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TITLE Adaptive Sampling Program Support for Expedited Site Characterization

ABSTRACT

Expedited site characterizations offer substantial savings in time and money when assessing hazardous waste sites. Key to some of these savings is the ability to adapt a sampling program to the "real-time" data generated by an expedited site characterization. This paper presents a two-prong approach to supporting adaptive sampling programs: a specialized object-oriented database/geographical information system for data fusion, management and display; and combined Bayesian/geostatistical methods for contamination extent estimation and sample location selection. This approach is applied in a retrospective study of a subsurface chromium plume at Sandia National Laboratory's Chemical Waste Landfill. Retrospective analyses suggest the potential for characterization cost savings on the order of 60% through a reduction in the number of sampling programs, total number of soil bores, and number of samples analyzed from each bore.

INTRODUCTION

Characterizing hazardous waste sites is an expensive and time-consuming process that typically involves successive sampling programs. The total cost per sample taken can be prohibitive when safety and health compliance costs, drilling or boring expenses, and sample analysis costs are all included. Expedited site characterizations present the potential for substantial savings in the time and cost associated with characterizing a site. Expedited site characterization techniques use recent advances in sensor technologies to generate "real-time" information on the extent and level of contamination. This information can take the form of non-intrusive geophysical survey results, down-hole and cross-bore sensor information, and field laboratory data. By using field laboratory techniques, expedited site characterizations reduce the cost per unit of information collected. By using information that is generated and analyzed in real-time, sampling programs can be guided interactively, reducing the number of samples taken to only those absolutely necessary to satisfy characterization needs. Finally, expedited site characterizations can often be brought to closure after one or two field visits, eliminating the mobilization costs associated with the staged, repetitive characterization approach traditionally used.

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For expedited site characterizations to exploit the second and third cost savings fully, adaptive sampling programs are required. "Adaptive" refers to the ability to change, or adapt a program while underway to accommodate new data as it is being generated. Adaptive sampling programs demand a means of rapidly integrating, visualizing and analyzing data. This paper describes the combined application of a commercial object-oriented database(OODB)/geographic information system (GIS) specifically designed for site assessment work and a smart sampling strategy methodology to the problem of supporting decision-making in expedited site characterization programs (Figure 1). The OODB/GIS provides real time data fusion, management and visualization. In this role, the OODB/GIS offers an immediate, qualitative image of where contamination might be expected, and how it is spatially related to other site features such as the water table, geological strata, etc. The smart sampling strategy methodology quantitatively fuses "hard" and "soft" information regarding contamination extent, estimates the extent of contamination and the uncertainty associated with those estimates, measures the expected impact derived from obtaining additional samples, and indicates where the best new sampling locations might be. In this role, the smart sampling strategy methodology provides quantitative support for adaptive sampling programs.

[insert Figure 1 here]

QUALITATIVE SUPPORT FOR ADAPTIVE SAMPLING PROGRAMS

Past approaches to data integration, management and visualization historically have revolved around data archiving systems for data management, and standard GIS systems for displaying data with spatial attributes. While data archiving systems and standard GIS applications have an important role to play in site restoration activities, they have fundamental limitations in the context of adaptive sampling programs. Traditional data archiving systems are typically built around relational database packages. They are meant to preserve information, guaranteeing its quality, security and integrity. Before data can be entered into such systems, it must satisfy lengthy quality assurance and quality control procedures. Once entered, access is controlled. Environmental data archiving systems seldom provide users anything more than tabular aggregates of data for analysis.

Standard GIS applications enhance data archiving systems by allowing the display of spatially-oriented data in maps. However, they too have inherent limitations in the context of adaptive sampling programs. Raster-based GIS systems are ideal for data that is rich in location, but sparse in data available at each location (i.e., satellite imagery). Site characterization data are typically sparse in location, but rich in information at each location. For example, a particular site may have a handful of soil bores, but the information available at each bore may include stratigraphic data, down-hole sensor results, laboratory results for soil samples, etc. Site characterization data are also typically three dimensional in spatial location. Traditional GIS systems treat data as two-dimensional layers, making it hard to visualize three dimensional subsurface structures such as contaminant plumes, or stratigraphic features. Because of the type of data generated by expedited site characterizations, specialized graphics are required that include bore logs, fence diagrams, and profile views, as well as the plan views provided by standard GIS systems. Finally, most GIS systems were designed primarily for data display and not data management. Consequently, most GIS systems have very limited inherent data management facilities.

Expedited site characterization programs demand data integration, management, and visualization that is dynamic, interactive, and graphically-based. A hybrid OODB/GIS specifically designed for site characterization is ideally suited for the task (1). Object-oriented data management systems organize information by object rather than table. Object classes are defined in an object dictionary, and as new data are included, new instances of a particular object class are created. Examples of object classes for expedited site characterizations are soil bores and soil samples. The power of object-oriented databases lies in the ability of new objects to inherit the attributes associated with their class definition. One example of this inheritance is the set of data fields that need to be filled for a particular object class. Another is the display capabilities associated with an object class. For example, a soil bore might possess the ability to participate in the creation of a bore log, but a lagoon would not. Or, a series of water samples taken from the same well over a period of time might be displayed in a "time view", but a set of soil bores could not.

A dynamic data integration, management and visualization system is one whose graphics are dynamically linked to the underlying data. As new data are included or old data changed, the graphics displaying those pieces of data are automatically updated. This capability is important for expedited site characterization programs where data is continually being generated, and images of the site must immediately reflect all available data. Graphically-based means that all data can be displayed and manipulated in some visually meaningful way. These graphics might take the form of plan views of the site, profile views showing subsurface characteristics, bore logs, fence diagrams, time views, or whatever is pertinent to the characterization.

Finally, interactive means that the OODB/GIS user has easy access to data contained in displays, and that the processes required for incorporating new data and generating new displays are quickly learned and simple to execute. Implied in interactive is a menu, mouse and icon driven system based on a standard graphical user interface that is easy to learn and easy to use. The paradigm of centralized computing facilities does not fit into an expedited site characterization system. Technical staff directing an expedited site characterization program will likely have considerable expertise as geologists, hydrologists, or geochemists, but will probably have limited computer knowledge. They, however, are the ones that need access to the data and graphics a OODB/GIS provides.

QUANTITATIVE SUPPORT FOR ADAPTIVE SAMPLING PROGRAMS

Contamination events generally possess two key characteristics. First, they are spatial processes that are dominated statistically by spatial autocorrelation. This simply means that the results from one sampling location will be similar to results from a neighboring sampled point, but may differ completely from a third sample taken further away. Second, there typically exists substantial "soft" information regarding probable contamination extent, even if little hard sample data are initially available. This information might come from past experience with similar sites, from historical records documenting release size, from non-intrusive geophysical surveys, or from preliminary transport modeling results.

Quantitative support for adaptive sampling programs should provide estimates of contaminant extent, measures of the uncertainty associated with those estimates, indications of how much additional information might be gained from further sampling, and direction as to where additional samples should be placed so as to maximize the value of the information they produce. To do this, quantitative sampling strategy support must accommodate spatial autocorrelation present in sampling results, and somehow quantitatively merge "soft" information with "hard" sample data as it is produced by an adaptive sampling program. Bayesian analysis provides a natural framework for quantitatively fusing hard and soft data, while some form of spatial statistical analysis can help with incorporating spatial autocorrelation.

Bayesian analysis is rooted in Bayes Theorem:

$$P(X|Y) \propto P(X) \cdot P(Y|X) \qquad \text{(Eq 1)}$$

This equation says that the probability of encountering state X given a set of Y values is proportional to the product of the probability of state X and the probability of encountering the set of Y values given state X. P(X) is called the prior probability density function (pdf) for X, and P(X | Y) is called the posterior pdf. In the context of sampling to delineate contamination, P(X) would be associated with the probability of contamination extent before one samples, and P(X | Y) its probability given the results of sampling. A prior such as P(X) could be constructed out of either hard or soft information. Bayes Theorem provides the mechanism for quantitatively updating P(X) with new sampling information as it becomes available.

To apply a Bayesian approach to delineating contamination events, one must interpolate from points where sampling data exists to areas where no samples have been collected. Spatial autocorrelation provides the rationale for interpolation; spatial statistical techniques provide the mechanism. Kriging is an interpolation procedure based on spatial statistical analysis. Kriging provides the "best" linear interpolated value at an unsampled point given a set of sampled points, where best is defined as the unbiased estimate with least expected estimation error. If one is delineating contamination events, then indicator kriging is appropriate. Indicator kriging considers just the presence or absence of contamination above a prespecified threshold. Indicator kriging has several advantages over ordinary kriging in the context of contaminant delineation (2). It can work with indicator data generated by field screening technologies. The variograms it uses tend to be more robust. Its interpolated values are also immune to outlying data points.

Using this approach, one defines a grid of "decision points" over a region of interest. As a sampling program develops, one will want to assign a probability of contamination to each point, and ultimately decide if the point is contaminated or not. One can define at each point a Beta distribution for the probability of contamination. In the context of Bernoulli trials, Beta distributions are conjugate priors, which means that as new samples are taken and the Beta distributions at each decision point updated, the results are posterior pdfs that are also Beta distributions with changed parameters. If a decision point is sampled, the probability of contamination at that point will be driven to either zero or one depending on the outcome of the sampling. If it is not sampled but new samples were taken close by, indicator kriging is used to apply the results of those samples to the particular decision point under consideration to obtain an updated value of its probability of contamination. The details of this updating process can be found in Johnson (3).

The probabilities of contamination at each decision point can be used to classify whether the point should be considered contaminated, clean, or state uncertain. For example, every decision point whose probability of contamination is greater than 0.8 might be considered contaminated, with probability of contamination less than 0.2 as clean, and with probability of contamination between those two values as uncertain. A natural choice for measuring the impact of additional sampling points with this classification system would be to calculate the expected effect a new sampling point would have on the total number of decision points classified as state uncertain---the more decision points expected to be pushed to the "clean" or "contaminated" categories, the greater the expected impact. One could then look for the sampling location or set of locations that maximize this impact, and drive an adaptive sampling program based on the search results. Figure 2 shows the logical flow of this process.

[insert Figure 2 here]

The one thing lacking at this point is a defensible stopping criteria---criteria that would allow the manager of an expedited site characterization program to decide that enough information had been gathered, and that sampling could stop. The EPA has espoused Data Quality Objectives as one basis for constructing stopping criteria (4,5). Data Quality Objectives use the probability of making Type I and Type II errors for stopping criteria. If one were attempting to classify a set of decision points as either contaminated or clean, with the initial assumption that they were all clean, then a Type I error would occur if a decision point were classified as contaminated when in fact it was clean. A Type II error would occur if a point were classified as clean when in fact it was contaminated. The probabilities of contamination at each decision point supplied by this methodology lend themselves naturally to a Data Quality Objectives type of analysis.

CASE STUDY

The above approach was applied in a retrospective study to the delineation of a chromic acid plume underneath the chemical waste landfill at Sandia National Laboratory, Albuquerque, New Mexico, as part of the Mixed Waste Landfill Integrated Demonstration (MWLID). The U.S. Department of Energy (DOE) supports the MWLID through its Office of Technology Development (OTD). The Mixed Waste Landfill Integrated Demonstration features innovative boring techniques, non-intrusive geophysical survey methods, field-screening analytical techniques for detecting metals, and sampling strategy support methodologies applied to mixed waste landfill characterization in arid environments. The ultimate purpose of the MWLID is to transfer promising technologies to environmental restoration programs at DOE facilities.

The specific contamination event targeted was a chromium plume beneath an unlined chromic acid pit (UCAP) within Sandia National Laboratory's chemical waste landfill. Figure 3 shows the relative location of the UCAP within the chemical waste landfill. Figure 4 shows a planview of the UCAP's immediate vicinity, and a profile view of an east-west transect of the pit based on seven soil bores completed in 1987. The shaded area in the profile view shows the extent of chromium contamination in this east-west transect using the sampling results from the 1987 borings. When the MWLID began work in 1992, there was no information about the north-south extent of contamination, or its current depth of penetration.

[insert Figure 3 here]
[insert Figure 4 here]

The first step in applying the methodology to the UCAP was to garner all historical data available for the UCAP, and fuse it in an appropriate OODB/GIS system. The system used was called SitePlanner^{TM}, a commercial software package designed specifically for site characterization work. The object dictionary used by SitePlanner^{TM} was modified to handle the soil bores, monitoring wells, landfills, directionally drilled bores, and soil samples expected to be included. A SitePlanner^{TM} virtual site was then constructed using base maps for the chemical waste landfill extracted from ArcInfo^{TM} coverages, monitoring well information (construction data, stratigraphic data, depth to water table measurements, etc.), and existing soil bore and sample information. Once the base virtual site had been created, the OODB/GIS was ready to accept additional data as new bores were sunk and samples analyzed by the MWLID.

The OODB/GIS played three key roles: database, data visualization, and reality check for/link to the sampling strategy support methodologies used. Figure 4 shows the OODB/GIS functioning in the first role. In Figure 5, soil bore UCAP-3 has been selected and its data displayed. From the scrolling list of objects attached to this bore, soil sample 10073 has been selected and its data retrieved, including both locational information and chemical results. Figure 6 is an example of data visualization. A plan view provides a bird's eye overview of the site, while a bore log, profile view, and fence diagram provide subsurface pictures of stratigraphic structure and contamination location. In every view, objects are represented by icons that are immediately available for selection via a mouse. For example, in the bore log, profile view and fence diagram, the icons running the length of the bores indicate the locations of soil sample objects.

[insert Figure 5 here]
[insert Figure 6 here]

The initial goal of the MWLID sampling program was to determine the best new vertical bore locations for delineating the extent of the chromium contamination, and to position sampling points along those bores. To facilitate this analysis, a three-dimensional grid of decision points was superimposed over the region of interest---16 points along the east-west axis, 16 points along the north-south axis, and 15 along the vertical axis for a total of 3840 decision points, with 2.09 meters separating each point. The extent of this grid was based on the belief that the solid it defined completely contained any potential contamination. Based on the location of the pit and results from earlier exploratory bores, an initial prior pdf was assigned to each decision point that reflected the expected probability of finding contamination at that decision point. These initial prior pdfs were then updated with the available 1987 sampling data. The MWLID staged two sampling programs in the summer of 1992, first completing two TEVES bores north of the unlined chromic acid pit, and then returning to install three additional UCAP bores along the western boundary of the pit.

After each sampling program, an "impact surface" was created to determine the areas where maximum impact on contaminant delineation could be expected if additional bores were installed. Impact at specific location is measured as the expected number of decision points currently classified as state uncertain that would be reclassified as either clean or contaminated given a new vertical soil bore at that location. In Figure 7 impact is grey-scale coded, ranging from white (minimum impact) to black (maximum impact). Based on just the 1987 data, the regions with the greatest potential for new bore locations lie north and south of the pit. With the completion of the TEVES bores, the value of additional bores north of the pit is insignificant compared to that south. After the UCAP bores were installed, much of the value of additional sampling lies southeast of the pit.

After each sampling program, each decision point was reclassified as either clean (less than 0.2 chance of contamination), contaminated (greater than 0.8 chance of contamination), or state uncertain (probability of contamination between 0.2 and 0.8). Figure 8 graphically shows how allocation of decision points to these categories changed as each sampling program was completed. The 0.5 line indicates the percent of decision points that would have been categorized as contaminated if a decision point had probability of contamination greater than 0.5. This is equivalent to forcing a clean/contaminated decision at each decision point, regardless of the probability for erroneous classification. Finally, Figure 9 shows how the horizontal extent of contamination looks at a depth of approximately six meters after each sampling program. The shading in Figure 9 ranges from white (zero probability of contamination) to black (probability of contamination equal to one).

[insert Figure 7 here]
[insert Figure 8 here]

[insert Figure 9 here]

These three sampling programs comprised twelve bores and 197 samples sent for analysis. The selection of bore locations and their positioning had little to do with attempting to keep characterization costs to a minimum. An obvious retrospective question is: if the original program had been designed to limit the number of sampling programs, bores and sampling points using the proposed methodology, how well could have one done? Using the initial prior pdfs for each decision point, a set of five bores was located and samples placed along their length so that maximum impact on the percent of decision points categorized as state uncertain was obtained. Figure 10 shows the locations of these five bores relative to the twelve bores that were actually sunk. Based on the initial prior pdfs for the set of decision points, approximately 68% of the decision points would have been classified as state uncertain. Upon completion of the three sampling programs actually conducted this value had been dropped to 32% of the volume. In contrast, by strategically placing the five bores comprising a total of thirty five samples, the number of decision points classified as uncertain could be dropped to 14%. Besides having a substantially greater impact than the actual sampling programs, this would have represented a 66% savings in sampling program mobilization costs, a 58% savings in boring costs, and an 82% savings in sample analysis costs (assuming the analyses were done in a laboratory using techniques comparable to those used during the actual sampling programs). If field screening techniques had been used on the majority of samples, with only a few sent to the laboratory for confirmatory analysis, the savings in sample analysis costs would have been even greater.

CONCLUSIONS

Expedited site characterization programs have the potential for significant cost and time savings during a site characterization process. To realize this potential, however, requires adaptive sampling strategy support. Adaptive sampling strategy support guarantees that technical staff conducting an expedited site characterization program attain a complete understanding of their site as quickly as possible, that they have their data readily available as it is being generated, that they place their new sampling locations as best as possible, and that they know when enough sampling is enough for their characterization purposes. A hybrid object-oriented database/geographical information system designed for site characterization work fulfills the role of integrating, managing and displaying site characterization data. Smart sampling strategy methodologies that combine Bayesian analysis with spatial statistics provide quantitative support for estimating contaminant extent, measuring the benefits to be expected from additional sampling, and identifying where those samples should be placed.

This approach was applied in a retrospective analysis at the unlined chromic acid pit, part of the chemical waste landfill belonging to Sandia National Laboratory. The analysis suggests significant cost and time savings could have been realized if this approach had been adopted from the outset.

ACKNOWLEDGEMENTS

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5. United States Environmental Protection Agency, "Data Quality Objectives for Remedial Response Activities: Example Scenario", Office of Emergency and Remedial Response and Office of Waste Programs Enforcement, Washington, D.C. (1987).

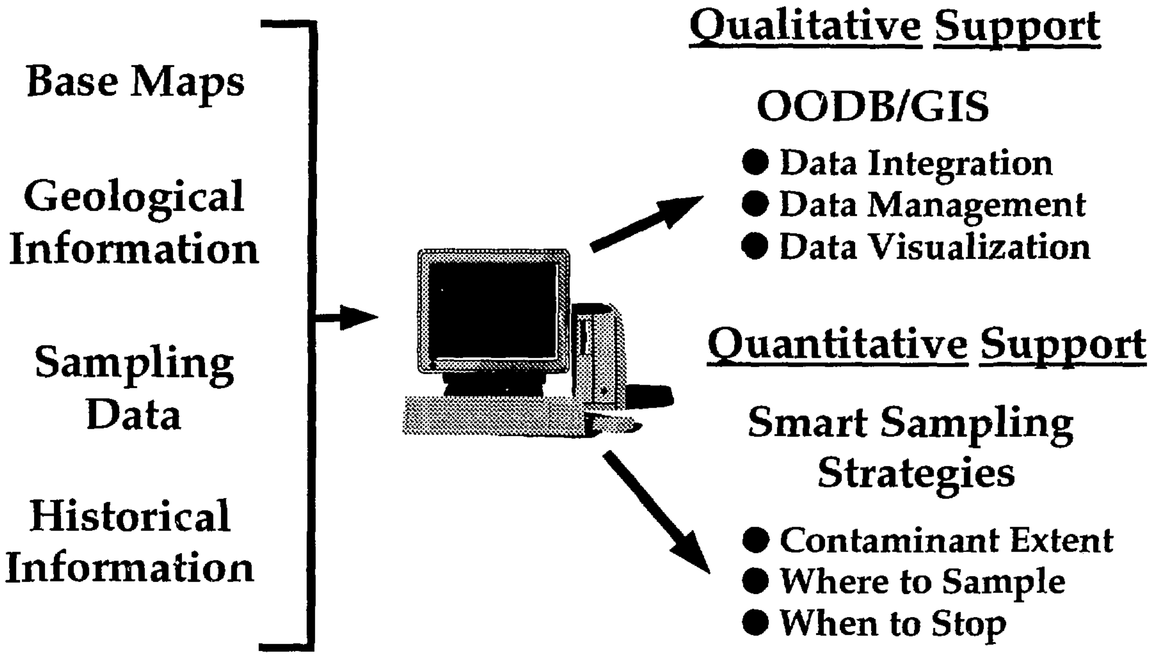


Figure 1 Framework for Adaptive Sampling Program Support

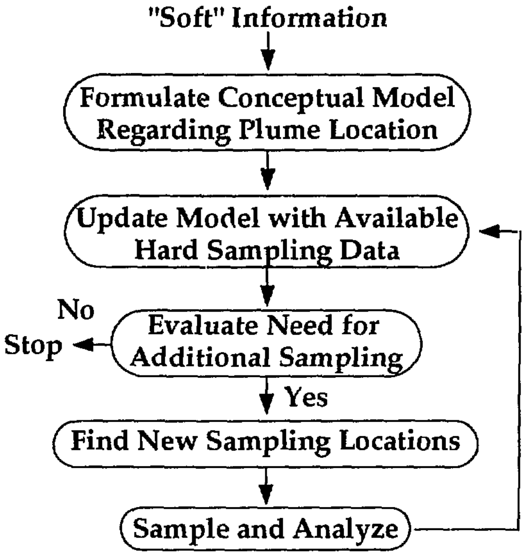


Figure 2 Decision Process for Adaptive Sampling Programs

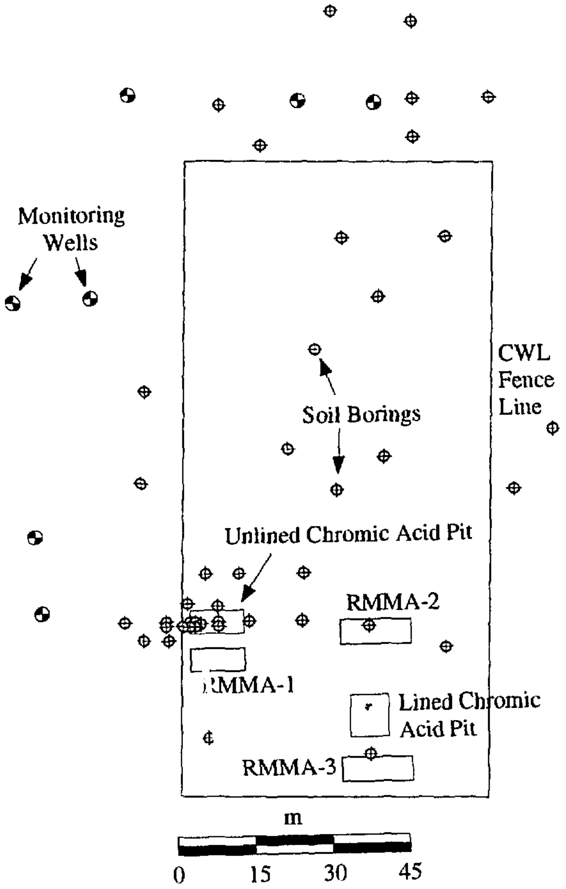


Figure 3 Chemical Waste Landfill

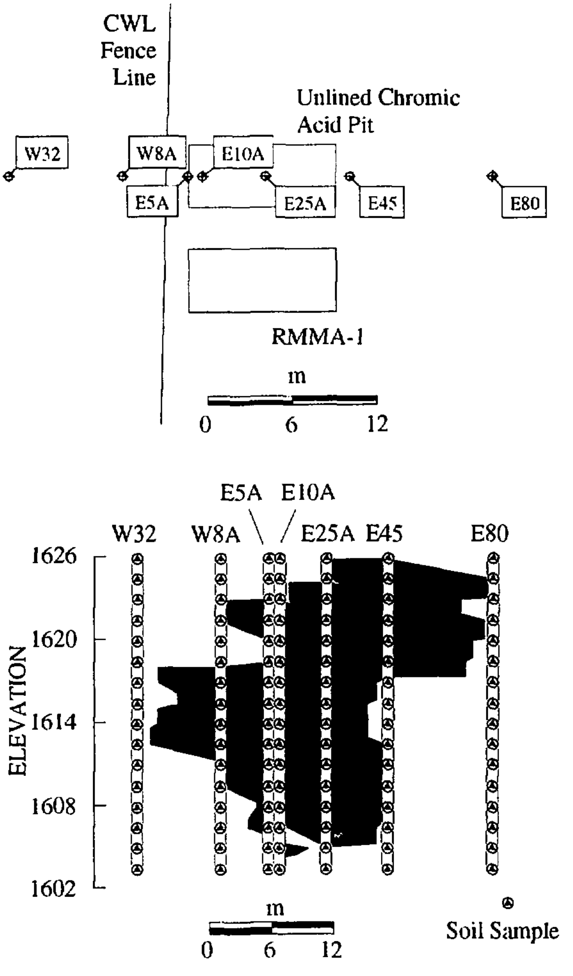
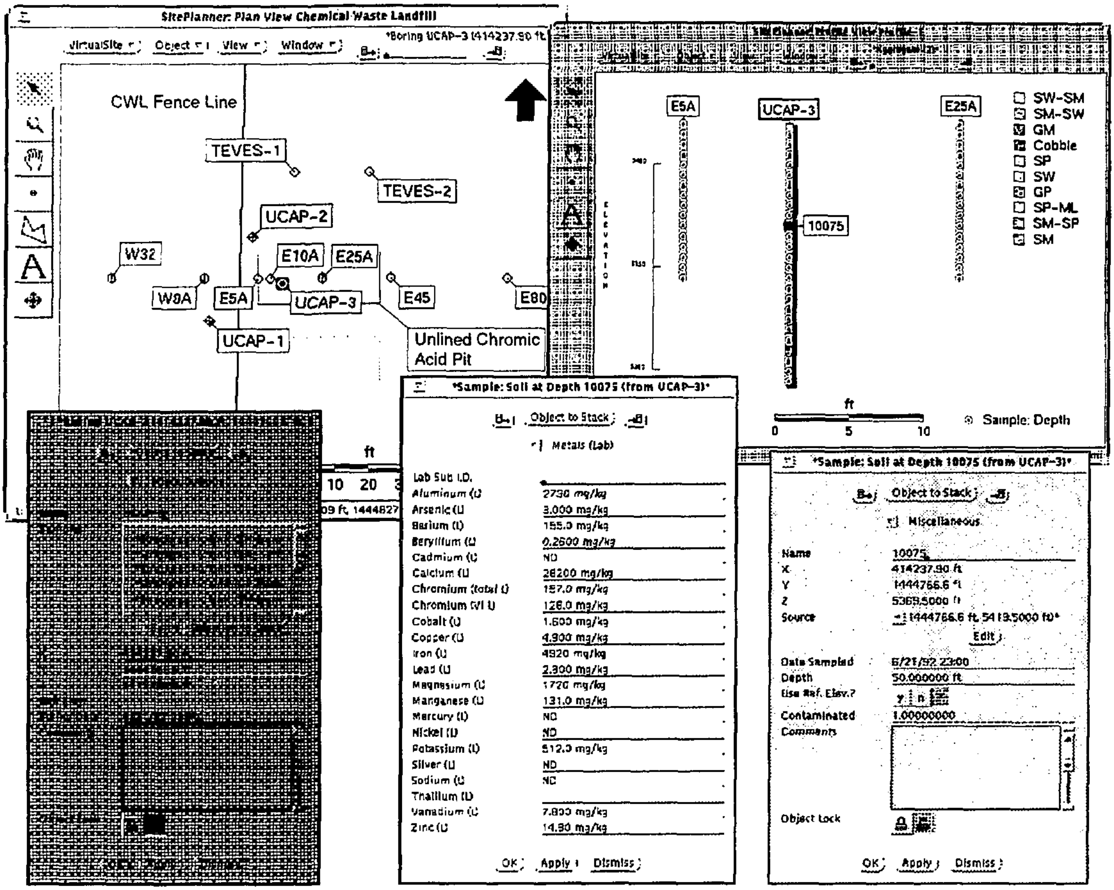


Figure 4 UCAP Plan and Profile Views



Sample: Soil at Depth 10075 (from UCAP-3)

Object to Stack

Metals (Lab)

Lab Sub I.D.	
Aluminum (U	2730 mg/kg
Arsenic (U	3.000 mg/kg
Barium (U	155.0 mg/kg
Beryllium (U	0.2600 mg/kg
Cadmium (U	ND
Calcium (U	28200 mg/kg
Chromium (total U	157.0 mg/kg
Chromium (VI U	126.0 mg/kg
Cobalt (U	1.600 mg/kg
Copper (U	4.900 mg/kg
Iron (U	4920 mg/kg
Lead (U	2.300 mg/kg
Magnesium (U	1720 mg/kg
Manganese (U	131.0 mg/kg
Mercury (U	ND
Nickel (U	ND
Potassium (U	512.0 mg/kg
Silver (U	ND
Sodium (U	NC
Thallium (U	
Vanadium (U	7.800 mg/kg
Zinc (U	14.90 mg/kg

OK Apply Dismiss

Sample: Soil at Depth 10075 (from UCAP-3)

Object to Stack

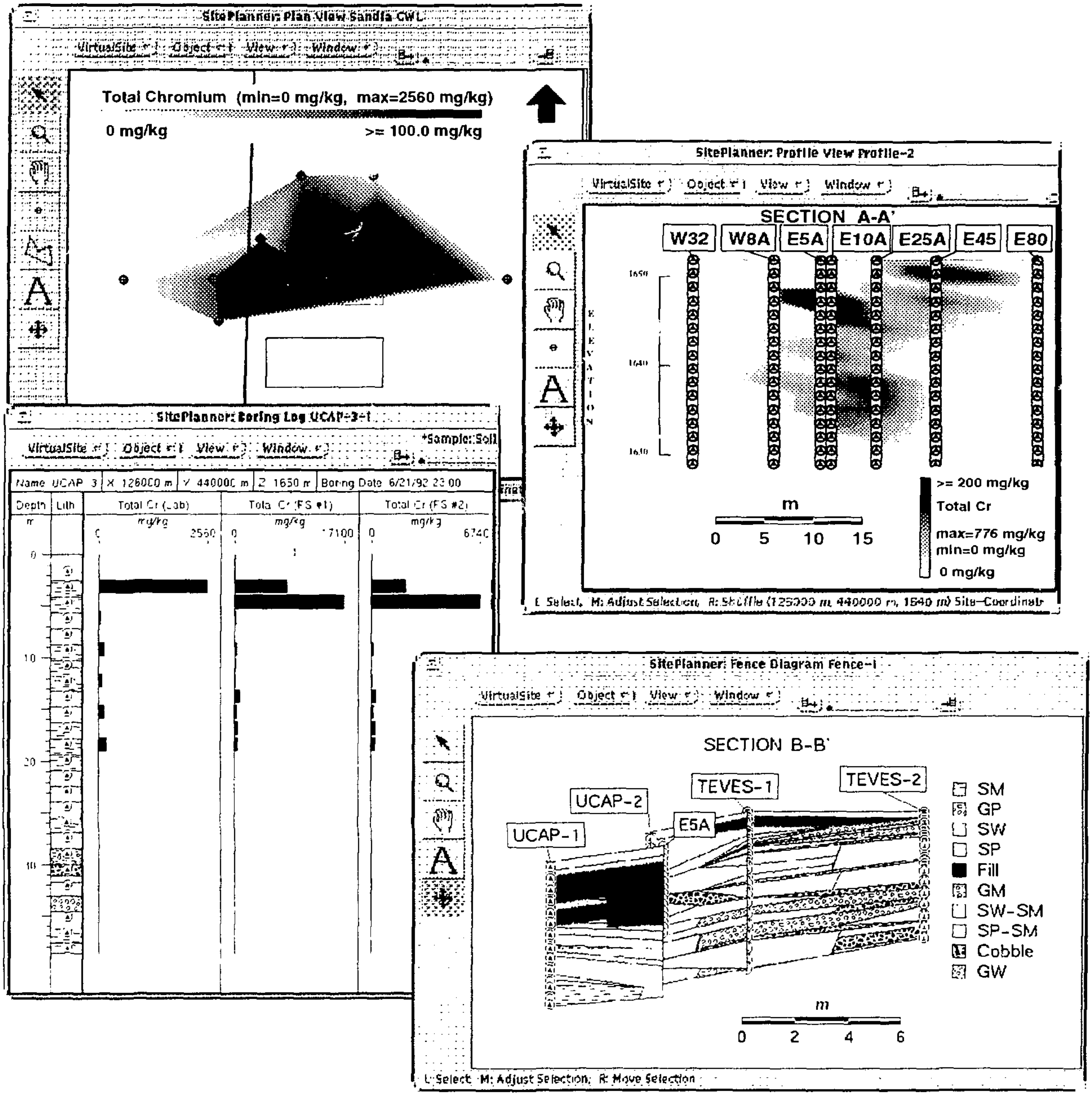
Miscellaneous

Name	10075
X	414237.90 ft
Y	1444766.6 ft
Z	5369.5000 ft
Source	1444766.6 ft, 5419.5000 ft)*
Date Sampled	6/21/92 23:00
Depth	50.000000 ft
Use Ref. Elev.?	y n
Contaminated	1.00000000
Comments	
Object Lock	

Edit

OK Apply Dismiss

Figure 5 OODB/GIS as Database



Name UCAP 3 | X 126000 m | Y 440000 m | Z 1650 m | Boring Date 6/21/92 23:00

L Select, M: Adjust Selection, R: Shuffle (125000 m, 440000 m, 1640 m) Site-Coordinate

L: Select M: Adjust Selection; R: Move Selection

Figure 6 OODB/GIS as Data Visualizer

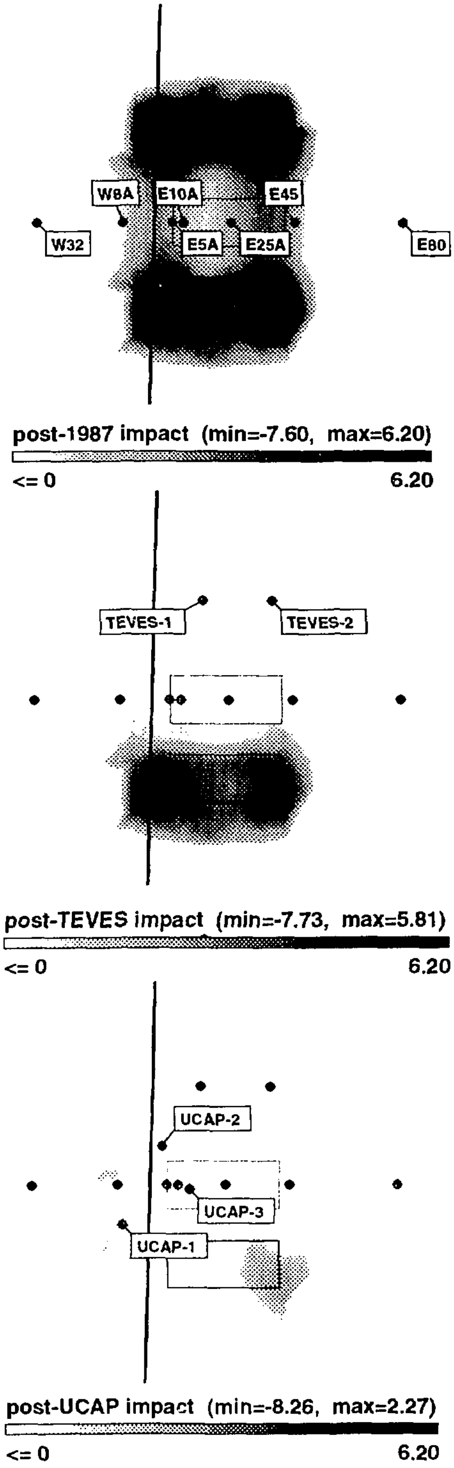


Figure 7 Expected Impact of New Vertical Bores

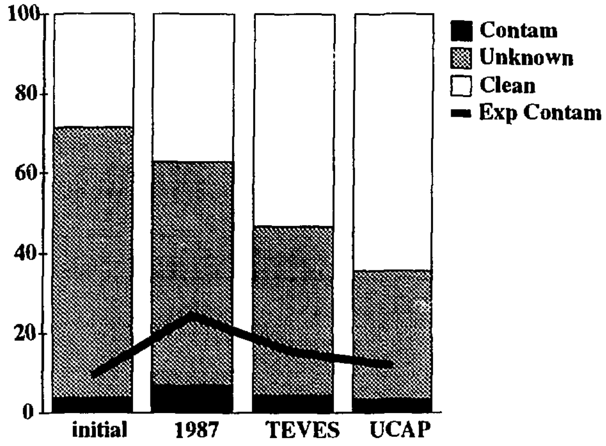


Figure 8 Classification of UCAP Decision Points

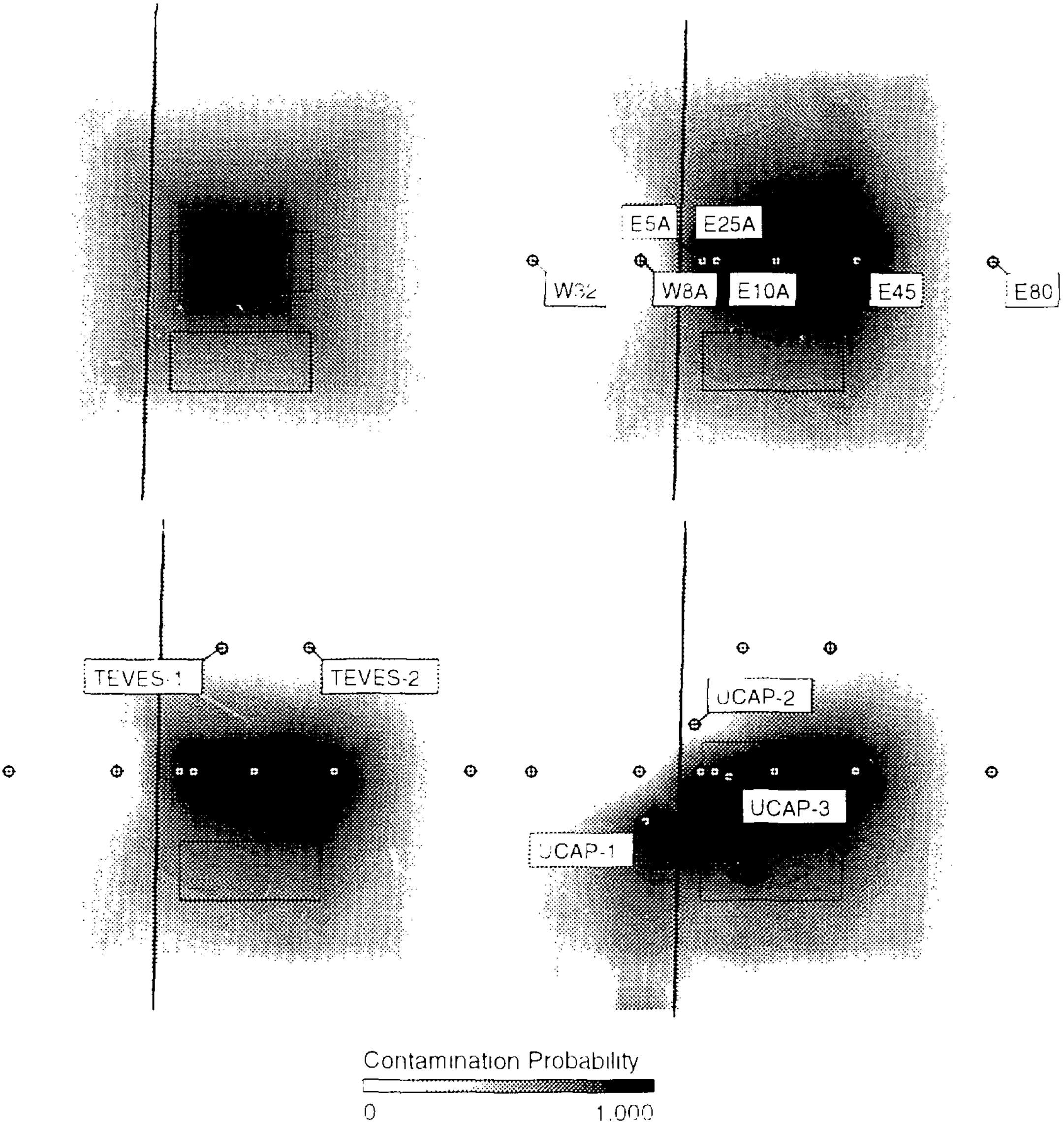


Figure 9 Lateral Contamination Extent at 6 meters