Konikow (1990) suggest that recharge variability may have a significant effect on the field-scale transport of hazardous wastes through the subsurface. Consequently, we are currently investigating ways to include recharge variability in our site characterization procedure.

4. Conclusions

The stochastic site characterization procedure described in this paper is intended to provide reliable descriptions of subsurface contamination at heterogeneous sites where field data are limited. The procedure is based on the concept of combining field measurements with predictions obtained from mathematical models of ground-water flow and solute transport. Since heterogeneity and uncertainty are represented probabilistically, the characterization procedure works with statistical measures such as the mean, variance, and correlation scale of solute concentration. An initial (or "prior") statistical description of the site is derived from a physically based stochastic model which treats hydraulic conductivity and source concentration as random functions of location. This prior description is updated whenever field measurements become available. Uncertainty is reduced after updating, particularly in areas near sampling locations.

The site characterization procedure is most efficient when it is applied sequentially, over a series of discrete sampling rounds, so that each new round of sampling decisions can benefit from information gained in previous rounds.

The site characterization example we have used to illustrate our procedure confirms that a model-based characterization can be useful in realistic field settings. Our characterization procedure helped to guide sampling decisions throughout the site investigation, and it was sufficiently flexible to deal with logistic constraints and differing professional priorities. The computer computations required, while demanding, can be completed in several hours on a readily available desktop workstation (e.g., a DECStation 3100).

The case study also reveals a number of important limitations which need to be overcome before our site characterization procedure can be widely applied. One of the most obvious is the two-dimensional approximation. Data collected at our study site, as well as many other contaminated ground-water sites, indicate that vertical variability is significant and that two-dimensional vertically averaged descriptions do not capture many of the important features needed to predict contaminant movement and plan cleanup programs. Although our approach is not inherently limited to two-dimensional site descriptions, it does become computationally demanding when extended to three dimensions. For this reason we are placing great emphasis on the development of more efficient numerical schemes for deriving the prior statistics required by our procedure. The nonstationary spectral method of Li and McLaughlin (1991) is one promising alternative. A truly three-dimensional characterization procedure would provide a systematic way to select sampling locations in the vertical dimension. Three-dimensional maps of concentration uncertainty could help site investigators decide where to install well screens and where to place multilevel sampler ports. They could also provide valuable guidance for hydraulically oriented remediation strategies.

The current version of our characterization procedure is also limited by the sources of uncertainty it considers. The procedure currently recognizes uncertainties contributed by spatial variations in hydraulic conductivity and by poorly defined source characteristics. At many sites there are undoubtedly other important sources of uncertainty, including recharge variability, variability in sorption and biodegradation properties, and uncertainty about the effects of hydrologic controls such as streams and seepage faces. Also, the procedure deals only with soluble contaminants and does not provide for the special properties of fractured media. The relative importance of these complicating factors depends on the site under investigation. In the case of our coal tar study site, we feel that recharge variability is particularly important, although sorption and biodegradation variability may prove to be significant during remediation.

The case study considered in this paper focuses on
characterization of an existing steady-state contaminant plume. The procedure we propose can also be used to predict the behavior of a changing plume which is responding either to natural gradients or to remedial activities. A simulated example is provided in Graham and McLaughlin (1989a, b). Dynamic effects can be included by using a time-dependent version of the stochastic model summarized in (1) through (4). Time-dependent site characterization introduces an interesting set of new sampling design questions since we must decide when as well as where to sample. As in the steady-state case, the sampling program should be designed to achieve the greatest possible reduction in uncertainty. Dynamic site characterization is particularly important during remediation since updated plume descriptions could be used to select pumping rates and other control variables which might influence the success of a cleanup effort. This is a topic which deserves further investigation.

Our case study illustrates that it is possible to apply advanced statistical concepts to a real-world field investigation. The general approach outlined here can provide a more systematic framework for site characterization, one which complements the skills of field personnel by giving them better information. We believe that this approach will help us achieve more with the limited resources generally available for site characterization and related remedial activities.

5. Acknowledgments

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6. References


