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# PERFORMANCE-BASED, COST- AND TIME-EFFECTIVE PCB ANALYTICAL METHODOLOGY

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## ABSTRACT

Laboratory applications for the analysis of PCBs (polychlorinated biphenyls) in environmental matrices such as soil/sediment/sludge and oil/waste oil were evaluated for potential reduction in waste, source reduction, and alternative techniques for final determination. As a consequence, new procedures were studied for solvent substitution, miniaturization of extraction and cleanups, minimization of reagent consumption, reduction of cost per analysis, and reduction of time. These new procedures provide adequate data that meet all the performance requirements for the determination of PCBs. Use of the new procedures reduced costs for all sample preparation techniques. Time and cost were also reduced by combining the new sample preparation procedures with the power of fast gas chromatography. Separation of Aroclor 1254 was achieved in less than 6 min by using DB-1 and SPB-608 columns. With the greatly shortened run times, reproducibility can be tested quickly and consequently with low cost. With performance-based methodology, the applications presented here can be applied now, without waiting for regulatory approval.

## INTRODUCTION

The philosophy of analytical procedures has progressed over the years from descriptive to prescriptive to performance based. Descriptive procedures tell what the researcher did, but they often leave out important details and also leave room for adaptation by others applying the procedure. Prescriptive procedures are described as "cookbook recipes"; deviations are not allowed. Performance-based procedures examine quality objectives for each sample to evaluate the performance of the procedure. Often, performance-based procedures permit greater flexibility for adaptation. The result is flexibility in conducting required environmental monitoring, expedited use of new and innovative techniques, and cheaper and faster approaches to conducting required site characterization, monitoring, and measurements.

The initial steps for acceptance of performance-based procedures appeared in October 1997 in the *Federal Register* (62, 52098) (Kinney and Caliandro, 1998); the Environmental Protection Agency (EPA) published a notice that will expand the range of acceptance monitoring technologies and procedures for use in compliance monitoring of air, soil, and water. The outcome will be an emphasis on the analytical chemistry needs of specific monitoring projects, rather than the required use of specific technologies; a consistent way of expressing method performance criteria that is independent of the type of technology or method; and increased new technology development, as well as improvement in existing methodologies.

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New cost-effective methods that meet program requirements and performance criteria are needed. The analysis of PCBs is an example of the need for development of performance-based methodologies. The PCBs are widespread, highly visible environmental pollutants. Their analysis is a very high-volume requirement across the country, and the current methods are widely acknowledged to need improvement. Too often, PCB methods are adapted from methods for chlorinated pesticides. Despite the fact that PCBs are such prominent analytes, inadequate attention is given to quality control (e.g., all matrix spike compounds are pesticides), qualitative identification, and quantitation related to PCBs. In addition, the method approved by the EPA for the determination of PCBs in transformer fluid, waste oil, and soil (Bellar and Lichtenburg, 1982) is performed on an unnecessarily large scale. The EPA methods for determination of PCBs in various matrices have not changed to accommodate the current trend toward microscale analysis and the incorporation of waste minimization, pollution prevention, solvent substitution, and new technologies.

The early analysis of PCBs was performed by packed-column gas chromatography (GC). Subsequent improvements in GC have historically emphasized separation or resolution. The research emphasis on increased resolution has largely ignored the time requirements of GC analysis. Nearly all PCB analyses take 20-60 min per run. (Extraction and cleanup procedures take considerable additional time.) Because analysis time translates directly into analysis cost, analyses completed within a few minutes by fast GC are desirable. Many articles have been published about the theory of fast GC (Hyver and Phillips, 1987; Van Es et al., 1987; Akard and Sacks, 1994), but only recently has fast GC been applied to air monitoring (Ke et al., 1992) and analysis of volatile organic compounds (Klemp et al., 1994; Sacks and Akard, 1994).

Fast GC shows potential for reducing PCB analysis time to a just a few minutes. With the greatly shortened run times, reproducibility can be tested quickly and consequently with low cost. However, the reduction in analysis time is accompanied by a significant loss in chromatographic resolution, a decrease in the number of components that can be separated, and increased probability of peak overlap.

The objective of this project was to investigate, develop, evaluate, and implement new procedures for preventing or minimizing primary and secondary waste, reducing costs, and minimizing time for the analysis of PCBs. Laboratory applications for the analysis of PCBs in environmental matrices such as soil/sediment/sludge and oil/waste oil were evaluated for potential reduction in waste, source reduction, and alternative techniques for final determination.

## EXPERIMENTAL DESIGN

### Instrumentation

The fast GC used in these experiments was a Varian 3600 Star system (Sugar Land, Texas) with a cryointegrator from Chromatofast™, Inc. (Ann Arbor, Michigan). High-purity hydrogen (AGA, Hammond, Indiana) was used as carrier gas, and high-purity nitrogen (AGA) was the make-up gas for the electron capture detector (ECD). Typical carrier gas velocities ranged from 95 to 250 cm/s.

The first injector in the two-injector system was a regular split/splitless injector set at 250°C, followed by a cold trap cooled by a continuous flow of liquid nitrogen at -90°C and resistively heated by a current pulse from a capacitor discharge power supply. The two injectors were connected by a fused-silica transfer line. To control analysis time, preconcentration, injection mode, and desorption time, the instrument has a build-in series of relays (standby, sample, purge, and analyze) for each function. For each of these relays, conditions were optimized for the final analysis.

The ECD was set at 300°C and a frequency of 40 Hz to detect fast transient signals from the analytes. Initial and final column temperature and rate of increase were optimized in each case. Two different columns were used. The initial experiments were carried out with a DB-1 column (Varian; 3 m long, 0.25 mm I.D.). Later experiments used an SPB-608 column from Supelco (Bellefonte, Pennsylvania; 3 m, 6 m, or 10 m long and 0.25 mm I.D.).

### Reagents

Aroclor standards were from ULTRA Scientific (North Kingston, Rhode Island). The standard mixture came in 1-mL ampules at an Aroclor 1254 concentration of 100 µg/mL in hexane. Other standards and solutions used for the dilution and cleaning were Ultra Resi-Analyzed from J.T. Baker (Phillipsburg, New Jersey).

## RESULTS AND DISCUSSION

Separation of PCBs from the matrix is generally accomplished by solvent extraction. For water samples, the solvent of choice has for decades been methylene chloride (dichloromethane), because it has good extraction properties and is heavier than water, making separatory funnel extraction mechanically easy. Methylene chloride, other chlorinated solvents, and selected nonchlorinated solvents are under increasing scrutiny because of their potential health hazards to workers and because of concerns about environmental pollution. Although solvent substitution and elimination have been aggressively addressed by industries involving semiconductor manufacturing and coatings, analytical laboratories have been far slower to confront the issue.

Once extraction has eliminated the bulk matrix, additional interfering chemicals are separated from the PCBs by a variety of cleanup techniques, including chemical degradation and column chromatography. The column chromatographic techniques continue to use large, wasteful columns that are unnecessary even with the present large sample volumes. Major improvements in time savings and reagent minimization can be realized by appropriate scaling of the cleanup adsorbent and solvent volumes; further improvements can be realized by application of more specific separations using appropriate sorbent-solvent combinations.

Improvements in GC are needed to minimize the time of analysis without detriment to the quality of the results. Typically, separation times for PCBs approach 40-60 min. To save time and minimize cost, duplicates and confirmation injections are usually omitted during standard analyses. Fast GC presents an option to minimize time without adverse results and to improve data quality objectives.

## Solvent Substitution

Solvent substitution has been studied for the determination of PCBs in soils. Solvent substitution can achieve results comparable to standard methods and can eliminate environmentally less desirable solvents, as illustrated in Table 1. Widely varying solvents were used as extractants, generally without significant comparative evaluations among potential solvent systems. Technically acceptable solvents are those that yield quantitative extractions of the analyte (as measured by the spiked sample). Solubility of the PCBs and wetting of the soil matrix are contributing factors to the efficacy of the solvent. Our results indicate that many common solvents and solvent mixtures can yield quantitative extractions. Hexane is the solvent of choice for our future work.

## Macroscale Extractions

Macroscale and microscale extractions were performed for samples of oil, waste oil, and soils. For macroscale extractions, EPA method 600/4-81-045 and method 8080 were used for the determination of PCBs in transformer fluid and waste oils and in soil samples, respectively. The chromatographic columns used for the macroscale procedure for the analysis of oil samples were 50 cm long with 250-mL reservoirs. The columns were filled with approximately 20 g of Florisil™ heated overnight at 160°C, as described in the EPA method. The loaded column was preeluted with 75-100 mL of hexane. The 2-mL aliquot of sample was placed on top of a sodium sulfate layer. The sample was eluted with 280 mL of hexane, as shown in Table 2. For extraction of soils, the

**TABLE 1** Solvent Recoveries for Soxhlet Extraction of Soil Samples

| Extraction Solvent | Recovery of Aroclor 1254 (%) |
|---|---|
| Hexane | 101 |
| Acetone | 101 |
| 1:1 Hexane:acetone | 105 |
| 3:1 Hexane:acetone | 109 |
| 3:1 Acetone:hexane | 94 |
| Methylene chloride | 89 |
| 1:1 Methylene chloride:acetone | 104 |
| 9:1 Hexane:methylene chloride | 99 |
| 10:1 Toluene:methanol | 101 |

**TABLE 2** Macroscale and Microscale (SPE) Florisil™ Extraction of PCBs from Motor Oil

| Parameter | Macroscale | Microscale |
|---|---|---|
| Reagent | | |
| Florisil™ (g) | 20 | 1 |
| Hexane (mL) | 280 | 25 |
| Oil sample (g) | 1.5 | 0.2 |
| Total Waste (mL)[a] | ~ 300 | ~ 26 |
| Time (min) | | |
| Dilution/cleanup | 120 | 20 |
| Eluate concentration[b] | 50 | 50 |
| GC analysis time | 45 | 45 |
| Total | 215 | 115 |
| Cost ($) | | |
| Florisil™ | 2.61 | 2.37 (SPE syringe) |
| Hexane | 3.28 | 0.29 |
| Apparatus[c] | 0.52 | - |
| Total[d] | 6.41 | 2.66 |
| Yield (% ) | 100 | 100 |

[a] Assumes no recycling; does not include gloves and other ancillary waste.

[b] Nitrogen blowdown technique used for concentration of eluate. Time required is based on volume of solvent evaporated.

[c] Glass chromatography column with reservoir amortized over 100 uses (i.e., column investment of $52) for the macroscale procedure. Microscale procedure requires no comparable apparatus.

[d] Based on manufacturers' catalog prices or actual purchase requisitions; assumes complete consumption of amount purchased.

sample was dried over anhydrous sodium sulfate. The amount of sample used was relative to the percent humidity of the sample. The sample was extracted with approximately 300 mL of a hexane-methylene chloride mixture.

## Microscale Extractions

Two different approaches were used for the determination of PCBs in oil matrices: solid-phase extraction (SPE) and disk extraction. The SPE Florisil™ (activated $Mg_2SiO_3$) columns were used as specified in J.T. Baker Bakerbond Application Note EN-014. SPE sulfonic acid ($C_6H_5SO_3H$) and SPE silica gel (SiOH) microscale columns were used, as described in J.T. Baker Bakerbond Application Note EN-015. For soil matrices, a microscale Soxhlet system was used, decreasing solvent consumption and extraction time. Microscale extractions can cut the scale of the analysis by at least a factor of ten, as illustrated in Tables 2-4.

**TABLE 3** Comparisons of Soxhlet, Micro-Soxhlet, and Shakeout Extractions

| Parameter | Soxhlet | Micro-Soxhlet | Shakeout |
|---|---|---|---|
| Sample size (g) | 10 | 1 | 0.5 |
| Sodium sulfate used (g) | 10 | 1 | 0.5 |
| Extraction solvent volume (mL) | 300 | 15 | 15[a] |
| Extraction time (hr) | 16-24 | 5 | 0.25 |
| Concentration technique | Kuderna-Danish | Nitrogen blowdown | Nitrogen blowdown |
| Concentration time (min) | 10-20 | 10-20 | 10-20 |
| Florisil™ used for cleanup (g) | 20 | 1 | 1 |
| Solvent used for cleanup | Methylene chloride | Hexane | Hexane |
| Final concentration volume (mL) | 10 | 1 | 1 |
| Waste volume (mL)[b] | 610 | 25 | 24 |
| Apparatus cost ($)[c] | 2.50 | 1.40 | 0.19 |
| Reagent cost ($)[d] | 12.76 | 2.76 | 2.76 |

[a] The 15 mL was in three 5-mL extractions, each lasting 5 min.

[b] Assumes no recycling at this point; does not include gloves and other ancillary waste.

[c] Based on manufacturers' catalog prices or actual purchase requisitions. Soxhlet and micro-Soxhlet were amortized over 100 uses (with a Soxhlet investment of $250).

[d] Based on manufacturers' catalog prices or actual purchase requisitions; assumes complete consumption of amount purchased for sodium sulfate, Florisil™, and solvent.

**TABLE 4** Scale and Costs of Sulfonic Acid and Silica Gel Microscale Extraction

| Parameter | Quantity | Cost ($) | Time (min) |
|---|---|---|---|
| Reagent | | | |
| Sulfonic acid SPE column | 1 | 1.64 | |
| Silica gel SPE column | 1 | 1.56 | |
| Hexane | 11 mL[a] | 0.19 | |
| Connectors | 1[b] | 0.23 | |
| Dilution/cleanup | | | 20 |
| Eluate concentration[c] | | | 20 |
| GC analysis | | | 45 (6 min for fast GC) |
| Total Waste | 6 mL and 2 columns | | |
| Total Cost | | 3.62 | |
| Total Time | | | 85 (46 min for fast GC) |

[a] The method calls for dissolving 1.5-2.0 g of oil sample in 50 mL of hexane. However, such a scale is unnecessary, and both of the figures can be cut by a factor of ten. The data in the table are calculated for this methodology.

[b] Connectors may be used repeatedly. The price of one connector is amortized over 10 uses.

[c] Eluate concentration time is reduced over both of the Florisil™ procedures because the analyte is eluted in a total volume of only 5 mL, whereas the analyte from the Florisil™ procedures is concentrated from 25 mL.

## Waste Volume Reduction

Microscale extraction can cut the volume of waste generated by at least a factor of ten, as shown in Tables 2 and 3. This reduction is increasingly important as we move toward full cost accounting, including waste disposal costs, in the analytical chemistry laboratory.

## Fast Gas Chromatography

Figure 1 shows the fast gas chromatogram of Aroclor 1254. Initial studies used a 3-m DB-1 column (0.25 mm I.D.) programmed from 100 to 150°C at 12.5°C/min. A 1-µL sample (0.5 µg/mL), injected into a split/splitless injector in the splitless mode at 250°C, flowed to a cryogenic trap at -90°C prior to introduction into the column. The preconcentration time was 30 s. Although results were very promising, total separation of the PCB congeners was not achieved.

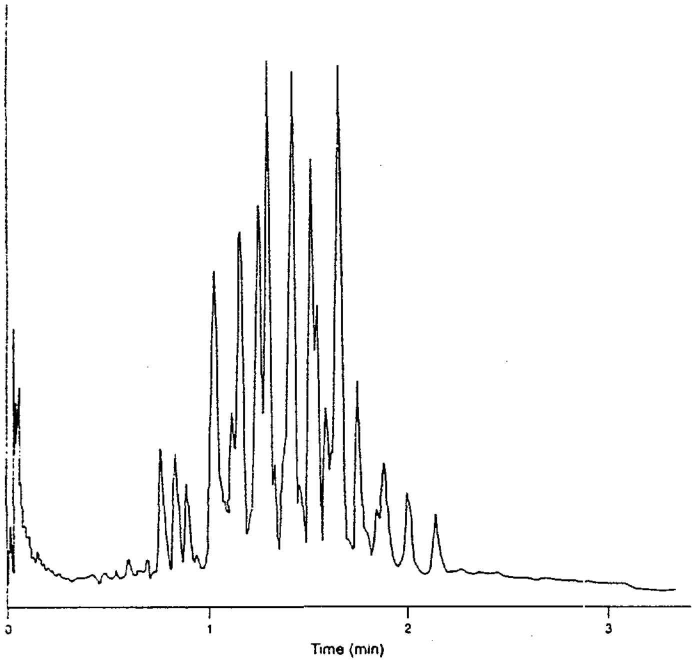

**FIGURE 1** Fast Gas Chromatogram of Aroclor 1254 with a DB-1 column (3 m, 0.25 mm I.D.) Programmed from 100°C to 150°C at 12.5°C/min (Hydrogen carrier gas velocity was 100 cm/s. A 1-µL sample at 0.5 µg/mL was injected into a splitless injector.)

Figure 2 shows the fast gas chromatogram of Aroclor 1254 for a run using a 10-m SPB-608 column (0.25 mm I.D.) and temperature programming starting at 190°C and finishing at 260°C. The initial temperature was kept at 190°C to accommodate the separation of congeners from other Aroclors (e.g., Aroclor 1248) with early elutions. Similarly, the final time was increased to allow the separation of high-molecular-weight congeners such as Aroclor 1260.

The application to PCBs is an excellent illustration of the power of fast GC, because the separation of an identifiable Aroclor pattern without full resolution of congeners often provides adequate data without the typical GC turnaround time of 20-40 min. Further, PCBs represent a different analytical challenge to the fast GC than do gases and volatile organic compounds, which have often been used to illustrate the inherent power of the technique. Separations, as shown in the figures, took less than 6 min, and the chromatograms met all requirements for the analysis of PCBs in environmental samples.

Fast GC holds significant promise, once the operational problems that limit its reproducibility and usability are overcome. An obvious advantage of the speed of fast GC is throughput of more samples per day, eliminating the need for a whole bank of GCs in a production laboratory environment. A corollary advantage would be rapid turnaround time in a field laboratory that is supporting on-line decision making in a remediation effort. However, this is a limited-use

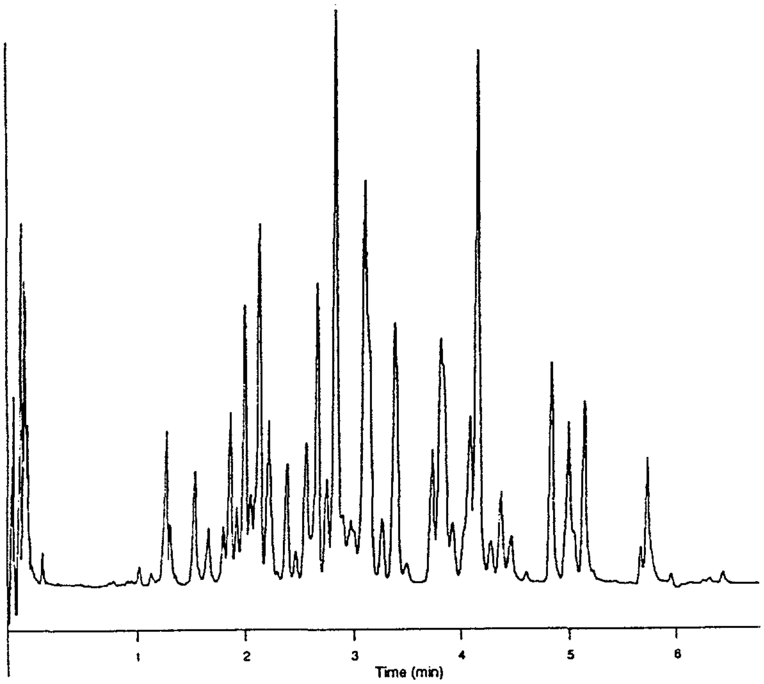

**FIGURE 2** Fast Gas Chromatogram of Aroclor 1254 with a SPB-608 column (10 m, 0.25 mm I.D.) Programmed from 190°C to 260°C at 15°C/min. (Hydrogen carrier gas velocity was 125 cm/s. A 1-µL sample at 0.5 µg/mL was injected into a splitless injector.)

application, because sample preparation is often the rate-limiting factor. Where fast GC is likely to become advantageous is in improving data quality. Few laboratories will have a sample load of several hundred injections per day per instrument; rather, we can reinvent GC analysis to include more calibration replicate injections and to permit signal averaging and standard addition. These common quality control techniques, routinely practiced in other areas of analytical chemistry, have been recommended in several interlaboratory study reports on PCB analysis in environmental samples. Another area that will be facilitated by fast GC is multidimensional analysis to exploit retention-time information for improved compound identification. Thus, fast GC represents an opportunity for a paradigm shift in our approach to improving the quality of GC analysis, rather than simply a tool for increasing throughput and cutting cost.

## Cost Considerations

Microscale extraction significantly reduces the costs of apparatus, reagents, and labor. The cost reduction for the apparatus and reagents are illustrated in Tables 2-4. The labor costs were not quantified but can be inferred directly from the tables. A cost impact will occur during the transition to microscale extraction, in that new glassware and instrumentation will be purchased, method validation will require some overhead time (see below), training will require some down time, and some efficiencies will be seen only after a break-in period.

### Quality Assurance

Any adaptation of a method requires some sort of internal validation and data quality objectives to demonstrate performance. The changes discussed here are no different. Any laboratory adapting its routine methods to microscale techniques and fast GC needs to validate the changes with the appropriate quality control samples to demonstrate that the laboratory is providing data of known and consistent quality. In addition, quality control measures must be modified as necessary to clearly monitor the performance of the analyses.

## CONCLUSION

The application of microextraction techniques to PCB analysis is an excellent illustration of the application of new technologies in a performance-based measurement system. We investigated new extraction and cleanup procedures for the analysis of soils and oils, incorporating solvent substitution, miniaturization of extractions, minimization of reagent consumption, reduction of energy consumption, reduction of cost per analysis, and reduction of time by applying new fast GC technology.

The methods developed here have direct applicability to routine PCB analyses, such as those used by the utility industry and in environmental characterization and monitoring programs. With performance-based methods, the applications presented here can be applied now, without waiting for regulatory approval.

## ACKNOWLEDGMENTS

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# ADDRESSING DATA QUALITY ISSUES THROUGHOUT THE SITE CHARACTERIZATION PROCESS TO MINIMIZE DECISION ERRORS

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## ABSTRACT

Making an incorrect decision concerning the need for cleanup at a hazardous waste site can result either in leaving a potentially harmful situation in place or unnecessarily committing large sums of money to cleaning up a site that otherwise poses no significant threat. Site management decisions are unavoidably associated with some degree of error because: (1) decisions are always rendered based on incomplete information and (2) data used to support decisions are subject to uncertainty. However, there are also many questionable practices that are commonly employed throughout the site characterization process that increase decision error beyond the unavoidable minimum.

A variety of common practices that can contribute substantially to decision error are identified below and evaluated both to identify conditions under which they lead to erroneous conclusions and to quantify the rate that such errors can occur. It will also be shown how these problems can be avoided by paying close attention to data quality issues throughout the site characterization process including, particularly, use of the data quality objectives (DQO) process to focus the planning of site investigations. Importantly, the problems introduced by the practices discussed are insidious; unless one addresses data quality issues throughout the site characterization process, one will never know whether a decision error has been committed.

## INTRODUCTION

Under the Federal Superfund program, state analogs to the superfund program, and (increasingly) hazardous waste sites in general, site risk assessments are employed to determine whether hazardous waste sites pose unacceptable risks to human health and/or the environment and, therefore, whether cleanup is warranted. Cleanup costs commonly reach tens of millions of dollars at the largest of such sites. Thus, making an incorrect decision can result either in leaving a potentially harmful situation in place or unnecessarily committing large sums of money and limited resources to cleanup a site that otherwise poses no significant threat. It is therefore important to minimize errors in the procedures used to determine the need for cleanup.

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The conclusions of a risk assessment are typically drawn by comparing estimated risks either to each other or to fixed targets. Comparisons between estimated risks, for example, may be used to rank the magnitude of problems at multiple sites. When fixed targets are selected to represent maximum acceptable risk, comparisons between estimated risks and fixed targets are typically performed to determine whether risks posed by a particular site (or source) are acceptable. When risks are found to be unacceptable, cleanup is generally required. For the indicated comparisons, the probability that conclusions from a risk assessment are "correct" is a function of the degree to which risks estimated in the assessment are accurate and precise or, at a minimum, the degree to which any biases introduced in the risk assessment process are consistent across risk estimates and target values.

In turn, the degree to which estimated risks are accurate and precise (or the extent to which biases are consistent) are functions of the quality of the underlying data and the appropriateness of the procedures used to derive risk estimates from such data. Over the years, however, several practices have been adopted that may compromise the quality of the data used to support risk assessments so that the conclusions drawn from such data should be considered unreliable. Although a numerical result can always be calculated by a manipulation of data, there is no assurance that such a result bears any relationship to true conditions in the field, unless one considers data quality. The problem is insidious.

When evaluating data to support risk assessments and render site management decisions, some degree of error is unavoidable. This is because:

(1) decisions are always rendered based on incomplete information; and

(2) data used to support decisions are subject to uncertainty.

However, there are also many questionable practices that are commonly employed throughout the site characterization process that can increase decision error beyond the unavoidable minimum. These include use of procedures that generate data that are not optimal for the purposes to which the data are applied and use of statistical procedures to evaluate data that are not appropriate for the characteristics of the data being evaluated. Questionable practices that result in the use of non-optimal data include:

- using data generated in a study designed for one purpose in an evaluation intended for a different purpose;
- combining data from multiple investigations without considering the compatibility of the multiple data sets for a given purpose;
- designing sampling plans that generate unintentionally biased data;
- using data from biased investigations to develop estimates that are intended to be unbiased; and

- using inappropriate procedures to "adjust" data sets to account for non-detects.

Questionable practices that result in the application of statistical procedures that are inappropriate for the characteristics of the data being evaluated include:

- not properly matching decision rules to the characteristics of the data before proceeding with an evaluation;
- using "default" procedures without due consideration of their appropriateness to a particular situation; and
- misapplying the laws of inequalities when constructing decision logic.

In recent years, several colleagues and I have evaluated the kinds of problems that can be created by carelessly employing the practices listed above. In a series of recent publications, we have characterized the conditions under which such practices lead to erroneous conclusions and, in some cases, to quantify the rate that such errors can occur. An overview of the results of these studies and their implications for site characterization is presented in the Discussion Section below. This follows a brief background discussion to introduce relevant terms and concepts.

## BACKGROUND

Before exploring the ways in which questionable practices can contribute to decision errors, it is necessary to introduce the formalism typically employed when using field measurements to support field data. The types of decision errors that can occur and the manner in which they are controlled are also introduced.

### Decision Rule Formalism

In most site risk assessments, the decision whether to remediate ultimately reduces to determining whether the arithmetic mean, "m," of some contaminant concentration within a defined area or volume element of the environment exceeds a critical target value, "Q" (USEPA 1992). In this context, m is the *true* arithmetic mean of the contaminant concentration and Q typically represents the boundary between acceptable and unacceptable conditions (i.e., the boundary between acceptable concentrations and those that are large enough to present unacceptable risks). The manner in which such comparisons fit into the larger scheme of a risk assessment has been described previously (Berman 1995).

The comparison between Q and estimates of m represents a test in which a *null* hypothesis (e.g. that $m < Q$, which might indicate that a site is "clean") is assumed to be true unless conditions at the site warrant rejecting the null in favor of an alternate hypothesis (e.g. that $m \geq Q$, which might indicate that cleanup is required). It is equally valid to begin with the assumption that the site is "contaminated" (i.e. that $m > Q$) and to test whether this null can be rejected in favor of an alternate (i.e. that $m \leq Q$) to "prove" that a site is clean. In fact, current guidance favors this latter formulation when making decisions at Superfund sites (USEPA 1992). As shown in the Discussion Section, however, these two hypothesis formulations are equivalent so that the probability of reaching an incorrect conclusion is not affected by the choice of the formulation of the null hypothesis.

In the absence of error (uncertainty) in an estimate of m, a direct comparison between m and Q provides a perfect test of the null hypothesis. However, the true value of m can never be known exactly. This is due primarily to the limited ability of a finite number of samples that are collected from a large and variable environmental medium to completely represent the characteristics of that medium. Also, methods employed for sampling and analysis are subject to error and this introduces additional uncertainty in the estimates of m. Thus, summary statistics that are biased estimates of m (such as upper or lower confidence limits) are typically derived from field measurements and compared to Q to determine *with some predefined level of confidence* whether m is likely to exceed Q. In fact, a variety of summary statistics can be (and have been) used to test hypotheses concerning the true mean of a field distribution of concentrations and each offers various advantages and limitations (Berman et al. 1998a and 1998b).

The nature of the summary statistic selected to represent the mean, m, the manner in which it is calculated from field measurements, and the formulation of the hypotheses employed to compare that statistic to the target, Q, constitute a "decision rule." The probability that a decision rule leads to an incorrect decision (i.e. the error rate) is a function of the characteristics of the decision rule, the nature of the underlying true condition at the site and the degree to which the set of measurements employed to evaluate the decision are representative of the environmental medium that is the subject of the decision.

The degree to which a set of samples can be assumed to represent the sampled medium is a strong function of the process by which locations were selected for the samples collected, the number of samples collected, and the characteristics of the methods employed for sampling and analysis. The effects on decision errors associated with the data quality limitations imposed by each of these factors were explored in a previous study (Berman 1995) and are summarized in the Discussion Section under considerations associated with non-optimal data sets.

Even assuming that data are collected optimally, however, the choice of the decision rule can also contribute to decision error. The manner in which the choice of decision rule affects decision error has also been explored in previous studies (Berman et al. 1998a and 1998b) and is also summarized in the Discussion Section under considerations associated with use of inappropriate statistical procedures.

## Types of Decision Errors

Given a particular decision rule in which, for example, it is assumed that $m < Q$ as a null hypothesis and a comparison between Q and some summary statistic employed to represent m is used to decide whether to accept or reject the null hypothesis, there are four possible outcomes:

- m is truly less than Q and the comparison leads properly to a conclusion that m is less than Q;
- m is truly less than Q but the comparison leads falsely to a conclusion that m exceeds Q;
- m truly exceeds Q and the comparison leads properly to a conclusion that m exceeds Q; or
- m truly exceeds Q but the comparison leads falsely to a conclusion that m does not exceed Q.

The first and third of the above listed outcomes are correct results. The second and fourth are erroneous. Thus, there are two kinds of errors that can potentially occur during the application of a decision rule. A "Type I" error occurs when the null hypothesis is falsely rejected. In the illustration presented above, this corresponds to the second of the listed outcomes. A "Type II" error occurs when the null hypothesis is falsely accepted and corresponds to the last of the possible outcomes listed in the above illustration.

Note that, because Type I and Type II errors are defined based on whether the null hypothesis is accepted or rejected, the relationship between these types of errors and the specific outcomes of a comparison depends on the way that the null hypothesis is defined. Thus, for example, if a new decision rule is examined in which the null hypothesis is assumed to be $m > Q$ (the reverse of the illustration above), then the second of the four outcomes listed above becomes a Type II error and the fourth becomes a Type I error.

In the face of uncertainty, formal decision rules are applied to control decision error. Statistical control is achieved when, due to the inherent design of a particular statistical test, the null hypothesis is rejected at a *fixed and defined* rate at the decision point (i.e. when $m = Q$). The rate that the null is rejected at the decision point is termed the significance or $\alpha$ (alpha) level for the test.

Importantly, statistical control implies that the significance level of the test is independent of sample size and other characteristics of the data to which the decision rule is applied. However, the rate of rejection of the null hypothesis for true conditions other than the decision point (i.e. when $m \neq Q$), is generally a function of both the true condition (i.e. the value of m) and the sample size. The rate at which the null hypothesis is rejected for conditions under which rejection is correct (i.e. when $m \geq Q$) is termed the power of the test. If a statistical test is well behaved, the power of the test increases as sample size increases.

In practice, the intended statistical control of a particular test is achieved when the characteristics of the data to which the test is applied completely satisfy the validity criteria for the test. The validity criteria for a particular statistical test are the mathematical axioms that were employed to construct the test (e.g. some tests require that data distributions be symmetric). However, tests are frequently applied to data that exhibit characteristics that do not strictly satisfy such criteria. If deviations are small, the test may still behave reasonably and statistical control will be maintained. However, the characteristics of environmental data frequently fall at the fringe of acceptability for the kinds of spatially-independent statistical tests that are commonly applied. The conditions under which statistical control fails for various commonly employed statistical tests and estimates of the resulting error rates have been reported in the literature (Berman et al. 1998a and 1998b) and are summarized in the Discussion Section below.

## DISCUSSION

The manner in which each of the questionable practices identified in the Introduction can contribute to decision errors is considered below.

### The Consequences of Using Non-optimal Data Sets to Support Decisions

The first five of the questionable practices listed in the Introduction lead to use of non-optimal data to support decisions and the consequences of using non-optimal data are illustrated in a simulation that was previously reported in the literature (Berman 1995). The advantage of studying a simulated case (versus an actual case) is that the true conditions for the simulated case can be defined absolutely. Thus, the reliability of the conclusions drawn from characterization of a simulated site can be determined by comparing such conclusions to the underlying true conditions. For real sites, in contrast, the underlying true conditions can never be known with certainty.

In the simulation reported by Berman (1995), a hypothetical site was constructed in which an old landfill is rumored to exist at the end of an old, paved road. It is further assumed that trucks from a nearby plant would drive to the end of the paved road and dump a hazardous "Compound Q" at the edge of the landfill. A map of the hypothetical site is presented in Figure 1.

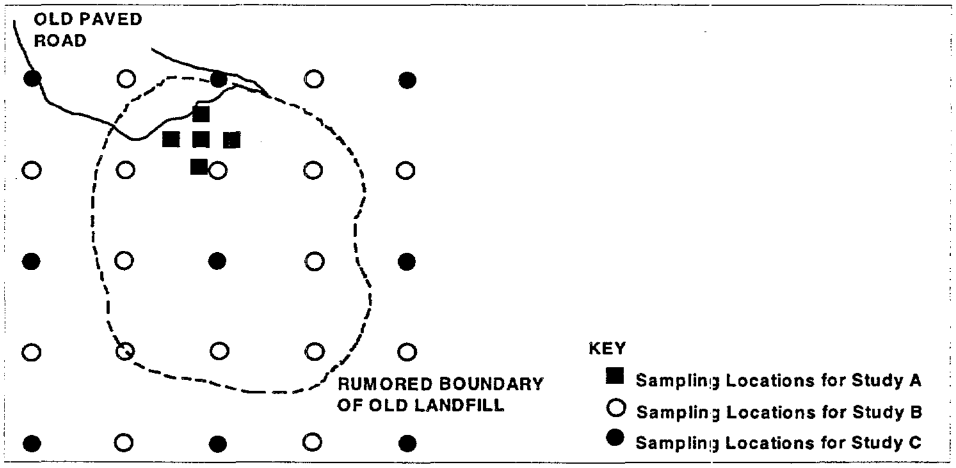

**FIGURE 1** Sampling Locations for a Hypothetical Landfill (Source: Berman 1995)

The underlying "true condition" was constructed for this simulation by defining a two-dimensional distribution of contamination that is consistent with the above-stated scenario. This distribution was then "sampled" by picking sampling locations and setting the value of the resulting "measured" concentration to the value of the concentration that exists within the synthesized distribution at the location sampled.

In a sequence that parallels the evolutionary path common to investigations of real sites, it is assumed in this simulation that the site is ultimately sampled three separate times for three separate purposes:

(1) to confirm the presence of the rumored Compound Q, a series of samples are collected from locations that are selected purposively in areas expected to be most highly contaminated (Study A). This creates a data set that is intentionally biased high;

(2) to estimate the "nature and extent" of contamination, the area within which the landfill is assumed to reside is sampled systematically (Study B); and

(3) to improve characterization of the "nature and extent" of contamination (to support remedial design), sampling is conducted over a systematic grid that is more closely spaced than that sampled in Study B (Study C).

The locations of the samples collected during each of the studies listed above are also depicted in Figure 1. Estimated concentrations derived using the measurements from each of the three studies are summarized in Table 1.

**TABLE 1** Summary of Findings for the Data Sets from Studies of a Hypothetical Landfill (in ppb)[a]

| Data Set | No. of Samples | Statistical Distribution[b] | Mean (generic)[c] | MLE Mean (log-dist)[d] | $UCL_{95}$ (log-dist)[e] | CV[f] |
|---|---|---|---|---|---|---|
| Study A | 5 | Lognormal | $4.7x10^5$ | $6.8x10^6$ | $1.8x10^8$ | 2.2 |
| Study B | 9 | Lognormal | $3.2x10^3$ | $2.1x10^5$ | $2.9x10^6$ | 1.98 |
| Pooled A and B | 14 | Lognormal | $1.7x10^5$ | $1.3x10^7$ | $1.6x10^8$ | 3.64 |
| Study C | 25 | Lognormal | $9.0x10^4$ | $9.3x10^5$ | $6.1x10^6$ | 3.4 |

[a] Adapted from Berman (1995).

[b] Based on Goodness-of-fit tests performed as described in Gilbert (1987).

[c] Arithmetic mean calculated using the sum of values divided by the number of values (Gilbert 1987).

[d] Arithmetic mean calculated using the simplified maximum likelihood estimator for a lognormal distribution (Gilbert 1987).

[e] Upper 95% confidence limit to the mean of a lognormal distribution (Land 1971).

[f] "CV" is the coefficient of variation, which is the appropriate independent variable for describing the variability of lognormally distributed data (Gilbert 1987).

As indicated in the first column of Table 1, the data sets evaluated include: results from Study A, results from Study B, a data set consisting of the pooled results from the combined Studies A and B, and results from Study C. The number of samples in each data set is listed in the second column of the table. The third column of Table 1 indicates the results of goodness-of-fit tests conducted on each data set to determine whether it might be adequately described by a normal or a lognormal distribution; all of the data sets listed can be adequately described by lognormal distributions.

The fourth and fifth columns of Table 1 provide "best" estimates of the mean of each data set calculated, respectively, using the general equation for the arithmetic average and the simplified maximum likelihood estimator (MLE) for the arithmetic mean of a lognormal distribution (Gilbert 1987). The sixth column of the table provides another kind of estimate for the mean for each data set. In this column, estimates are presented for the upper 95% confidence limit to the mean ($UCL_{95}$) of each data set. These were calculated using the Land Equation, which is appropriate for lognormally distributed data (Gilbert 1987). The last column of the table presents estimates of the coefficient of variation, which is a measure of the spread (variability) of the data (Gilbert 1987).

Several trends are immediately apparent from Table 1. It is clear, for example, that the estimates of the mean concentration for Compound Q vary by five orders of magnitude across the data sets for the kinds of estimates of the mean depicted (i.e., across all of the entries in Columns 4, 5, and 6). Even considering results based on any one procedure for estimating the mean (i.e., within each column), results vary by up to two orders of magnitude across data sets. Which is correct? The answer depends on what question is being addressed. For example, if the goal is to find the highest localized concentrations in the landfill, then mean estimates based on Study A may be appropriate.

If the goal is to determine the average concentration of Compound Q over the contaminated area of the landfill as a whole, Study C (the most dense of the data sets sampled systematically) provides an answer that is closest to the truth. The less dense of the data sets sampled systematically (Study B) also gives answers that are in relatively close agreement with Study C. In contrast, concentration estimates derived from the data set that was intentionally biased (Study A) can be as much as two orders of magnitude higher than that obtained from the unbiased Studies B or C. Concentrations estimated from the data set derived by pooling Study A and Study B are also as much as two orders of magnitude greater than the concentrations estimated for Study B alone.

It is also clear from Table 1 that estimates of the mean concentration for any specific data set vary by up to three orders of magnitude, depending on which procedure is employed for calculating the estimate (i.e., within any one row across Columns 4, 5, and 6). Because all of the data sets have been shown to be adequately described by lognormal distributions, the correct procedure for deriving a best-estimate of the mean is to use the MLE (Column 5). Although the general equation for estimating the mean (Column 4) is an unbiased estimator for any distribution, for lognormal distributions, it converges to the true mean more slowly than the MLE. Thus, when data are lognormally distributed, the traditional procedure for estimating the mean should not be used for small data sets (such as those evaluated in Table 1) because results will not be stable.

Estimates derived using the general equation for the arithmetic mean are presented in Table 1 to illustrate what can happen if the incorrect estimator for the mean is used during data evaluation. This commonly occurs, for example, if the characteristics of a data set are ignored when selecting the statistical procedure to be used for data evaluation. That the two best estimates of the mean derived for each data set (Columns 4 and 5 of Table 1) vary by an order of magnitude is a function of the lack of stability for the means estimated using the general equation (Column 4). The direction of the apparent bias between the two means is due simply to chance; for other data sets, the traditional mean can just as easily be orders of magnitude larger than the means calculated using the MLE equation (Gilbert 1987). Thus, biases introduced by the use of this type of incorrect statistical procedure will be inconsistent across risk estimates.

The $UCL_{95}$ is also presented in Table 1 because such upper bound estimates of the mean are more frequently employed in risk assessments than best estimates of the mean. These estimates are used because they can provide formal statistical control of uncertainty (as defined in the Background Section). Use of the $UCL_{95}$, for example, assures that there will be no more than a 5% chance that the true mean is underestimated. Therefore, if such an estimate is compared to a target value in a risk assessment, there would be no more than a 5% chance that a site is falsely determined to be clean.

Importantly, the correct procedure for calculating a $UCL_{95}$ varies depending on the characteristics of the data. Careless selection of an inappropriate procedure may result in calculating $UCL_{95}$ estimates that are orders of magnitude different than the appropriate value. Clearly, therefore, such misuse can contribute substantially to decision error. The $UCL_{95}$ estimates presented in Table 1 were derived using the appropriate procedure for lognormally distributed data, which appears appropriate for this case. The consequences of using inappropriate statistical procedures is discussed in a later subsection of this discussion.

The results in Table 1 indicate that estimates of concentrations derived from field measurements can vary by orders of magnitude depending on what data are used and how the data are evaluated. Clearly, employing inappropriately derived concentration estimates in a risk assessment can contribute substantially to decision errors. Given the above discussion, deriving appropriate concentration estimates requires that one employ data that are generated in investigations designed specifically for the purpose for which the data are intended (i.e., requires use of optimal data). Thus, one should generally avoid:

- using data generated in a study designed for one purpose in an evaluation intended for a different purpose;
- combining data from multiple investigations without considering their compatibility for a given purpose;
- designing sampling plans that unintentionally generate biased data; and
- using data from biased investigations to generate estimates that are intended to be unbiased.

Thus, to minimize the chance of increasing decision errors due to the manner in which data are collected and evaluated, the first four of the questionable practices listed in the Introduction should generally be avoided. The fifth of the questionable practices, use of improper adjustments to account for non-detects, is discussed below.

Note, deriving appropriate concentration estimates also requires that the procedures used to evaluate such data be matched carefully both to the objectives of the evaluation and to the characteristics of the data. Contributions to decision errors associated with the selection of data evaluation procedures are discussed later in this Section.

## Using of one-half of the Sample Quantitation Limits for Non-detects

It is common practice to substitute one-half of the sample quantitation limits for non-detects when evaluating a set of measurements to estimate concentration. The consequences of this practice were illustrated in a talk presented by Kenny Crump to the State of California Department of Toxic Substances Control (Crump 1993).

In his talk, Crump (1993) showed that, as long as more than a very small fraction ( a few percent) of the measurements in a data set are non-detect, the mean of the data set will be overestimated whenever values of one-half of the sample quantitation limits are substituted for non-detects in the data set. This is particularly true when data sets exhibit behavior that is characteristic of lognormal distributions, which is relatively common for environmental data (Berman 1994).

Crump (1993) showed further that overestimation likely increases as the fraction of non-detects increases. In some of the examples presented in his talk, the bias was as much as several orders of magnitude. However, unless the mean is also calculated using a less biased procedure (such as the maximum likelihood estimation procedure discussed in the talk), the magnitude of the bias introduced in the mean by the use of this common substitution is unquantifiable. In addition, because the bias varies as a function of the characteristics of the data, biases will be inconsistent across data sets and, correspondingly, across risk estimates.

The effect that use of one-half the sample quantitation limit has on upper bound estimates of the mean is even more confusing (Crump 1993). In this case, the bias introduced may be either positive or negative, depending on a number of factors and, once again, the magnitude is unquantifiable (unless an unbiased procedure for estimating the upper bound is also employed for comparison). Such biases are likewise inconsistent across risk estimates.

Given that use of one-half the sample quantitation limit can create errors in estimates of mean concentrations that can vary by orders of magnitude from estimates derived using more appropriate procedures, it is clear that indiscriminate use of these kinds of substitutions can contribute substantially to decision errors.

## The Consequences of Using Inappropriate Decision Rules

Even assuming that the data to be used to support a risk assessment have been generated in an optimally designed investigation, the chance of committing a decision error can still be increased substantially depending on the nature of the decision rule employed during the evaluation of the data.

The vast majority of procedures employed for evaluating site data are based on what is called "parametric analysis." In a parametric analysis, data are assumed to display a distribution that closely mimics the characteristics of a known statistical distribution (e.g. a normal or lognormal distribution) with defined central value and spread. In turn, the characteristics of the known distribution are assumed to closely parallel the corresponding characteristics of the data.

When there is good correspondence between a data distribution and the shape of a known distribution, then the properties of the known distribution closely match the properties of the data. However, when the correspondence is poor, the properties of the known distribution are unlikely to relate well to the properties of the data. To minimize decision errors, it is therefore important to closely match the data to be evaluated to the characteristics of the known statistical distribution that is selected to represent the data. Sometimes this is done formally using goodness-of-fit tests and we recommend that such tests be employed routinely during the analysis of data from hazardous waste sites. Frequently, however, the relationship between a particular data set and the statistical distribution chosen to represent it is simply assumed and this can lead to substantial decision errors.

The quality of the relationship between a known statistical distribution and a set of field data that the distribution is intended to represent is illustrated in Figure 2. Figure 2 shows a curve representing a lognormal distribution that has been fit to two sets of data (one on the right and one on the left). To indicate the quality of the fit, each data set has been ordered from its lowest to its highest value, the data have then been grouped into a series of narrow ranges, and the number of values within each range plotted as a histogram on the graph. Since these then represent the frequency distribution for the values of the data, they can be compared directly to the frequency distribution of the ideal, lognormal distribution that is represented by the curve on each graph.

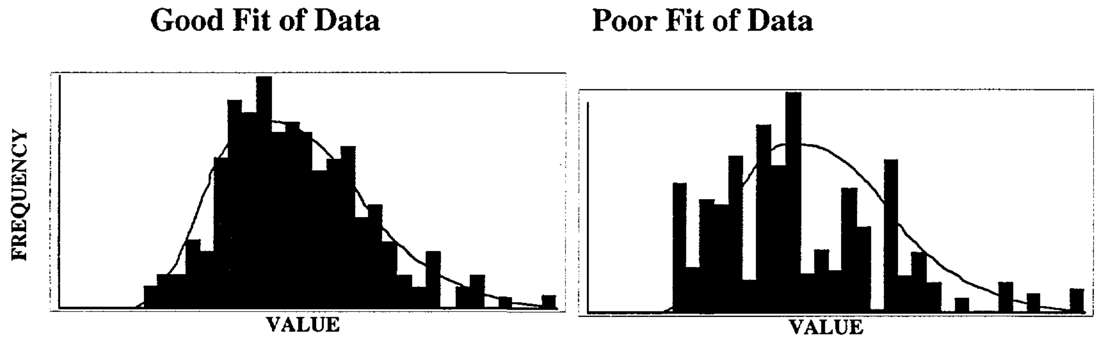
**Good Fit of Data** **Poor Fit of Data**

**FIGURE 2** Fit of Two Data Sets to a Lognormal Distribution

The fit of the curve to the data on the left graph in Figure 2 is a good fit. This is clear from the degree of agreement between the frequencies represented by the individual columns of the histogram and the curve representing the ideal, lognormal distribution. Consequently, the properties of the ideal, lognormal distribution can be expected to corresponding to the characteristics of the data set represented on the left graph. In contrast, the data presented on the right graph in Figure 2 is poorly fit by the curve representing the lognormal distribution. Therefore, one can place little confidence in the assumption that the properties of the curve correspond to the characteristics of the data set presented in this graph.

To more formally characterize the problems that can be introduced when data are evaluated using statistical procedures (decision rules) that are not properly matched to the properties of the data, it is useful to introduce the concept of a power curve. Before employing such curves to further discussion of the effects that choice of a decision rule have on decision errors, the properties and uses of a generic (hypothetical) power curve are described briefly below.

*Hypothetical Power Curve*

A power curve depicts the relationship between the probability of rejecting the null hypothesis and the true condition (i.e. mean and CV) for a given decision rule. To illustrate, a hypothetical curve is presented in Figure 3. The X-axis in Figure 3 indicates one dimension of the true condition (expressed in terms of the ratio of the true mean, m, to the target value, Q). Note that it is presented on a logarithmic scale. The Y-axis is the probability of rejecting the null hypothesis (i.e. that m < Q). A "perfect" power curve would indicate zero probability of rejecting the null hypothesis whenever the ratio of m to Q is less than one and the probability would rise to one for all values of this ratio greater than one. This "perfect" (errorless) power curve is depicted as a dotted line in Figure 3. Note that the terminology employed in this discussion was introduced in the Background Section.

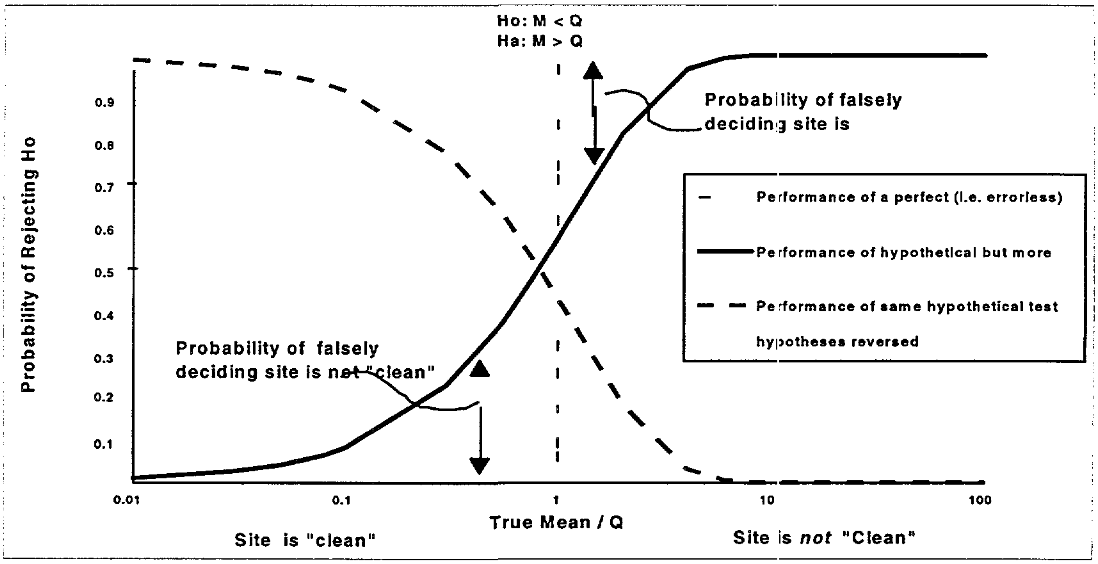

**FIGURE 3** A Hypothetical Power Curve (Source: Berman et al. 1998a)

A more realistic power curve is depicted as the solid line in Figure 3. By comparing the solid line to the dotted line, the effects of error become apparent. To the left of one on the X-axis, the vertical distance between the solid curve and the X-axis (which is also the line representing zero probability of rejecting the null) represents the rate at which a false positive (Type I) error can occur. Thus, for this hypothetical curve, when m is one tenth of Q (i.e. at 0.1 on the X-axis), the solid curve indicates an 8% chance of *falsely* rejecting the null. This error increases as the ratio m/Q approaches one.

Once m/Q exceeds one in Figure 3, the null hypothesis should be rejected. Therefore, to the right of one on the X-axis, the vertical distance between the solid line and the line representing unit probability of rejecting the null represents the false negative (Type II) error rate. As depicted, this error rate is vanishingly small when the m is 10 times Q but increases steadily as m approaches Q from the right. The power curves presented in the remaining figures, which depict the performance of the decision rules evaluated in this paper, can be interpreted in precisely the same manner as Figure 3.

One additional feature of Figure 3 deserves mention. The dashed line in the figure represents a power curve for a hypothetical decision rule that is identical to that assumed for the solid line except that the dashed curve represents testing a reversed set of hypotheses (i.e. the alternate hypothesis for the solid line that $m > Q$ is taken as the null for the dashed line with the old null serving as the new alternate hypothesis). This is presented to illustrate that reversing hypotheses serves precisely to transform the power curve by reflection across the line defined by 50% probability of rejecting the null. This relationship holds because the two (complimentary) decision rules would be tested using the same data set for the same true condition so that the value of the summary statistic would be the same. Thus, all that changes is that values formerly indicating rejection of the null now indicate acceptance of the null and vice versa. The relationship between a power curve for a particular decision rule and one for the same decision rule with the hypotheses reversed was confirmed during the simulations conducted in the previous study by Berman et al. (1998a).

### *The Performance of Decision Rules Applied to Real Data*

A set of power curves for the decision rule most commonly applied to environmental data is presented in Figure 4. This decision rule is a test of the null hypothesis that $m < Q$ in which the 95% upper confidence limit ($UCL_{95}$) to the mean of the data is compared to the target value (Q) to determine whether the null should be rejected. For this rule, the $UCL_{95}$ is calculated using the Land Equation (Land 1971), which is the appropriate statistical procedure for lognormally distributed data. The various curves that are presented differ by the number of samples included in the data set. As indicated by the key at the bottom, sample sizes of 5, 10, 20 and 100 samples are represented. These curves were generated from a simulation as part of a study that was previously reported (Berman et al. 1998a).

As indicated by the curves presented in Figure 4, the chance of falsely concluding that the null hypothesis should be accepted (i.e. that the site is clean) is limited to no more than 5% by this decision rule (under the conditions represented by the figure), no matter how many samples are included in the data set. This can be seen by considering that the null hypothesis can only be false when $m \geq Q$ (which represents the parts of each curve that lie to the right of one on the X-axis) and noting that the probability of rejecting the null hypothesis when $m \geq Q$ is never less than 95% for any of the curves depicted. In fact, all of the curves pass through the point representing 95% probability of rejection when $m = Q$ (i.e., at one on the X-axis) and approach unit probability of rejection to the right.

The behavior described in the last paragraph represents the kind of statistical control that is intended by use of the $UCL_{95}$, as previously discussed. Because this procedure is health protective in that it limits the chance of falsely concluding that a site is clean, it has been used widely to support cleanup decisions at hazardous waste sites. As indicated below, however, the indicated statistical control is seldom achieved in practice and, even when it is achieved, it comes at a cost.

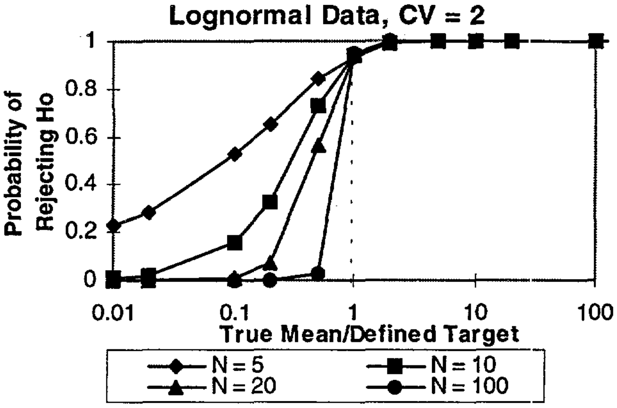

**FIGURE 4** Power Curves Indicating the Probability of Rejecting the Null Hypothesis (that m < Q) Using a Comparison Between the Estimated $UCL_{95}$ of the Mean and the Target for Lognormally Distributed Data (CV = 2)

If one examines the left side of Figure 4, it is readily apparent that the decision rule depicted is not very good at limiting the probability of falsely rejecting the null hypothesis (i.e., concluding falsely that a site requires cleanup). For example, when the true mean is as little as one fifth of the target and 10 samples are employed in the analysis, there is a 30% chance of falsely concluding that cleanup is required.

The probability of falsely concluding that cleanup is required also increases as the variability or spread of the data increases. The curves depicted in Figure 4 were developed assuming that the data exhibit a Coefficient of Variation (CV) of 2. However, environmental data frequently exhibit even greater variability; CV's as large as 5 or 10 are not uncommon and can be even larger (Berman 1994). With a CV of 5, the probability of falsely concluding that cleanup is required approaches 65% for a data set containing 10 samples when the true mean is no more than one fifth of the target. Even for a data set containing 20 samples (and exhibiting a CV of 5), the chance of falsely concluding that cleanup is required is still as large as 40% when the true mean is as small as one fifth of the target.

More importantly, the error rates associated with both types of error (i.e., either falsely accepting or falsely rejecting the null) increase when the underlying assumptions concerning the characteristics of the data are not satisfied. The curves in Figure 4 were generated from a simulation in which the data sets examined were drawn from ideal, lognormal distributions. Frequently, however, environmental data do not exhibit behavior that is characteristic of a lognormal distribution. When data that are not lognormally distributed are evaluated using the decision rule described above, the true error rates that occur are greater than the error rates indicated by the ideal curves depicted in Figure 4. This is illustrated in Figure 5.

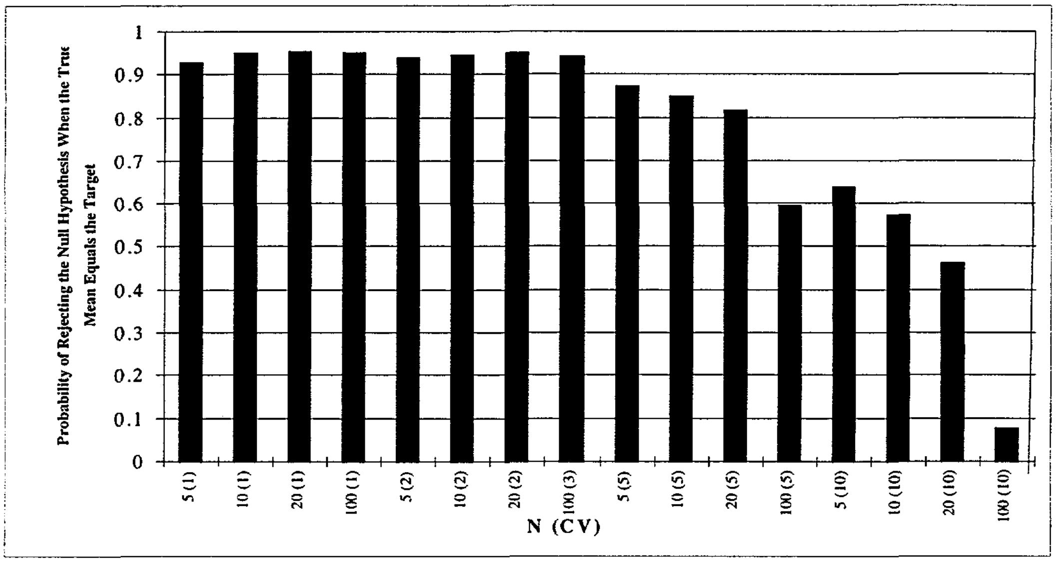

**FIGURE 5** Alpha Values for a Decision Rule Involving Comparison of the $UCL_{95}$ to the Target Applied To Data Sets Derived from a Lognormal Distribution Censored at 10% of the Target Value (Source: Berman et al. 1998b)

Figure 5 depicts the alpha value that is obtained for the decision rule described above when it is applied to data sets whose behavior varies from that of an ideal lognormal distribution. As indicated previously, the alpha value is the probability of rejecting the null hypothesis at the decision point (i.e., when m = Q). Also indicated previously, the alpha value for decision rule described above should be 95% when the intended statistical control is achieved.

The data sets depicted in Figure 5 vary from ideal lognormal distributions in that they are all censored at a value set equal to 10% of the target, Q. To censor the data, any samples derived from the underlying distribution whose values are less than 0.1 x Q, were set equal to 0.05 x Q. Thus, such a data set is designed to mimic an environmental data set containing non-detects that have been adjusted by adopting a value of one-half the detection limit for each of the non-detects.

Each of the bars depicted in Figure 5 represents a censored data set containing the number of samples, "N," and exhibiting the spread (CV) that are indicated by the numbers presented on the X-axis. The Y-axis in the figure indicates the alpha value (the probability of rejecting the null hypothesis that m < Q when m = Q) that is achieved for the data set indicated.

Although alpha values of 95% appear to be achieved for the first several of the data sets depicted in Figure 5, it is readily apparent that statistical control is lost for some of the latter data sets depicted in the figure. In fact, the alpha value for the last data set depicted in the figure (the one on the extreme right) is only about 8%. Generally, the alpha value (and therefore chance of falsely accepting the null hypothesis) increases as the spread of the data increases and as the number of samples in the data set increases. Thus, in addition to the limited ability of this decision rule to control the probability of falsely rejecting the null hypothesis, the intended control of the chance of falsely accepting the null hypothesis is also compromised when this decision rule is applied to data sets that exhibit characteristics more commonly observed among environmental data than the ideal lognormal distributions represented in Figure 4.

The performance of a variety of decision rules (in addition to the one discussed here) is reported by Berman et al. (1998a and b). Each of the decision rules evaluated are applied to simulated data sets exhibiting a broad range of characteristics that are commonly encountered among environmental data. Results from these studies indicate that, because environmental data do not typically exhibit characteristics that are sufficiently similar to the kinds of statistical distributions for which most of the available decision rules are defined, the error rates associated with application of such decision rules are generally greater than anticipated based on theory. It is further shown that decision error rates can generally be reduced by employing decision rules that are carefully matched to the characteristics of the data being evaluated. In many cases, non-traditional decision rules (which are rules that do not offer the kinds of formal statistical control that are inherent to the design of traditional rules) may sometimes be employed to reduce decision errors below that achievable using more traditional rules, as long as the non-traditional rules are carefully matched with the characteristics of the data to which they are applied.

## CONCLUSIONS

As indicated above, the questionable practices identified in the Introduction Section of this paper can cause decision errors to increase when they are carelessly applied during the investigation of hazardous waste sites and the subsequent evaluation of data. In turn, this can lead both to inadequate protection of public health or to needless expenditures for cleaning up sites that otherwise pose no significant threat.

The best way to avoid the problems associated with these and other questionable practices is to carefully address data quality considerations during all stages of the site characterization process. This includes, for example, using the data quality objectives process during the planning of site investigations (so that field work is optimized for cost-effectiveness). Generally, the choice of the number of samples; the locations from which the samples are collected; and the methods used for sample collection, handling, and analysis all affect the quality of the resulting data, which (in turn) affects decision error rates. Data quality considerations should also be addressed to guide selection of appropriate tools for data evaluation that are matched both to the specific objectives of the study and to the characteristics exhibited by the data evaluated.

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# DEVELOPMENT AND OVERVIEW OF THE ASTM PRACTICE FOR EXPEDITED SITE CHARACTERIZATION

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## ABSTRACT

The expedited site characterization (ESC) process developed by Argonne National Laboratory's Environmental Research Division has been formalized by the American Society for Testing and Materials (ASTM) in standard D6235, *Practice for Expedited Site Characterization of Vadose Zone and Ground Water Contamination at Hazardous Waste Contaminated Sites*. The ASTM *ESC Practice* received intensive review within the ASTM and by federal and state agencies responsible for environmental programs involving contaminated sites. A distinctive feature of the ESC process is the use of an integrated, predominantly geoscience-based, experienced, multidisciplinary team employing judgment-based sampling and measurements in the field to identify the critical features of the geologic and hydrogeologic setting that control groundwater and contaminant distribution and movement. This knowledge is used to guide sampling to determine the amount and extent of contamination.

## INTRODUCTION

Much money has been wasted at contaminated sites in the last 20 years as a result of traditional site characterization approaches that have tended to emphasize extensive sampling for contaminants and installation of a fixed number of groundwater monitoring wells that may or may not be in the right location to detect contaminants. A number of approaches have been developed recently to make characterization of contaminated sites more timely and cost-effective. The ESC process, originally developed at Argonne National Laboratory, is especially effective at sites with contamination in the vadose zone and groundwater. This paper describes the formalization of this process by the ASTM and provides an overview of the ASTM ESC standard.

## DEVELOPING THE ASTM ESC STANDARD

### The ASTM's Standard Development Process

The ASTM, currently celebrating the 100th anniversary of its initial organization, is one of the world's largest systems for voluntary standards development. More than 33,000 members in over 130 standards-writing committees have developed in excess of 8,500 standards that are published annually in 70 volumes.

In the last ten years, ASTM's various environmentally related committees, including D18 (Soil and Rock), D19 (Water), D22 (Sampling and Analysis of Atmospheres), D34 (Waste

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Management), E47 (Biological Effects and Environmental Fate), and E50 (Environmental Assessment), have been especially active in developing standards relevant to environmental site characterization. The latest annual revision of ASTM D5730 *Guide to Site Characterization for Environmental Purposes with Emphasis on Soil, Rock, the Vadose Zone and Ground Water*, lists more than 520 standard test methods, practices, and guides for use in the field and laboratory that could be pertinent for environmental site characterization.

The ASTM standards are developed through a consensus process designed to ensure that anyone with an economic or other interest in the standard has multiple opportunities for review and input. A task group or section in a committee, consisting of individuals with expertise in the subject matter of the standard, develops initial drafts. Formal balloting on a standard begins at the subcommittee level, with all negative votes requiring resolution before going on to committee and Society ballot. Resolution of negative votes usually occurs via revision to address the concern of the negative voter. Where negative votes cannot be resolved in this way, specific procedures must be followed to find a negative vote nonpersuasive. Typically, 1.5–2 years are needed for a new standard to be approved as a full consensus standard.

A full committee may authorize development of a *provisional* standard when there is a pressing need for speeding the standard development process. Provisional standards are balloted only at the subcommittee level; however, once approved, they must go through the full approval process within two years.

## Why an ASTM Standard on Expedited Site Characterization?

Office of Management and Budget Circular No. A-119, *Federal Participation in the Development and Use of Voluntary Standards*, first approved in October 1982 and revised in October 1993, provided an impetus for government participation in the ASTM's standards development process and for use of ASTM standards. The circular was codified in Public Law 104-113, Technology Transfer Improvements Act of 1995, which was signed into law by President Clinton on March 7, 1996. Section 12 of the Act requires federal agencies to participate in the development of, adopt, and use to the extent practicable, technical standards developed by voluntary, private sector, consensus standards bodies. On February 19, 1998, a final revision to OMB Circular A-119 was published in the *Federal Register*, rewritten in plain-English, question-and-answer style, to give guidance to federal agencies on ways to more effectively use voluntary standards and participate in their development.

In 1993 the U.S. Department of Energy (DOE) began funding demonstrations of technologies that could be used in the ESC process, which had been under development by Argonne since 1989. In 1996 DOE officials decided that the ASTM would provide a cost-effective route for formalizing the process and encouraging wider use at DOE facilities. At that time, DOE had about 1,500 release sites involving subsurface characterization where ESC was expected to be effective; the average cost savings of replacing traditional approaches with ESC were estimated at about $300,000 per site.

Consequently, DOE provided funding for a task group in ASTM Subcommittee D18.01 (Surface and Subsurface Characterization) and requested that a provisional standard be developed as quickly as possible, with subsequent development of a full consensus standard. The task group, chaired by the author, consisted of three other ASTM Subcommittee D18.01 members; two DOE representatives from Washington; and DOE representatives from Argonne, Ames Laboratory, and Los Alamos National Laboratory.

## Development Chronology for the ESC Standard

Appendix A provides a detailed chronology of events through approval of the full consensus ESC standard. Eight months elapsed between the first meeting with DOE representatives in April 1996 and approval of ASTM PS 85-96, *Provisional Guide for Expedited Site Characterization of Hazardous Waste Contaminated Sites*. An additional 13 months were required to obtain approval of ASTM D6235, *Practice for Expedited Site Characterization of Vadose Zone and Ground Water Contamination at Hazardous Waste Contaminated Sites*, as a full consensus standard.

For several reasons, the ASTM ESC standard received more extensive review than is strictly required by the ASTM's normal balloting procedures. First, the use of provisional standards to speed up the development of standards by some other ASTM environmental committees had become controversial, so more extensive review, especially during the preballot draft stage, was initiated to ensure that technical quality was not compromised as a result of the more limited review that provisional standards receive. Subcommittee D18.01, which approved the provisional standard, had about 80 members, whereas more than 900 members of Committee D18 received the ballot for the full consensus standard.

Second, the broad scope of the standard made it important to get input from task group and subcommittee chairs in other ASTM committees (especially Committees E50 and D34) to ensure compatibility with related standards development efforts. Finally, to facilitate regulatory acceptance at the federal and state levels, the standard was reviewed by individuals in appropriate program offices who do not normally participate in the ASTM's standards development process.

Preballot review drafts for federal agency review were distributed to key individuals in DOE, the Department of Defense (DOD; Army, Air Force, Navy), major program offices in the U.S. Environmental Protection Agency (EPA), and the Commodity Credit Corporation of the U.S. Department of Agriculture (CCC/USDA). Selected states received preballot review copies (California, Nebraska, Iowa, Ohio, and Texas), and the penultimate draft (6.0) received formal review by all the member states of the Interstate Technology Regulatory Cooperation (ITRC) group. The ITRC review resulted in more than 230 specific comments from 17 states (California, Colorado, Delaware, Idaho, Illinois, Kansas, Louisiana, Massachusetts, Nebraska, New Jersey, New York, Ohio, Pennsylvania, South Dakota, Texas, Utah, and Washington).

Altogether, the standard went through seven major drafts, with numerous intermediate versions, several title changes, two subcommittee ballots for approval as a provisional standard, and two full committee ballots for approval as a full consensus standard. All negative votes that addressed the content of the standard were resolved to the satisfaction of the voter. A number of negative votes addressing matters of ASTM policy, received on the final ballot, could not be resolved by making revisions to the standard. These negatives were found to be nonpersuasive by Committee D18 on January 14, 1998. A revision to the standard was balloted in April 1998 to address additional comments on the approved standard that require substantive, but minor, changes. The published version of ASTM Practice D6235 should be available from the ASTM in the fall of 1998.

# OVERVIEW OF THE ASTM ESC PRACTICE

The ASTM ESC process formalizes an approach to characterizing sites with contamination in the vadose zone and groundwater that was developed by Dr. Jacqueline Burton's group at Argonne. The principles of this approach, based on oil and mineral exploration methods, were first developed and applied at several landfills on Bureau of Land Management land in New Mexico and have since been refined at more than 30 CCC/USDA former grain storage sites in Nebraska and Kansas and at DOE and DOD facilities in California, Texas, Illinois, and Oklahoma.

The ASTM standard defines ESC as follows:

> A process for characterizing vadose zone and groundwater contaminated sites using primarily judgment-based sampling and measurements by an integrated, multidisciplinary core technical team, led by a technical team leader and operating within the framework of a dynamic work plan that gives the flexibility and responsibility to select the type and location of measurements to optimize data collection activities during a limited number of field mobilizations.

## ESC Philosophy: Technical Goals and Strategy

The technical goal of ESC is to *first* identify the critical features of the geologic and hydrogeologic setting that control groundwater and contaminant distribution and movement. This knowledge *then* guides delineation of the amount and extent of contamination. This approach contrasts with traditional site characterization approaches, which tend to focus on sampling for contaminants before the geologic and hydrogeologic system is well understood.

The technical strategy for ESC has three main elements: (1) the program is dominantly driven by geoscience experts, (2) multiple complementary methods are used to resolve essential features of the site conceptual model, and (3) data collection emphasizes quality rather than quantity.

Early on, the ASTM ESC Task Group decided that its objective was to formalize a process for introducing good science into the characterization of contaminated sites through use of an experienced multidisciplinary team and multiple complementary geologic and hydrogeologic characterization methods. Consequently, the ASTM *ESC Practice* clearly states that it is *not* tied to any particular regulatory program, site characterization method or technology, chemical analysis method, risk evaluation method, or computer modeling code.

## Where and When to Use the ESC Approach

Although the basic principles of the ESC process are applicable to any scientific investigation where geologic and hydrogeologic characterization are primary objectives, the ASTM *ESC Practice* focuses on sites where contaminant migration in the vadose zone and groundwater is a concern. The ESC process is inappropriate for use at sites with no data or no known problem. Some prior investigation is required to determine that vadose zone and groundwater contamination at a site is a matter of concern. Use of the ESC process is essential at contaminated sites where vadose zone and groundwater systems are highly heterogeneous or there is a potential for complex behavior of contaminants. Figure 1, adapted from the ASTM *ESC Practice* (ASTM D6235), is a flow diagram for determining the appropriateness of the ESC process.

The ESC approach is likely to be appropriate for (1) CERCLA remedial investigations/ feasibility studies (RI/FS), (2) RCRA facility investigations/corrective measures studies (RFI/CMS), (3) DOD base closure actions, (4) environmental site assessments (ESAs) for real estate property transactions where conditions described above apply, (5) large petroleum release sites such as refineries, and (6) sites or facilities with radioactive subsurface contamination that are not regulated by RCRA or CERCLA.

## Essential Features of the ESC Process

At the most basic level, the ESC process has the following five features:

- The ESC process is *goal oriented* (to close the site) rather than task oriented (to install a specified number of monitoring wells or collect a specified number of samples).

- The ESC process *focuses on contamination in the vadose zone* (areas in the subsurface that are not permanently saturated) *and groundwater* because they represent the contaminant migration pathways that are most difficult to characterize.

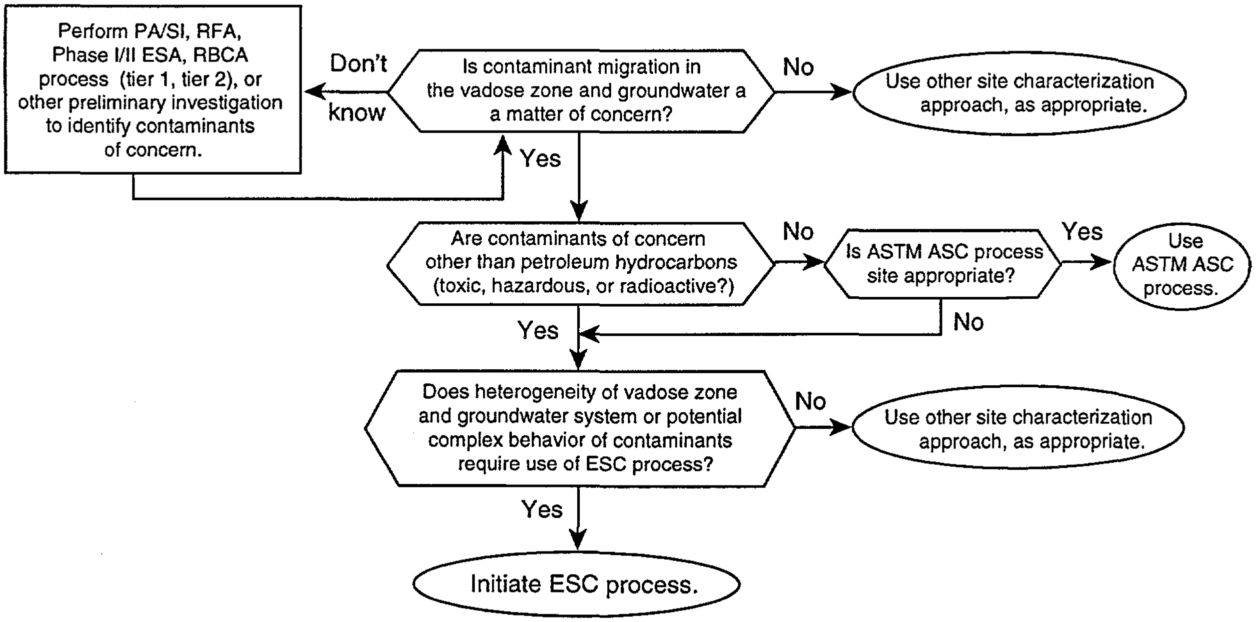

**FIGURE 1** Flow Diagram for Initiation of Expedited Site Characterization Process (Adapted, with permission, from the *Annual Book of ASTM Standards*, copyright ASTM, 100 Barr Harbor Drive, West Conshohocken, PA 19428.)

- An *integrated multidisciplinary project team in the field*, led by a *technical team leader* with training and experience in geosciences, uses an *on-site technical decision-making process* that promotes timely and efficient data collection and interpretation and ensures *quality control of all data* (geologic, hydrogeologic, chemical, etc.).

- The ESC process *relies primarily on judgment-based sampling and measurement* to develop a conceptual site model of contaminant migration pathways for use in focusing the subsurface contaminant sampling in areas where contamination is likely to be detected.

- An integrated multidisciplinary project team working in the field, using judgment-based sampling and measurements, allows characterization of vadose zone and groundwater contamination in a *limited number of mobilizations*. The ASTM *ESC Practice* assumes the typical need for two major mobilizations. Phase I focuses on essential features of the geologic and hydrogeologic system, while Phase II focuses on delineating the distribution and concentration of contaminants.

The ESC process is not the only approach that has been developed with the objective of accomplishing expedited, accelerated, or rapid site assessment. For example, ASTM Committee E50 has developed PS 03, *Provisional Guide for Accelerated Site Characterization of Confirmed or Suspected Petroleum Releases*. Consequently, the ASTM ESC Task Group developed minimum criteria for evaluating whether a characterization project satisfies the requirements of the ASTM ESC practice. Table 1, adapted from the ASTM *ESC Practice* (ASTM D6235), presents a checklist of ten items that identify these minimum criteria. Other site characterization approaches may include many of the items on this checklist, but they tend to place less emphasis on understanding the geologic and hydrogeologic system before contaminant sampling and often rely more heavily on screening-level than on definitive data for contaminant analysis. No other site characterization approach explicitly requires quality control procedures for *all* aspects of data collection and handling, including field work for geologic and hydrologic characterization.

## Overview of Seven Steps in the ESC Process

Figure 2, adapted from the ASTM *ESC Practice*, provides an overview of the steps in the ESC process as formalized by the ASTM. These steps are as follows:

- *Step 1: Initiate ESC Process.* As noted earlier, some prior investigation work is required to determine that the ESC process is appropriate. ESC is not intended to determine whether there is a problem with vadose zone and groundwater contamination.

- *Step 2: Establish ESC Project Team.* The ASTM *ESC Practice* uses the term "technical team leader" to emphasize that the person in charge of the investigation is technically qualified and leads the team both in the office and in the field. The team leader and an integrated multidisciplinary team with expertise in geologic, hydrologic, and chemical systems work together, as the areas of

**TABLE 1** Minimum Criteria for a Project Using the ASTM ESC Process

___ 1. A technical team leader oversees the ESC project and leads the ESC core technical team.

___ 2. Project objectives, data quality requirements, and performance criteria are defined by some process that includes ESC client, regulatory authority, and stakeholders.

___ 3. The technical team leader and an integrated multidisciplinary core technical team with expertise in geologic, hydrologic, and chemical systems work together, as the areas of expertise are needed, in the field and throughout the process.

___ 4. Intensive compilation, quality evaluation, and independent analysis and interpretation of prior data are used to develop a preliminary site model.

___ 5. A dynamic work plan, approved by the ESC client and regulatory authority, provides the framework for use of multiple complementary, site-appropriate geologic and hydrologic investigation methods, along with rapid site-appropriate methods for contaminant analysis.

___ 6. The ESC project is founded primarily on judgment-based sampling and measurements to test and improve the concepts and details of the evolving site model.

___ 7. Quality control procedures are applied to all aspects of ESC data collection and handling, including field work for geologic and hydrologic characterization.

___ 8. Field data collection is initially focused on geologic and hydrologic characterization of vadose zone, groundwater, and other relevant contaminant migration pathways (and on identifying contaminants of concern, if they are not already known), followed by delineating the distribution, concentration, and fate of contaminants on the basis of knowledge of the relevant contaminant migration pathways. This effort typically requires no more than two field mobilizations.

___ 9. Field data are integrated, analyzed, and interpreted daily to refine the evolving site model and are used to optimize the type and location of subsequent field data collection until project objectives have been met.

___ 10. The final site model provides the ESC client, regulatory authority, and stakeholders with the information required to choose a course of action based on risk analysis or regulatory standards-based cleanup criteria.

**NOTE**: Other site characterization approaches may include many of these elements, but all must be present for an investigation using the ASTM ESC process.

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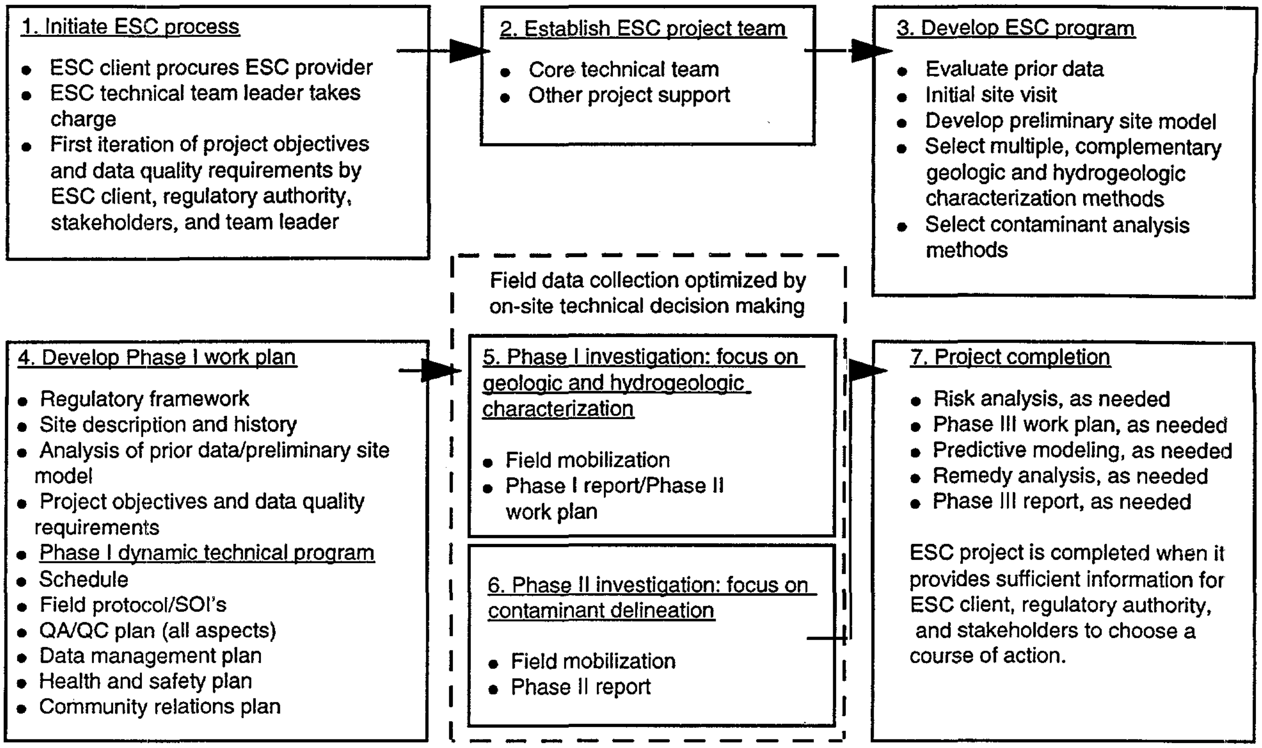

**FIGURE 2** Overview of Expedited Site Characterization Process (Adapted, with permission, from the *Annual Book of ASTM Standards*, copyright ASTM, 100 Barr Harbor Drive, West Conshohocken, PA 19428.)

expertise are needed, in the field and throughout the process. Figure 3, adapted from the ASTM *ESC Practice*, illustrates key ESC project team relationships.

- *Step 3: Develop ESC Program.* Activities in this development step are identified in Figure 2. The ASTM ESC practice emphasizes the importance of thorough data compilation, data quality evaluation, and initial interpretation of prior data in the development of the preliminary site conceptual model and to guide collection of new data.

- *Step 4: Develop Phase I Work Plan.* Distinctive features of the work plan include (1) the *dynamic technical program*, in which the types of data and data collection methods are described, without specifying the exact locations and number of measurements and samples, and (2) a quality assurance/quality control plan for geologic and hydrogeologic characterization methods, not just for chemical analyses (as is typical of most site investigation work plans). The Phase II work plan is normally included in the Phase I investigation report.

- *Steps 5 and 6: Phase I and Phase II Investigations.* The technical team leader and other members of the core technical team, as needed, are in the field throughout the field investigations. Phase I focuses on geologic and

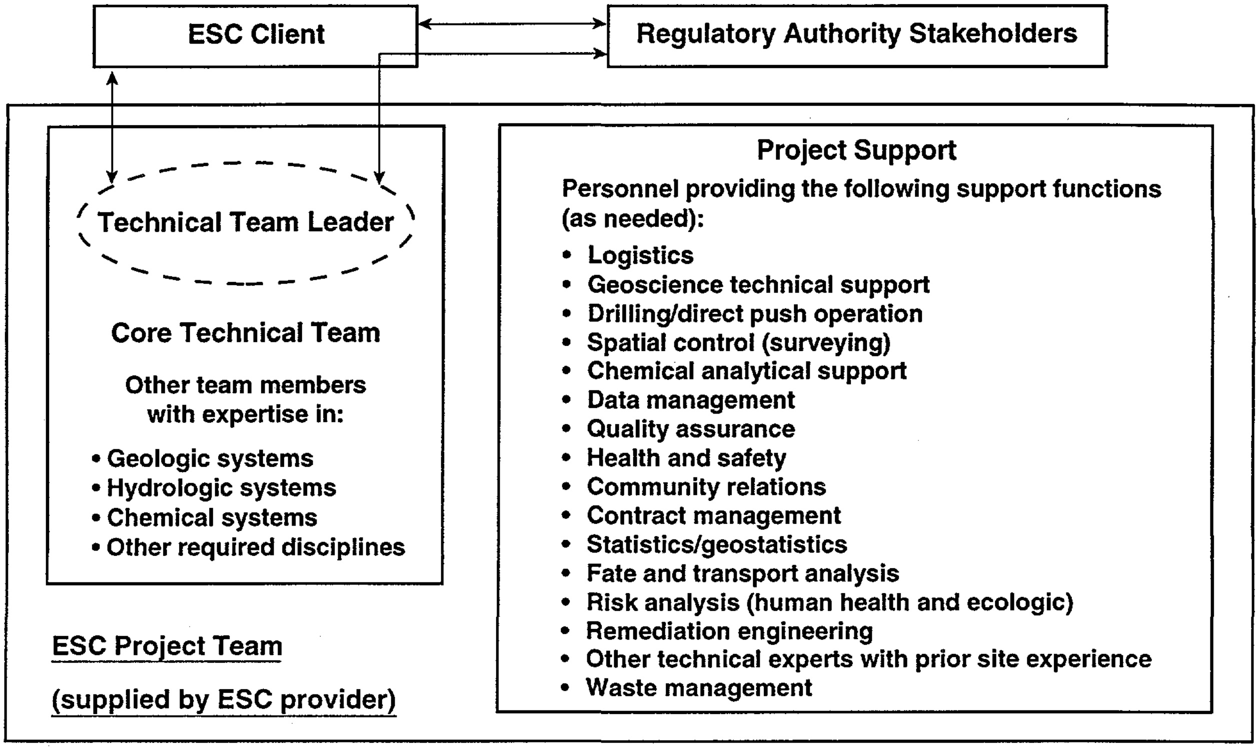

**FIGURE 3** ESC Project Team Relationships (Adapted, with permission, from the *Annual Book of ASTM Standards*, copyright ASTM, 100 Barr Harbor Drive, West Conshohocken, PA 19428.)

hydrogeologic characterization, with sampling for contaminant analysis occurring to the extent that it contributes to understanding relevant contaminant migration pathways. Phase II focuses on contaminant delineation. Central to the field investigation phases is the *on-site technical decision-making process*, in which field observations and measurements are continuously evaluated and used to guide subsequent data collection efforts (see Figure 4).

- *Step 7: Project Completion.* Depending on the results of the Phase I and Phase II investigations and the regulatory framework (risk-based or regulatory-standards-based), project completion can take a number of directions, including Phase III investigation for predictive modeling and evaluation of remediation options. Ultimately, project completion occurs when the ESC project provides sufficient information to support the selection of a course of action that will lead to site closure. Options can range from no action to the design and operation of a remediation system allowing site closure within a predictable period of time.

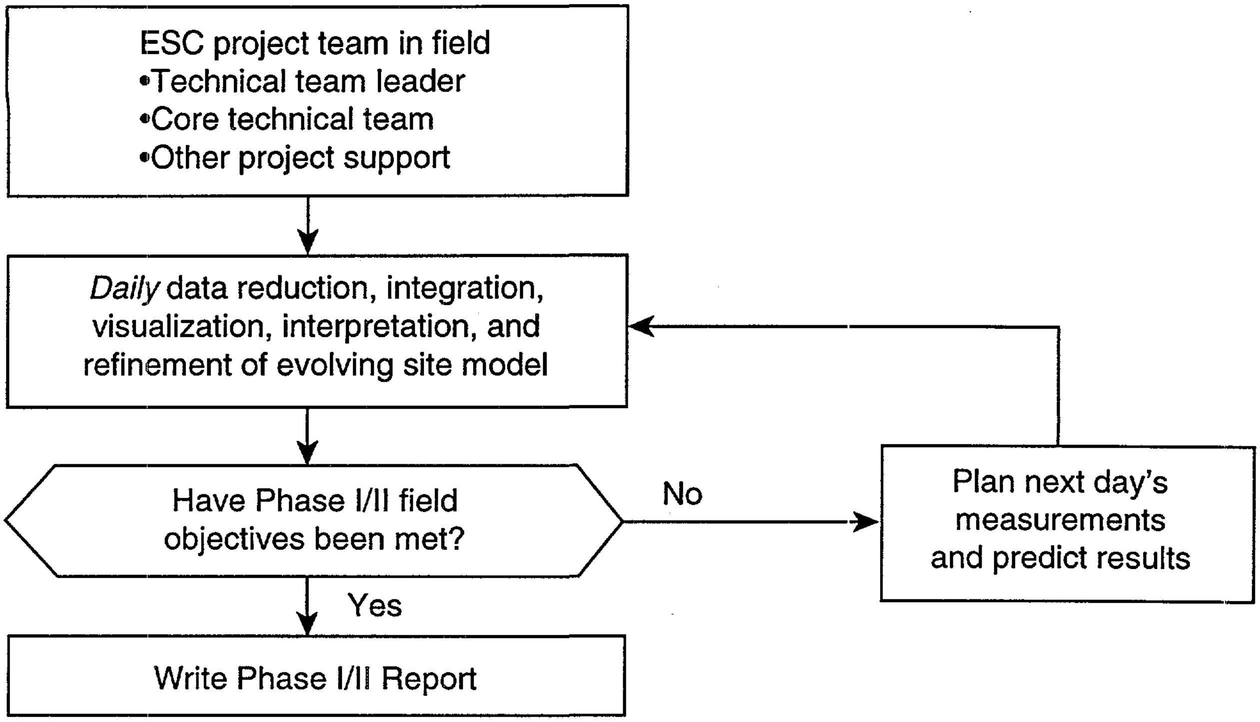

**FIGURE 4** On-Site Technical Decision Making Process

## APPENDIX A: CHRONOLOGY FOR ASTM EXPEDITED SITE CHARACTERIZATION STANDARD

**1996**

| | |
|---|---|
| 4/1 | Russell Boulding, chair of ASTM D18.01.01 (Committee on Soil and Rock, Subcommittee on Surface and Subsurface Characterization, Section on Environmental Site Characterization), meets with DOE representatives in Washington, D.C., to discuss possibility of establishing a task group to develop a guide for ESC. |
| 4/18-19 | Russell Boulding meets with DOE and DOE laboratory personnel in Santa Fe, New Mexico, to discuss first draft of a working outline for the guide. |
| 4/27-28 | First full ASTM ESC Task Group meeting in Boulder, Colorado, to discuss expanded third draft of working outline and develop first draft of ESC flow chart. Task group members are Russell Boulding (chair); Joe Downey, Ed Gutentag, and Ken Kolm (ASTM D18.01.01 members); Paul Beam (DOE EM-40); David Berg (DOE EM-50); Dr. Al Bevolo (Ames Laboratory); Dr. Jacqueline Burton (Argonne National Laboratory); and Dr. Tom Starke (Los Alamos National Laboratory). |
| 5/3-6 | Russell Boulding meets with Burton (Argonne, Illinois) and Bevolo (Ames, Iowa) for additional briefing on ESC process. |
| 5/8-10 | Russell Boulding attends ITRC meeting in Washington, D.C., and presents information on ESC Task Group's activities and plans. |

5/24 Draft 1.0 of ESC guide distributed to ESC Task Group members.

6/5 Draft 2.0 of ESC guide completed.

6/6-7 ESC Task Group meeting, Boulder, Colorado, to discuss Draft 2.0.

6/19 ESC Task Group receives approval from Committee D18 to develop ESC guide as a provisional standard, at a meeting in Orlando, Florida.

6/21 Preballot Draft 3.0 of ESC guide completed and distributed to more than 30 individuals outside the ESC Task Group, representing the following areas of expertise or perspective: geophysics, hydrogeology, direct-push technology, chemistry, federal agencies (EPA, Air Force, Army, Navy), states (California, Iowa, Nebraska [prior to formal ITRC review]), and selected individuals in ASTM Committee E50.

7/8 Draft 4.0 of ESC guide completed in response to comments on preballot review draft received to date.

7/15 First D18.01 Subcommittee Ballot on Draft 4.0 (*Provisional Guide for Expedited Site Characterization of Vadose Zone and Ground Water Contamination*) mailed.

8/14 Draft 4.0 sent to selected ITRC state members: California, Colorado, Idaho, Nebraska, New Jersey, New Mexico, Ohio, Tennessee, Texas, Washington.

8/15 First D18.01 Subcommittee ballot closes with 35 affirmative votes (8 with comments), 1 negative vote, and 26 abstentions.

9/23-24 ESC Task Group meets at ASTM headquarters, West Conshohocken, Pennsylvania, to discuss Draft 4.5 and meet with ITRC review panel (Colorado, Idaho, New Jersey, Ohio, and Washington). Written comments from California were also discussed.

9/25 ITRC meeting, Philadelphia, Pennsylvania. Accelerated Site Characterization Subteam develops work plan for FY 1997 that includes ITRC-ASTM partnership with formal, full ITRC review of ESC guide.

10/18 Emergency ESC Task Group meeting, Golden, Colorado, to address concerns of ASTM E50 Task Group on Accelerated Site Characterization. Conference call with E50 Task Group resolves issues, one being a change in title.

10/24 Draft 5.0 completed (retitled *Provisional Guide for Expedited Site Characterization of Hazardous Waste Contaminated Sites*).

11/6 Second D18.01 Subcommittee ballot on Draft 5.0 mailed.

12/8 Draft 5.0 of ESC guide sent out to full ITRC membership for review.

12/11 Ballot closes with 30 affirmative votes (9 with comments), no negative votes, and 22 abstentions. The ESC guide, with editorial revisions in response to one withdrawn negative, is approved as provisional standard PS 85-96.

**1997**

| | |
|---|---|
| 1/13-15 | ASTM D18 Committee meeting in New Orleans; ESC guide discussed at D18.01.01 Section meeting. |
| 2/19-20 | ESC Task Group meets in Golden, Colorado, to discuss Draft 5.5 and ITRC review comments. |
| 2/24 | Draft 6.0 completed (addresses ITRC comments received by that time). |
| 3/7 | Draft ESC Task Group responses to ITRC comments received to date from California, Colorado, Delaware, Illinois, Kansas, Louisiana, Massachusetts, Nebraska, New Jersey, New York, Ohio, Pennsylvania, Texas, Utah, Washington, and two stakeholder ITRC members. This draft is posted on the ITRC Web site. |
| 3/21 | Draft 6.0 mailed for concurrent D18 and D18.01 ballot. |
| 3/25 | Russell Boulding joins ITRC-ASTM subteam responsible for writing report on ITRC-ASTM partnership activity. |
| 4/30 | Second Draft of ESC Task Group response to ITRC comments completed as a result of ESC Task Group review of first draft and additional comments received from South Dakota. |
| 5/2 | D18-D18.01 ballot closes with 146 affirmative votes (2 with comments), 12 negative votes, and 322 abstentions. |
| 5/7 | Second Draft of ESC Task Group response to ITRC comments sent to all states and stakeholders who provided comments. |
| 5/30 | Draft 6.5 completed; includes revisions in response to additional ITRC state comments and ASTM ballot results. |
| 6/2-4 | ITRC meeting, Washington, D.C.; discussion of major issues identified in ESC Task Group response to ITRC comments. |
| 6/10 | Followup ESC Task Group conference call to discuss Draft 6.5. |
| 6/17 | Section D18.01 on ESC discusses Draft 6.5 at ASTM D18 Committee meeting in St. Louis, Missouri. |
| 6/25 | Draft 6.7 completed; revised sections distributed to ESC Task Group members. Final title changed to *Practice for Expedited Site Characterization of Vadose Zone and Ground Water Contamination at Hazardous Waste Contaminated Sites.* |
| 7/25 | Draft 7.0 submitted to ASTM headquarters for balloting. |
| 8/4 | Draft final ITRC-ASTM report submitted to full ITRC membership; includes as an appendix the final ESC Task Group response to ITRC comments. |

8/26 Second D18-D18.01 ballot on Draft 7.0 mailed.

10/14 D18-D18.01 ballot closes with 163 affirmative votes (1 with comments), 5 negative votes, and 321 abstentions (5 with comments).

**1998**

1/12-14 ESC practice approved as full consensus standard at ASTM Committee D18 meeting, San Diego, California.

# CHARACTERIZATION OF BEDROCK TOPOGRAPHY AT ARGONNE NATIONAL LABORATORY'S RAYMOND SITE

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## ABSTRACT

Two geophysical techniques were implemented at Argonne National Laboratory's Raymond, NE site: high redundancy P- Wave refraction and high resolution S- Wave reflection. The purpose of high redundancy refraction was two fold: first, to delineate the saturated zone above the Dakota formation and second, to map the topography of the bedrock. A high resolution seismic shear wave (S- Wave) reflection profile was performed to quantify sediments above the Dakota bedrock. Both techniques are capable of defining possible pathways for groundwater to follow bedrock and sedimentary topographic lows. Total refraction survey line length is 12,363 feet with a total of 179 seismic records and 17,184 channels recorded. Total reflection survey line length is 1,204 feet.

## INTRODUCTION

As part of an ongoing project for the Commodity Credit Corporation of the U.S. Department of Agriculture, Argonne National Laboratory has been investigating a contaminant plume of carbon tetrachloride used to preserve grains stored at various facilities. One of these abandoned facilities shown in Figure 1 was located approximately 1 mile East of Raymond, Nebraska. The soils in the Raymond Site area are predominately glacial tills overlying the Dakota sandstone. The complexity of the till combined with the weathering of the Dakota complicated vertical and horizontal ground water migration at the Raymond Site.

## SEISMIC REFRACTION

During Phase II of the Raymond Site investigation a seismic refraction survey was conducted to delineate bedrock topography and potentially the depth to water table. The survey was conducted using reflection seismic equipment to record highly redundant data. Ninety-six channels were recorded with a split spread geometry. Thirteen foot stations were used with a single 8 Hertz geophone planted at each station. Source locations were every sixth geophone (78 feet). A 1/3-lb. Kinnepak® explosive source was placed 4 feet below ground surface.

The data was acquired in exactly the same manner as a reflection survey. The spread geometry was kept consistent about each shot point. The spread was rolled up with each consecutive shot. The purpose of using the reflection equipment (i.e., spread cables, roll switch) was to increase the efficiency with which the seismic refraction data could be acquired. A single shot (Figure 2) essentially creates a 48 channel forward and reverse spread at each shot position. After sorting the shot data, a continuous profile with redundant forward and reverse arrivals is generated. This redundant data is highly suitable to the GRM method of travel time inversion. Figures 3a, 3b, and 3c show the travel time curves for Lines 1, 2, and 3 respectively, as well as depth inversions utilizing

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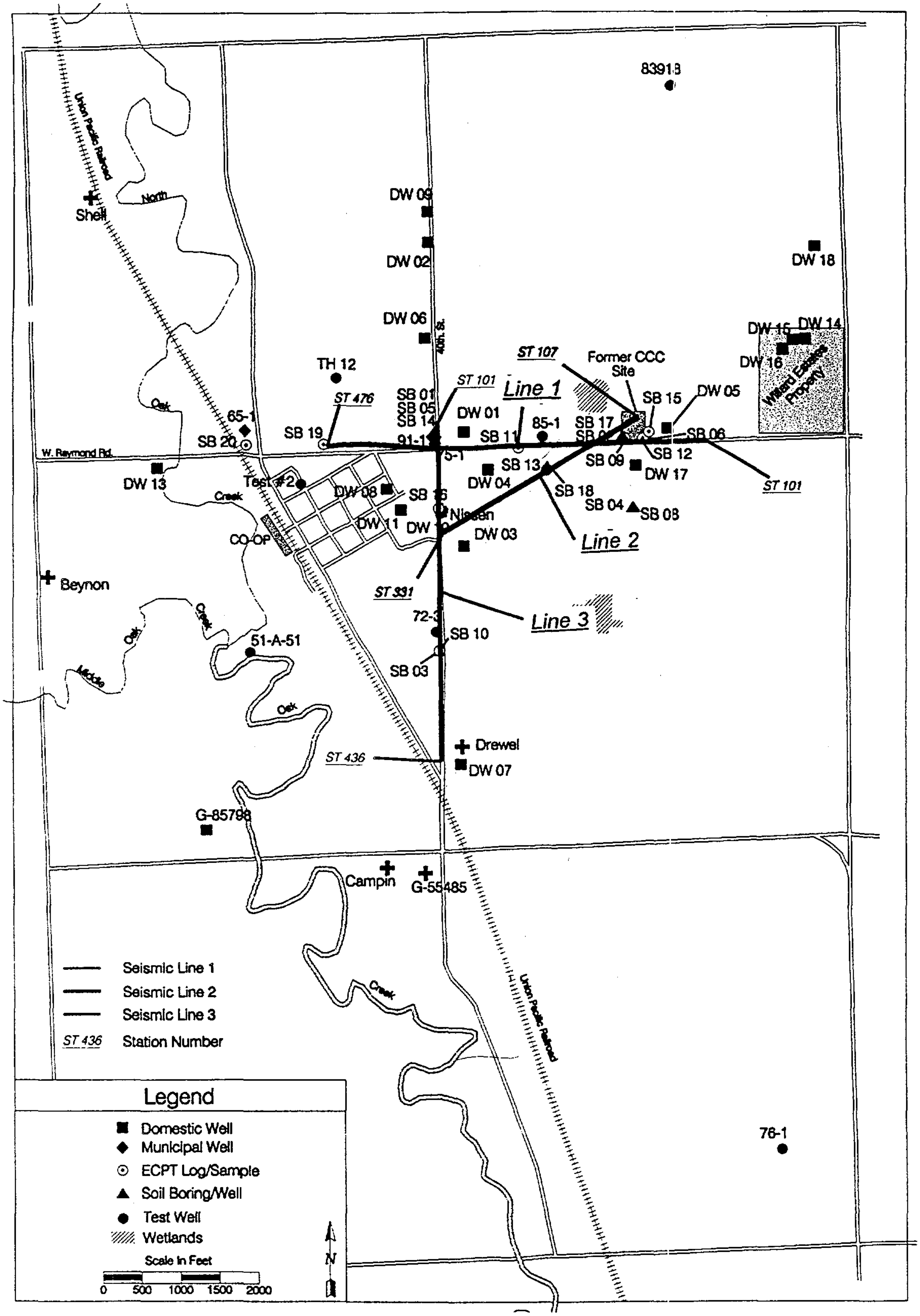
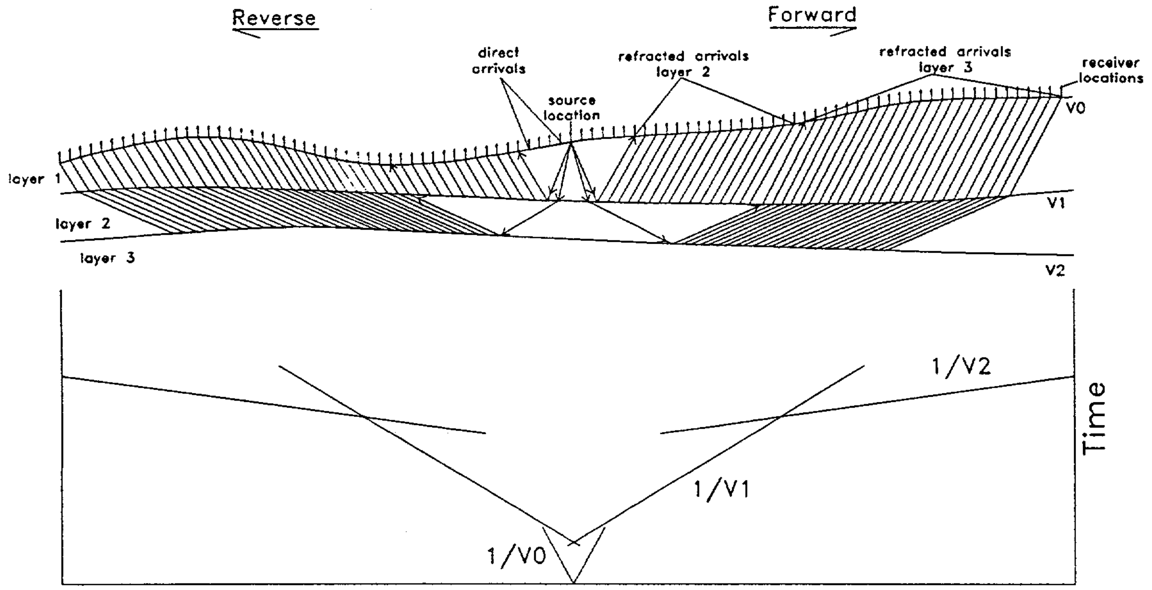
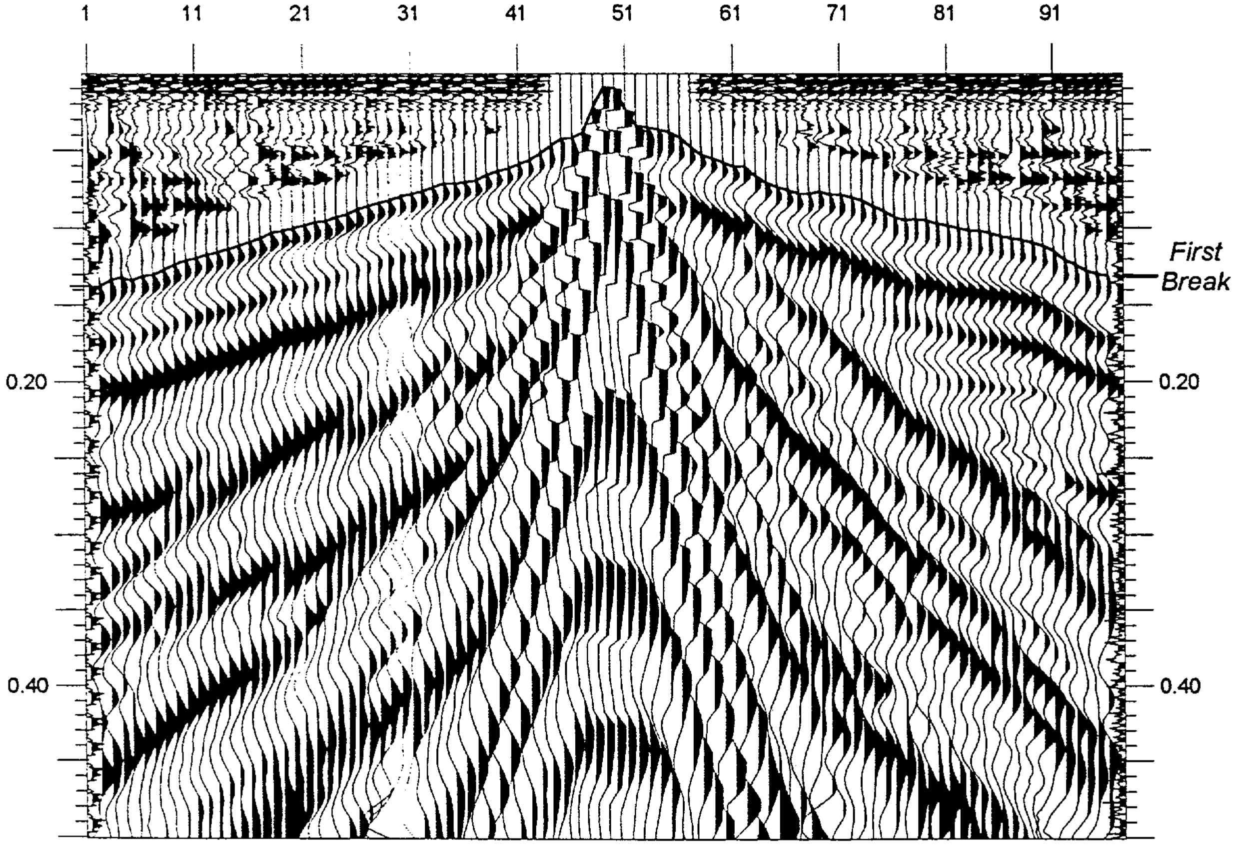


*Figure 1. Raymond Site map with seismic refraction surveys Line 1, Line 2, and Line 3 posted (Argonne 1997).*



Refraction Schematic



P- Wave refraction record 100ms AGC (2D Line)

*Figure 2. Schematic of seismic refraction 3 layer case. Sample refraction record from the Raymond Site plotted below. Schemtatic not relevant to Raymond Site.*

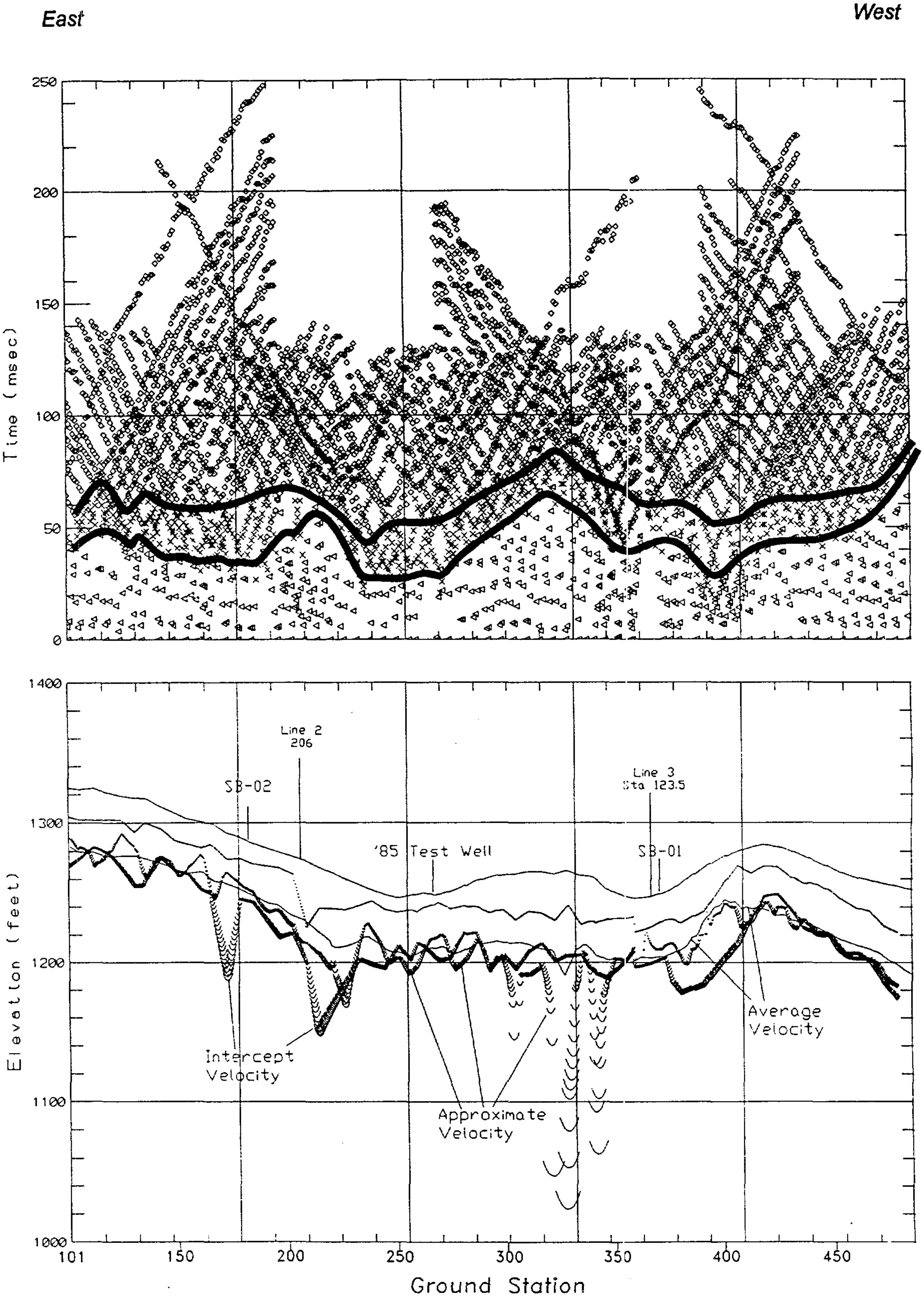


*Figure 3a. Seismic refraction solution for Line 1.*

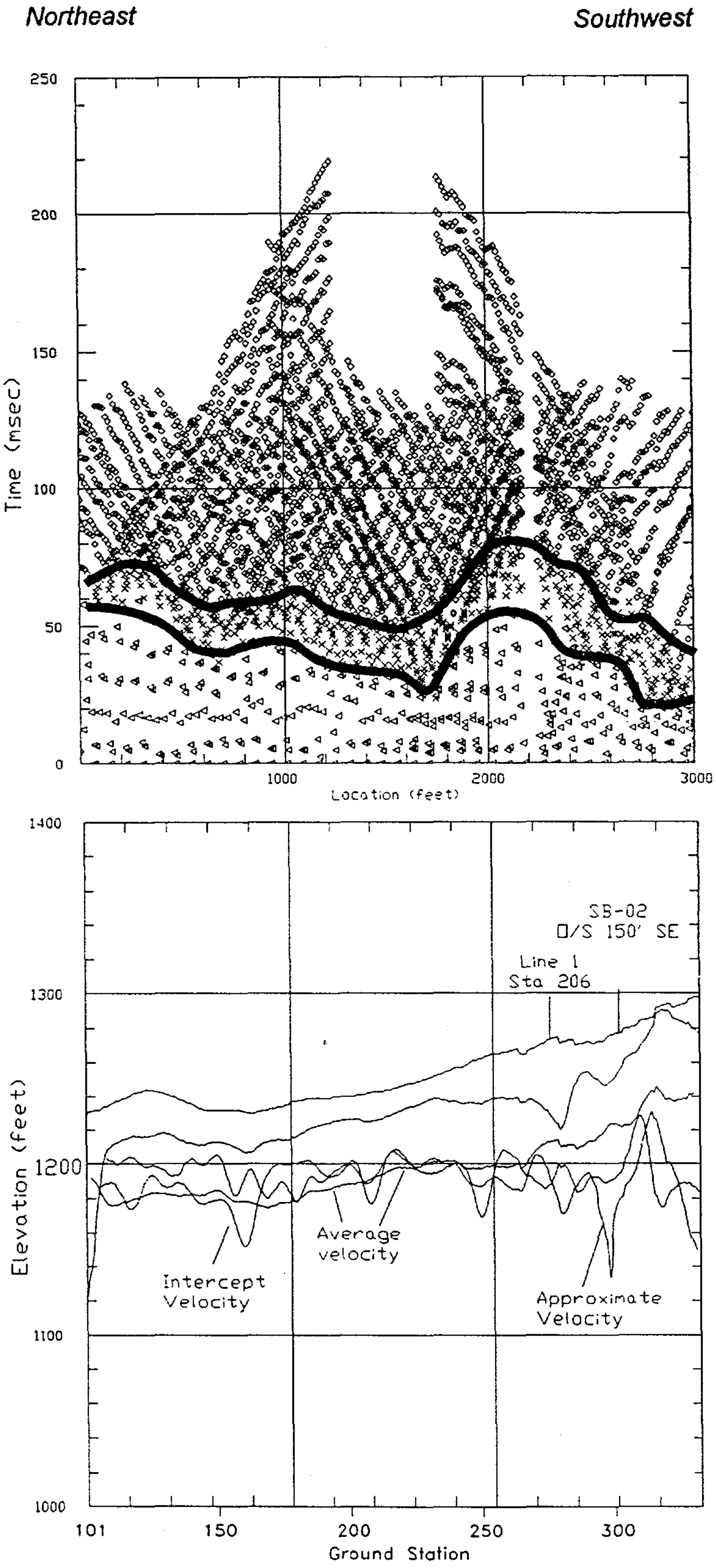


*Figure 3b. Seismic refraction solution for Line 2.*

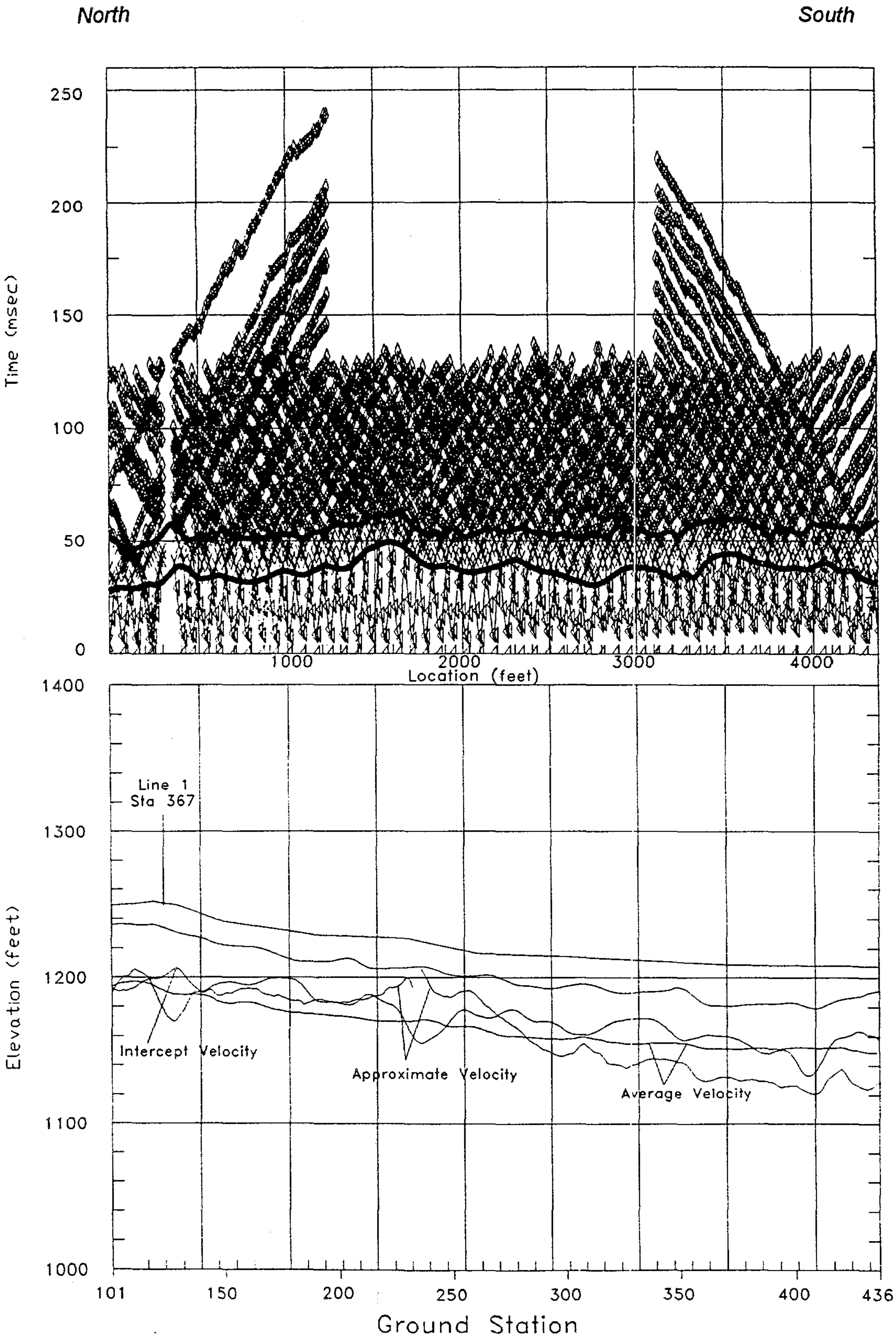


*Figure 3c. Seismic refraction solution for Line 3.*

three means of velocity inversion: average velocity, intercept velocity, and approximate velocity. The redundancy of arrivals is apparent. The depth inversion difference between the average velocity method and the other methods is a result of the redundancy and statistical first arrival analysis.

Refraction data was processed and interpreted as the data was acquired using ViewSeis®. Two days after the beginning of the survey for Line 1, a location for soil boring SB-2 was chosen as a result of the quick interpretation of the refraction data. The soil boring encountered bedrock as predicted by the refraction survey up to this point, however, the ground water elevation was not predicted accurately. The processed refraction data revealed a three layer case with the second layer being approximately 15-30 feet in depth with an average velocity of 4,500 feet/second and the third layer averaging 50 feet and running to an excess of 100 feet in some places. The average velocity of the third layer was 7,000 feet/second.

The analysis of borehole data was completed after the acquisition and subsequent processing of the refraction data. Line 1 had the greatest occurrence of borehole information and was the focus of great scrutiny. While the depth to bedrock and water table was accurate along the East portion of the line, the refraction data suggested that bedrock was deeper by approximately 25 feet near boring SB-01. Figure 4a is the interpreted geologic cross section from borehole data with Line 1 refraction solution posted. A subsequent analysis of the soil borings and geophysical logs indicated that a thin, calcified, high velocity layer within the glacial till caused this discrepancy.

Figure 4b is the interpreted geologic cross section derived from borehole data with Line 3 refraction solution posted. The refraction solution shows bedrock to be 26 feet deeper than the borehole data suggests at the north end. An extension of Line 3 to the north would resolve this discrepancy. The refraction solution extrapolates bedrock topography at the ends of seismic refraction lines. Bedrock depth is in error with the geologic cross section at the ends of refraction due to the lack of intercept times here. Figure 5 is a depth to bedrock contour map utilizing the seismic refraction data only. A possible valley providing a conduit for groundwater migration above the bedrock is identified in this figure.

## SEISMIC S- WAVE REFLECTION

In order to more precisely image the components of the glacial till and the erosional surfaces of the Dakota sandstone, a high-resolution shear wave seismic reflection survey was conducted along a portion of refraction Line 1 as shown in Figure 6.

The acquisition of the S- Wave seismic reflection line was similar to that of the refraction acquisition mentioned above. The station and source interval was 4 feet using a single 40 Hertz horizontal geophone for receivers and an Industrial Vehicles International (IVI) mini-vibrator for a source. A symmetrical split-spread geometry was used such that the near and far offsets were maintained at 2 and 190 feet, respectively. A maximum fold of 48 was achieved. Recording parameters were a 1.0 millisecond sample rate and a 7 second recording time.

Sweep tests were performed to ensure limited ground roll (Love waves) and achieve the highest frequency possible. After observing different sweep configurations, ground roll

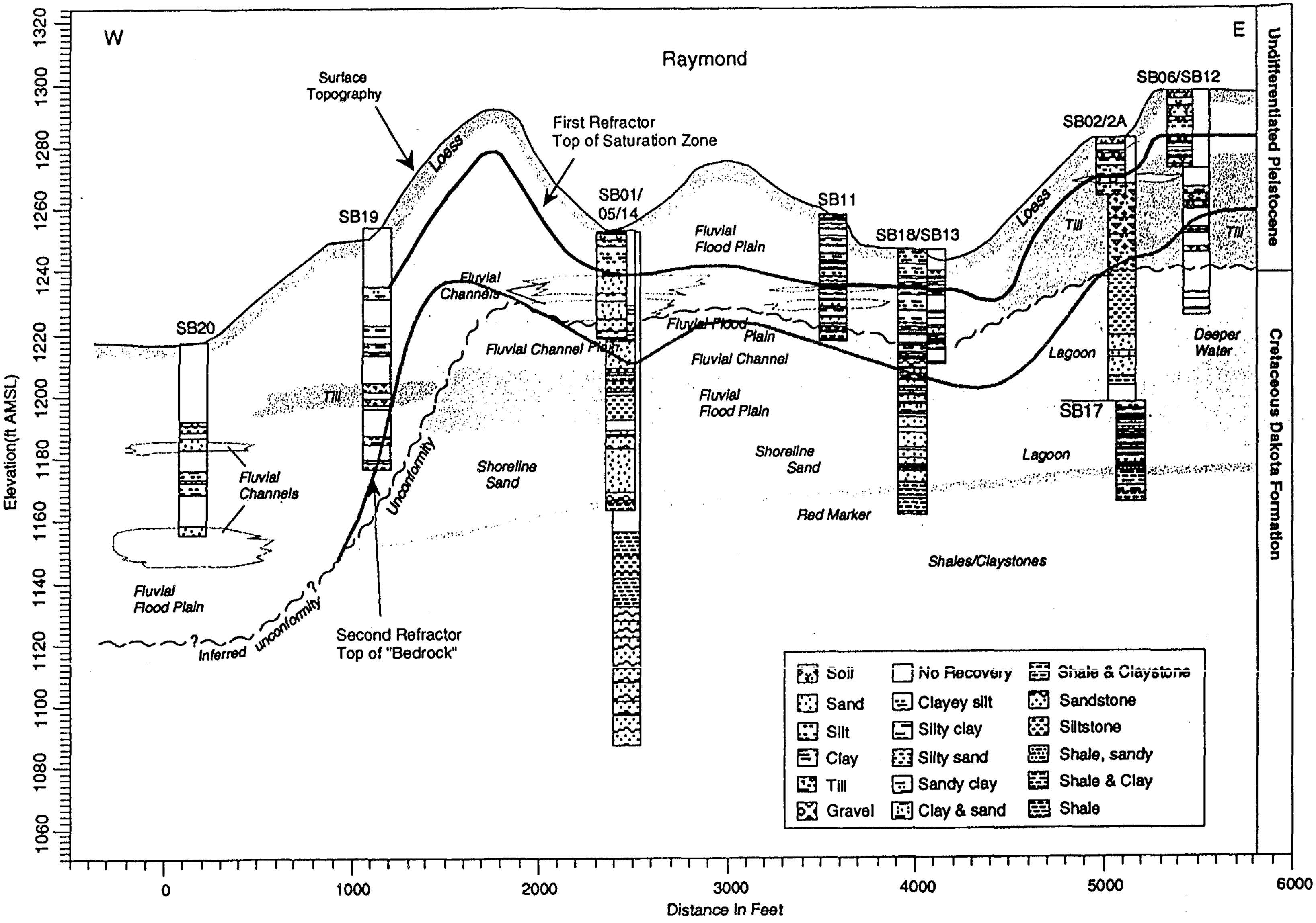


*Figure 4a. Geologic cross section of A-A' with seismic refraction depth to bedrock solution (Argonne 1997).*

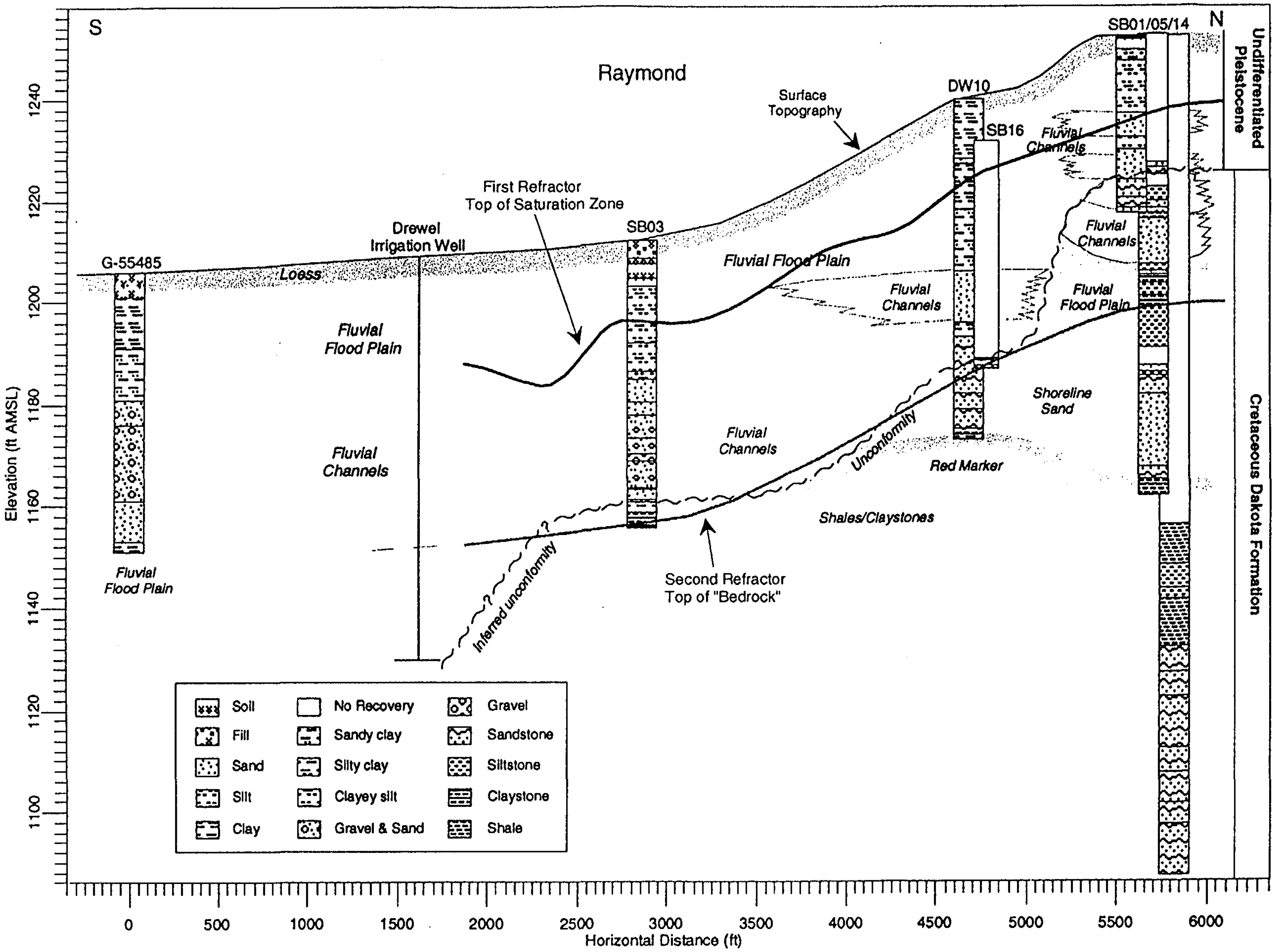


*Figure 4b. Geologic cross section of C-C' with seismic refraction depth to bedrock solution (Argonne 1997).*

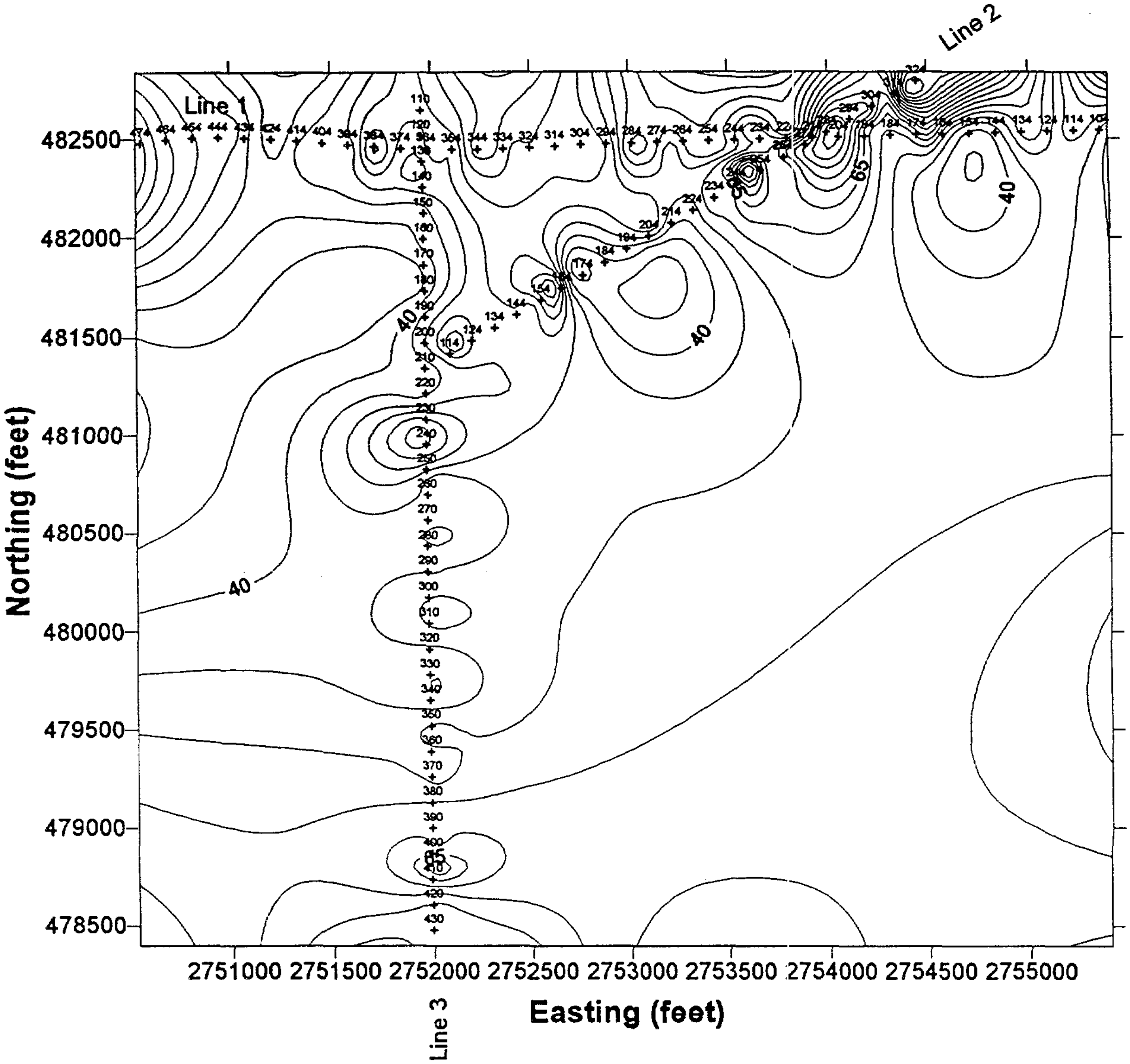


*Figure 5. Depth to bedrock contour map in feet below ground level. Contour interval 1 foot.*

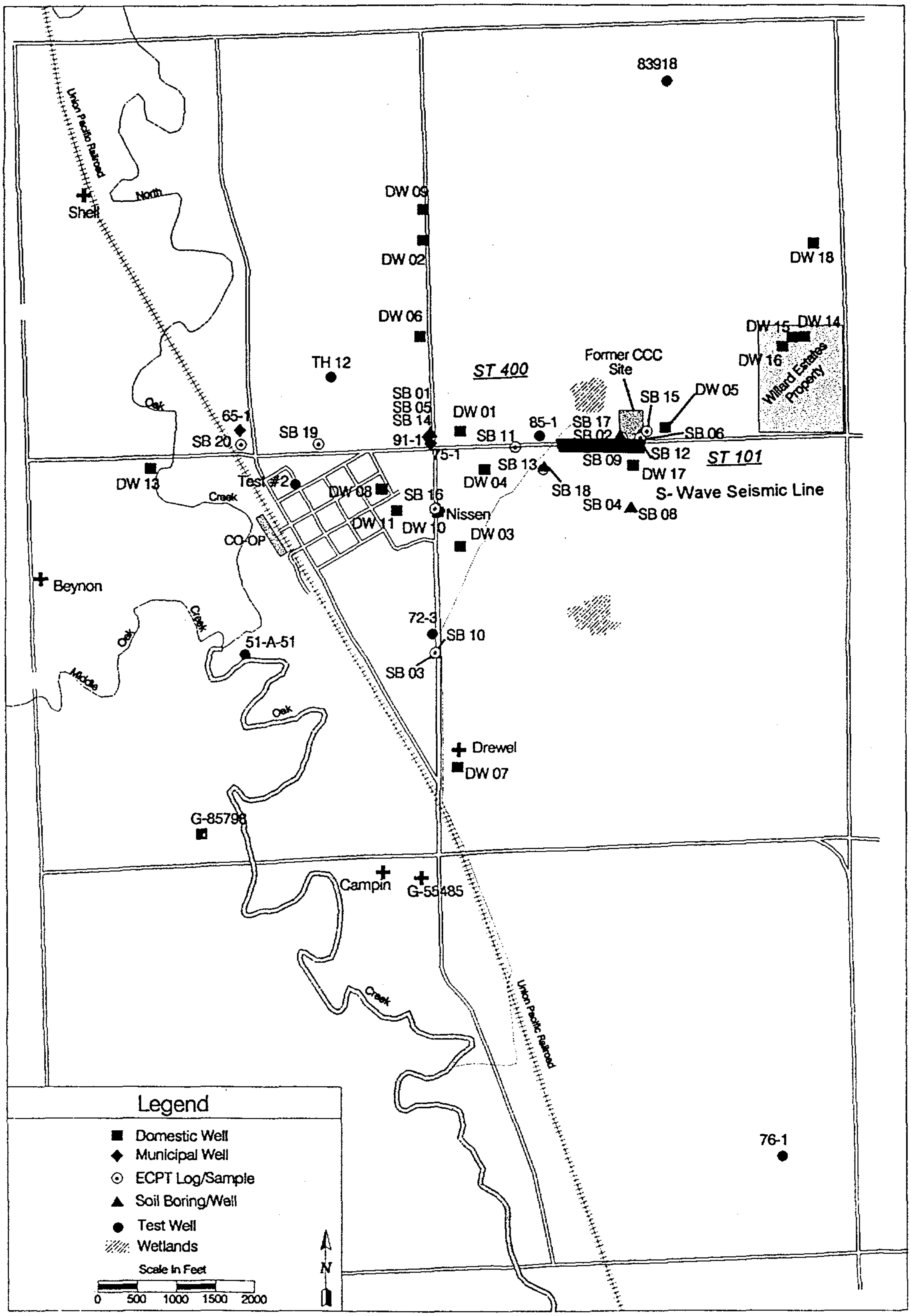


*Figure 6. Raymond Site map with S- Wave seismic survey posted (Argonne 1997).*

was minimal. Frequencies of greater than 200 Hertz were obtained. Final sweep parameters were set to 15-256 Hertz, 6 second sweep length, 400 millisecond start taper, 200 milliseconds end taper, and 4 sweeps per each source location. Drive level for the vibrator was set at 50 percent to prevent damage to the road surface. A sample S- Wave production seismic record from the Raymond Site is displayed in Figure 7. Reflected events are highlighted for demonstration. A ray trace model, not site specific, is plotted above the seismic record to show reflecting horizons and how energy raypaths are dispersed.

Data was processed by Sterling Seismic Services, Ltd. using ProMax® software. Vibroseis sweep correlation was performed before geometries and trace editing. Two iterations of surface consistent automated statics and velocity analysis were performed before stacking. Surface consistent deconvolution was run to reduce the earth filtering effects local to each geophone. Normal moveout corrections are applied to remove the hyperbolic character of horizontal reflectors highlighted in Figure 7. Final stacking of the common depth point gathers, filtering and gaining of the field data produces the final stacked S- Wave section.

Figure 8 shows the instantaneous phase of the seismic S- Wave stacked section. This section better displays the continuous and non-continuous events than the original stacked section. This figure shows events dipping to the West and impinging on top of the Dakota formation to the East. A depressed area noted on the East end of the section exhibits a possible fill within and is interpreted as a sand lens, labeled A. Undulations of strata above the Dakota describe the distribution of glacial till. Two channel like features within the Dakota are denoted in Figure 8 and centered at stations 170 and 380. There is a noticeable change in dip at the top of the Dakota at station 210 with dip increasing to the West.

Although the section exhibits extremely good resolution above bedrock, the actual structural position of the bedrock remains in question. The hinge point in the Dakota is in question because of highly variable near surface S- Wave velocities. High variability of near surface S- Wave velocities is the primary impediment to the interpretation of high resolution reflection data. At the time of this abstract preparation, we are awaiting the acquisition of a VSP to verify the identification of the Dakota and to verify the depths of strata above the bedrock.

## CONCLUSION

The high redundancy seismic refraction survey conducted at the Raymond, NE Site was successful in delineating the Dakota sandstone topography. Bedrock topography lows can be used to infer contaminant migration. The complexity of sediments deposited above the Dakota reduced the reliability of refraction interpretation in some areas.

The high resolution seismic S- Wave reflection survey provided good glacial till stratigraphy above the Dakota formation. The S- Wave reflection survey provided sufficient soil stratification information to close the gap between the refraction data and the confirmation of borehole data. S- Wave check shot surveys performed along this line can provide velocities to better estimate depths within the glacial till.

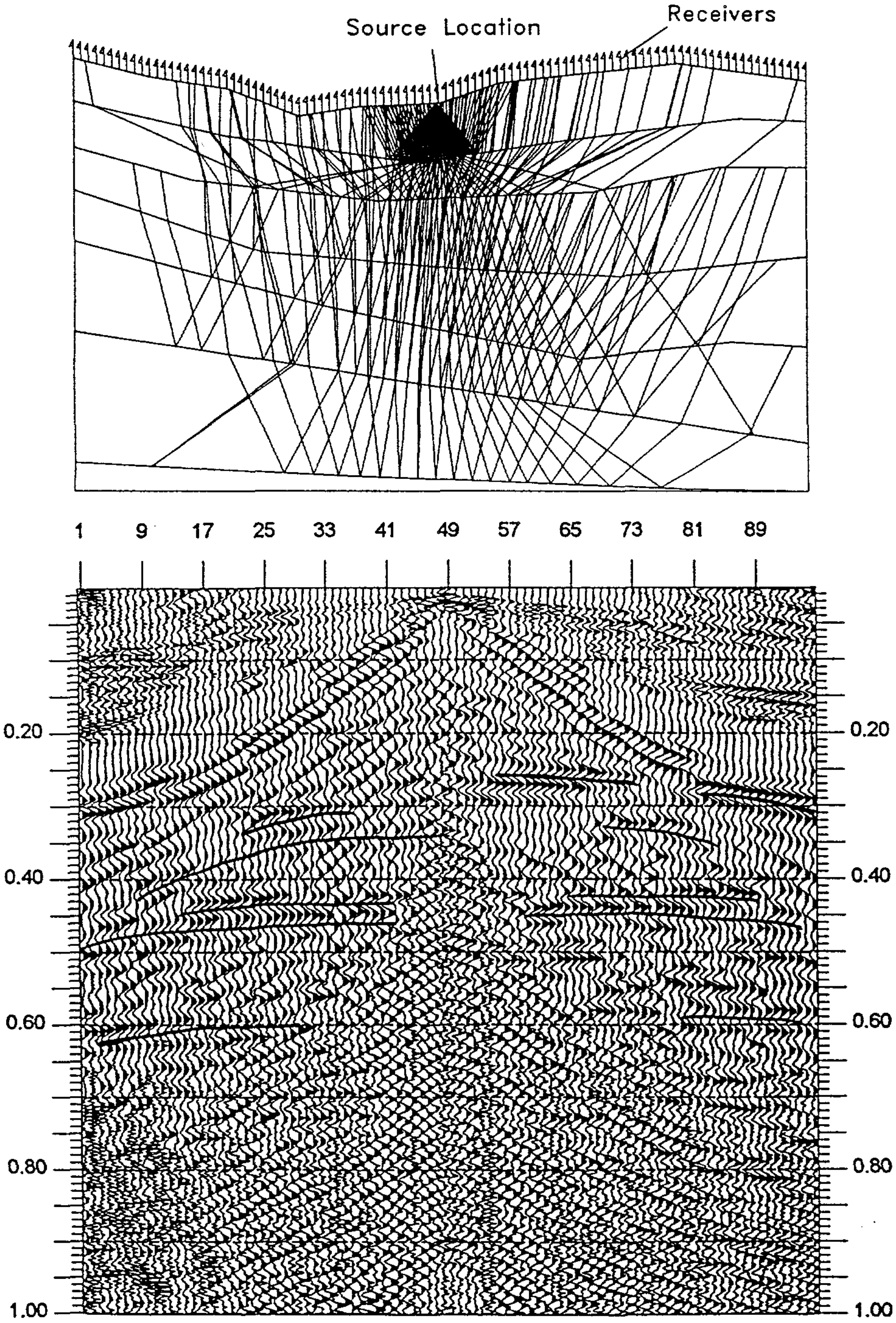


*Figure 7. Schematic representation of S- Wave shot record showing ray trace shot record and actual shot record.*

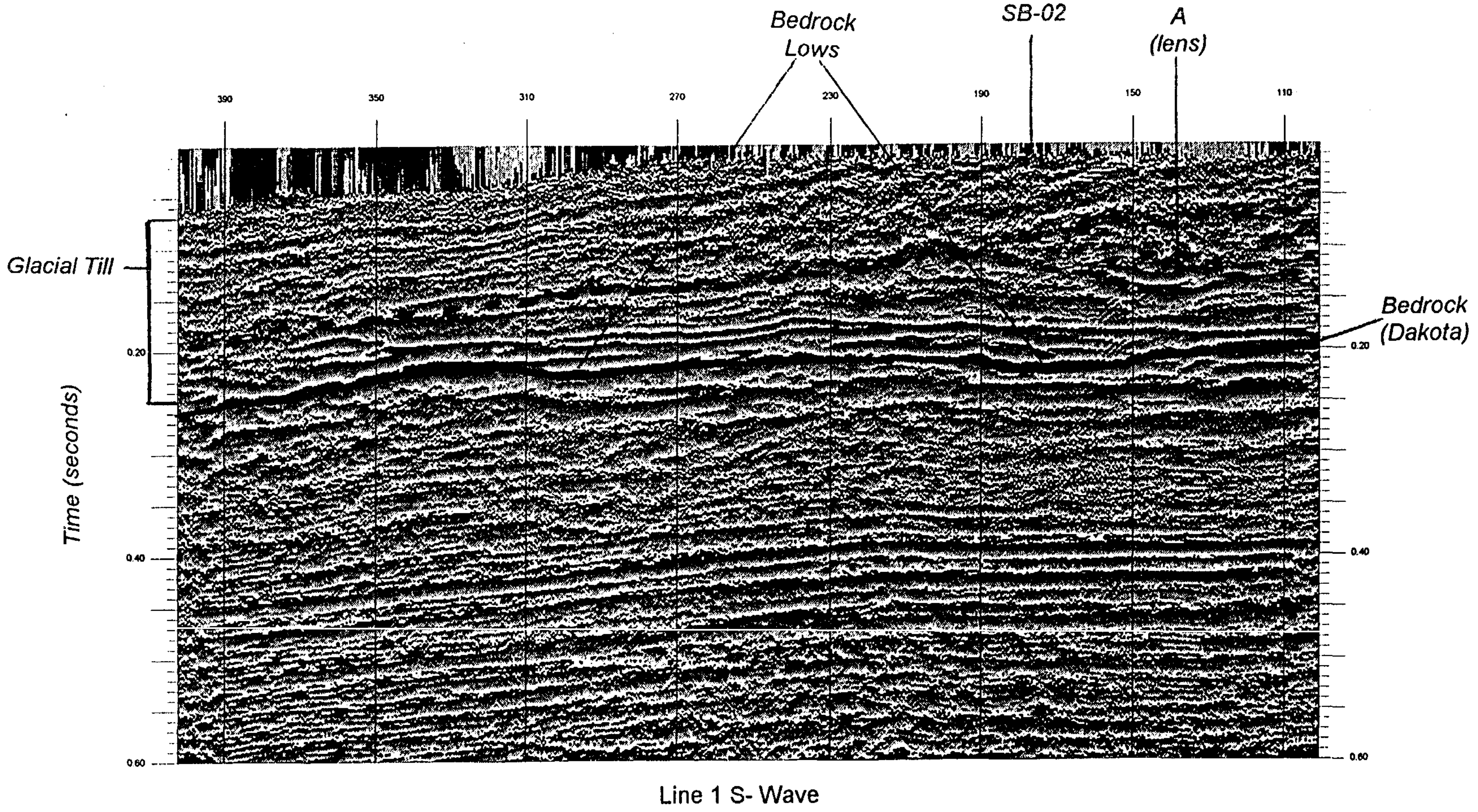


*Figure 8.* *S- Wave seismic reflection section plotted as instantaneous phase.*

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# EPA EFFORTS TO PROMOTE IMPROVED PROCESSES AND TOOLS FOR SITE CHARACTERIZATION AND MONITORING

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## ABSTRACT

The United States Environmental Protection Agency (EPA) advocates the use of innovative tools and methods to improve the cost-effectiveness and quality of hazardous waste site characterization and monitoring. This paper describes the efforts of various EPA offices within the Office of Solid Waste and Emergency Response to work toward this goal.

## INTRODUCTION

EPA promotes the use of innovative methods and technologies relevant to hazardous site remediation. As the environmental marketplace responds with the creation of tools to enable site characterization and cleanup to be performed "better, faster, and cheaper," it is essential that the various sectors of the engineering and regulatory communities keep pace. As described by the recent National Research Council report, *Innovation in Groundwater and Soil Cleanup: From Concept to Commercialization,* two ways that regulators can promote innovation within the remediation arena are by

- coordinating training, education, and dissemination of information about the appropriate use of innovative technologies to increase general regulatory acceptance; and
- coordinating verification and testing programs to define the boundaries of appropriate use, while eliminating duplicative demonstration projects.

The tools available for hazardous site remediation are undergoing rapid transformation. The regulatory, industrial, and public attitudes toward hazardous site remediation has become much more sophisticated since the 1980s, and the body of knowledge generated by research efforts and by practical experience is expanding so quickly that it is difficult to stay current.

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One result of these experiential and technological advances is that practitioners no longer find it necessary to always perform site work in a piecemeal fashion. It is no longer necessary to temporarily halt remedial activities while data is gathered and summarized into reports, and the interpretation of the data roundly debated before the next phase of work is begun. We often have enough experience now with certain site types that we can anticipate or "presume" the problems to be addressed and narrow the menu of technology options to consider. The result is that work at some sites can proceed seamlessly from investigation to remediation and closeout. With both careful planning and the use of rapid turn-around, on-site analytical technologies, investigation and cleanup objectives can be achieved in a fraction of the time and cost of traditional approaches which rely on a prescriptive, linear progression of phases and tasks. Considerable savings are realized both by reducing the number of distinct tasks and by performing multiple tasks simultaneously.

The challenge for advocates of innovative improvement is to begin to close the gap between what is possible through these "new" processes and techniques and what is accepted as "standard practice." We must synthesize successful innovations and pilot experiences into a more widely accepted (and practiced) paradigm which stresses thorough up-front planning of site work, stakeholder involvement, flexibility, and defensible data and decisions. This paradigm needs to be accepted and recognized institutionally within regulatory and legislative frameworks so that impediments to its use can be removed and incentives to its implementation created. We must also educate field practitioners and individual regulators to alleviate any misgivings they may have about new methods which may replace older, proven mechanisms to which they have grown accustomed and comfortable. It is essential that individual project teams have the tools at their disposal to fully understand and objectively review the application of these techniques at the site level.

EPA is attempting to meet this challenge. The Agency recognizes the progress that is occurring in EPA Regional Offices, other federal agencies, and state environmental agencies that demonstrates the success of this approach. The burden falls to EPA Headquarters to tackle impediments to widespread adoption of this paradigm by addressing issues such as budgetary and regulatory constraints, lack of information or education, and reluctance to break with past practices. This paper describes the roles of the various waste program offices within EPA Headquarters in this regard and it presents an overview of a number of specific EPA projects, supporting resources, and activities that signal progress toward meeting this challenge.

## EPA WASTE PROGRAM OFFICES' ROLES

The EPA Headquarters Office of Solid Waste and Emergency Response (OSWER) is the national program manager for the clean-up programs developed pursuant to the major legislative mandates in the area of hazardous waste and site clean-up. A number of these program offices play unique but interrelated roles in developing, promoting, and implementing activities that affect the manner by which site studies and cleanups are conducted. These offices and their respective roles are summarized as follows:

- **Technology Innovation Office (TIO):** Created in 1990 as an advocate for the use of innovative remediation technologies within OSWER, one of TIO's principal roles is to form partnerships between research programs and waste programs within EPA, as well as with other federal and state governmental organizations, universities and non-profit organizations, and private industry to encourage the exploration and acceptance of promising techniques useful for environmental remediation.

- **Office of Emergency and Remedial Response (OERR):** As the national program manager for the Superfund program, OERR is committed to finding ways to improve site assessment and investigation. OERR is currently working with TIO, the EPA Regional Offices, and the states to develop a number of tools to foster, and perhaps institutionalize, effective innovative site characterization practices. Since OERR is largely responsible for developing policies that govern the investigation and clean-up of Superfund sites, these initiatives are crucial to any efforts to cultivate widespread acceptance and institutional entrenchment of new practices.

- **Office of Solid Waste (OSW):** Equally critical in advancing the acceptance of new practices and techniques in EPA waste programs is the work of the OSW, which is the waste program office responsible for managing the Resource Conservation and Recovery Act (RCRA) regulatory and corrective action programs. Not only does the RCRA Corrective Action program provide national oversight for a large number of sites to be investigated and cleaned up, the guidance and regulations developed under RCRA have a profound effect on the practices employed in many waste clean-up program, both at the federal and state levels. OSW is actively involved on several fronts to support more efficient approaches to site characterization and measurement.

- **Office of Underground Storage Tanks (OUST):** This is the OSWER program office responsible for the regulatory program governing corrective actions for underground storage tanks, particularly petroleum tanks. OUST is developing a number of tools to assist states in their role of leading the investigation, monitoring, and cleanup of this potentially large universe of sites.

- **Federal Facilities Restoration and Reuse Office (FFRRO):** As the office responsible for EPA policy for the investigation and clean-up of facilities owned and operated by the federal government, FFRRO has significant influence over many sites undergoing environmental restoration. Thus, FFRRO has substantial impact on the ultimate acceptance and implementation of innovative processes at federal facility sites.

In addition to the OSWER program offices, the Agency's Office of Research and Development (ORD) is fully engaged in the area of improved technologies and techniques for site characterization and monitoring. The ORD National Exposure Research Laboratory (NERL), in particular, maintains the Agency's technology expertise for characterization technology. Through their research and technical management of Agency programs, NERL tests and evaluates new processes and technologies.

Each of the offices described above is undertaking a significant set of activities which promote the goal of improved site characterization and monitoring. These activities fall under two broad categories: policy and process improvements, and creating and disseminating better technology information. Together these activities work to create a climate and an institutional framework more receptive to improved technologies and processes in the Nation's waste clean-up programs.

## PROCESS AND POLICY INITIATIVES

### Performance-Based Measurement System

One of the most significant EPA initiatives to create a more flexible environment for conducting investigation and monitoring activities across all environmental media is the Performance-Based Measurement System (PBMS). PBMS embodies EPA's efforts to break down barriers to using new monitoring techniques and to implement the President's program for reinventing government and reforming regulatory policy. The Agency anticipates that PBMS will expedite development and acceptance of new technologies which may provide less costly options for environmental analyses. The PBMS initiative places regulatory emphasis on obtaining analytical results that provide adequate input into the regulatory decision, but leave the choice of analytical procedure up to the user. Adequate documentation is required to demonstrate that the testing protocol is truly adequate to meet the goal of regulatory compliance.

The Office of Solid Waste (OSW) has always subscribed to a flexible approach for analytical methods. This flexibility is emphasized within the EPA publication, *Test Methods for Evaluating Solid Waste-Physical/Chemical Methods* (commonly known as "SW-846"). The August 31, 1993 *Federal Register* states: "Any reliable analytical method may be used to meet [most] requirements in 40 CFR parts 260 through 270...[SW-846] functions as a guidance document setting forth acceptable, although not required, methods to be implemented by the user, as appropriate, to RCRA-related sampling and analysis requirements." (Emphasis added.)

Unfortunately, the flexibility inherent in the vast majority of SW-846 applications is frequently misunderstood by the environmental community. For this reason, OSW has increased its efforts to educate and inform the public and regulators about method flexibility and regulatory intent by means of national meetings and symposia, information request lines, training courses and workshops, and the development of guidance documents. More information is available from the OSW Methods Team Home Page, entitled *Monitoring Science in the RCRA Program*, on the World Wide Web at **http://www.epa.gov/epaoswer/hazwaste/test/index.htm**.

### State of the Practice in Site Assessment

In 1997, EPA prepared a review of the various independent approaches to rapid site assessment that depart from past practice. The goal of this study was to understand the range of work that various parties have done to improve and streamline the study of contaminated sites. The review paper contained the results of interviews and literature searches to identify and summarize uniquely described site characterization approaches within the U.S. There are at least 15 described strategies from a variety of sources, such as government agencies, academia, and professional organizations. Some commonalities underlie these approaches to expediting site characterization work:

- Formulate (at the *start* of the project, and with the involvement of stakeholders) a detailed description of what the site work is expected to accomplish.
  - What is the goal of this project? What is the site decision?
  - What level of uncertainty is permitted in the site decision? What level of documentation is required?
  - What level of funding is available?
- A team approach that includes representatives from various disciplines (risk assessment, engineering, chemistry, compliance, etc.) is vital to adequate planning and implementation of an efficient site characterization project.
- Determine data quality needs, i.e., what types and how much data are needed to answer the site question(s) to the level of uncertainty as formulated above?
- Develop a Conceptual Site Model (CSM).
  - What useful data are already available?
  - What data gaps remain?
  - How will the data gaps be filled?
- Consider data and documentation needs, funding, and regulatory aspects.
  - Will a traditional sampling and analytic scenario be required?
  - Can the use of field analytics and dynamic sampling plans save time and or money and meet all or some data needs?
  - Important: The choice of analytical methodologies must follow *from* the data needs.
- Prepare adequate and complete Sampling and Analysis Plans.
  - Address sampling design needs (e.g., statistical and uncertainty considerations, hotspots)
  - Address data quality needs (e.g., uncertainty considerations, interferences, detection limits, confirmation requirements).

On-site generation of data provides "immediate" decision-making capability which can rapidly and efficiently guide characterization efforts and focus remediation selection through an adaptive sampling strategy. Flexible or "dynamic" work plans maximize the power of field analytical methods to effect a cost-effective, successful conclusion. A well-written work plan will communicate the rationale for, and use of, each data point to be collected. Technical experts should be available on-site to implement the adaptive sampling strategy by evaluating analytical results and designing subsequent sampling protocols, and to address any problems that arise, such as unexpected analytical interferences.

This type of formalized or systematic planning process is especially vital to site characterization efforts that involve the use of field analytical methods. With standard "fixed lab" procedures and the EPA Contract Laboratory Program (CLP), there is an expectation of a certain minimum level of data quality and analyte detection limits. This "default" level of data quality can be expensive and time-consuming, and (possibly) wasteful if it is not needed for the specific decision objective. However, it does provide a data quality safety net that cannot be automatically assumed with the use of field analytics. Field analysis *can* realize substantial time and cost savings, while providing high quality data to support defensible site decisions, but this can be guaranteed *only* if sufficient advance planning is performed.

## Emerging Site Assessment Guidance: Presumptive Site Assessments

In conjunction with the above, EPA is undertaking several initiatives to strengthen and modify the Site Assessment process within the Superfund program. Among these activities is an effort to develop strategic site investigations for specific site types (e.g., manufactured gas plants, grain storage bins, steel manufacturers) that are designed to save time and money. These "presumptive"strategies would function as suggested protocols and could be combined into a compendium of assessments for the purpose of supporting several of EPA's recent initiatives including brownfields, site screening, and rapid site characterization.

Presumptive site assessments are derived from the most current practices. They focus the inspection activities on specific strategic objectives, use field analytical methods to satisfy data needs when possible, and emphasize a reduction in time and cost (as compared to a conventional site characterization approach) by combining activities. Some prior knowledge of site history would be necessary in order to select an appropriate assessment approach. Based on the type of site and its history, the presumptive site assessment would specify likely contaminants and their probable locations, as well as promising characterization strategies.

EPA hopes to develop example strategies in cooperation with EPA Regional Offices using the Superfund Technical Assessment and Response Team (START) contractors. Region 7 efforts have focused on grain storage sites. Region 6 is exploring creosote sites, aerial applicators, and dry cleaners. All Regions have been encouraged to assist in the development of presumptive site assessment guidance, which need to be practical and useful, reflecting the experience gained from past site assessment efforts. The Regional Offices are working with EPA Headquarters to help frame discussions on the development of these guidance and to deliberate on key policy issues. State requirements and experience will be considered as well. Preliminary discussions with the Association of State and Territorial Solid Waste Management Officials (ASTSWMO) indicate a strong interest. Kansas representatives have written a letter asking to participate. Some EPA Headquarters contract work related to this effort has been completed: four draft templates were prepared which considered dry cleaner operations, manufactured gas plants, steel manufacturing sites, and paint shops.

### Brownfields Site Assessment Guidance

A large portion of future site evaluation workload lies in brownfields programs, which link economic development with the environmental restoration of underutilized, abandoned, or idled properties, with the goal of beneficial reuse. A premium is placed on investigations that are less costly and performed more quickly than has been the case in more traditional settings. To provide assistance to state, tribal, and municipal officials, EPA is developing a guidance document entitled *Quality Assurance Requirements for Conducting Brownfields Site Assessments*. It will include a framework for determining the types and quantity of environmental data needed to make decisions regarding site characterization and redevelopment potential, as well as a template Quality Assurance Project Plan (QAPP), which describes the activities needed to ensure that collected data are of known quality to support reasonable, informed decisions.

### OERR Site Assessment Team

This team coordinates many of the above activities within the Superfund program, and is comprised of Site Assessment Regional Coordinators from the five OERR Regional Centers, as well as from the various Superfund program "Centers" (State and Tribal Site Identification, Information Management, Contracts Oversight, Community Involvement and Outreach, Program Analysis, and Resource Management). The Team's mission is to ensure consistency and communication across the Regions and to develop policies that facilitate the site assessment process.

### RCRA Corrective Action Strategy

In a May 1996 *Federal Register* Notice EPA introduced its strategy for promulgating regulations governing corrective action for contaminant releases at hazardous waste management facilities which are regulated under the Resource Conservation and Recovery Act (RCRA). This

Advanced Notice of Proposed Rulemaking (ANPR) emphasized areas of flexibility within the current program and described program improvements under consideration. Section III.C.2 (pp. 19444-19446) emphasizes the critical importance of carefully designed and implemented RCRA Facility Investigations (RFIs) to accurately characterize the nature and extent of site contamination.

Experience in corrective action implementation has demonstrated that poorly focused investigations can become a drain on time and resources and, in some cases, unnecessarily delay remedial actions. EPA emphasizes that remedial investigations should be tailored to the specific conditions and circumstances at the facility and focused on the units, releases, and exposure pathways of concern. A number of approaches were discussed in this ANPR as being particularly helpful in developing focused site investigations:

- The use of dynamic conceptual site models considerably aids planning and risk-based decision-making at a site.
- EPA encourages program implementors and facility operators to take advantage of the cost- and time-savings possible with innovative characterization technologies. Exploitation of innovative site characterization technologies (including on-site analytical techniques and adaptive sampling plans) offers many benefits which include
  - on-site decision-making and optimization of the investigation effort;
  - enhanced 3-dimensional understanding of the site;
  - better identification of actual or potential risks posed to human or ecological receptors; and
  - more rapid assessment of the need for interim actions.
- Tailoring data quality objectives (DQOs) to site-specific needs ensures that environmental data are scientifically valid and defensible for the intended use. EPA has found that site investigations can be expedited considerably when DQOs are carefully established.
- The use of existing information to streamline the remedial investigation can reduce costs and increase the speed of cleanups. Where DQOs have been established, the adequacy and usefulness of existing data is assessed by comparison with the project DQOs.
- Action levels (health- or environmentally-based concentrations derived from chemical-specific toxicity and protectively conservative exposure assumptions) can serve as a trigger mechanism for deciding whether additional investigation is warranted. Actions levels can be most beneficial if they are available during the planning stages of site investigations.
- If thorough advance planning is used, likely remedial strategies will become clear early in the site assessment process. To expedite the corrective action process, EPA encourages program implementors and facility owners/operators to focus data gathering during site characterization on information needed to support plausible remedies.

Additionally, a national RCRA Corrective Action Training Initiative is being developed that will emphasize results-based site management tools for accelerating schedules, improving efficiency, and focusing implementation on protective results. This training course is anticipated to address some of the innovative characterization approaches outlined in the May 1996 ANPR.

### Interagency Policy Initiative

The EPA Federal Facilities Restoration and Reuse Office (FFRRO) has been instrumental in organizing an Intergovernmental Data Quality Task Force which is currently composed of representatives from EPA, DoD, and DOE, with other federal entities expected to join. The Task Force was initiated to address an EPA Inspector General's audit concerning data quality issues at federal facility Superfund sites, but is evaluating whether its scope should eventually expand beyond Superfund to all environmental data quality concerns. Its current mission is to document a government-wide quality system focused, at least initially, on the hazardous waste programs. Because this is a new initiative, many details regarding this Task Force and its mission remain to be defined.

## CREATING AND DISSEMINATING BETTER TECHNOLOGY INFORMATION

### Partnering to Improve the Documentation of Technology Performance

Through efforts such as the Federal Remediation Technologies Roundtable, the Remediation Technologies Development Forum, and the Consortium for Site Characterization Technology, EPA and its federal and private sector partners have collaborated on technology demonstrations and the development of products to standardize the effective communication of technology capabilities. Spearheaded by the Technology Innovation Office, one such product was the Roundtable development of the *Guide to Documenting Cost and Performance for Remediation Projects*. The *Guide* established a baseline for the future collection of standard data elements for thirteen classes of remediation technologies. It is being used by member agencies to collect cost and performance information for incorporation into case studies on current remediation efforts. Continued use of the *Guide* should lead to a significant body of information to support cost comparisons and performance projections, which will, in turn, permit better remedy selection and remedial design at hazardous waste sites.

The lessons learned through the Roundtable efforts on remediation technologies are now being applied to site assessment and characterization. TIO and other Roundtable members are investing resources in products that support better understanding of the state of the practice for site study. To carry out this work, the Roundtable has formed a site characterization subgroup.

### Technology Evaluation and Performance Verification

A key component of promoting innovation is creating a body of credible data on the performance of commercially available, field-ready technologies. The Technology Innovation Office works closely with EPA's Office of Research and Development to implement a program that provides unbiased evaluation of vendor claims for field performance of analytical, sampling, monitoring, and characterization technologies. Managed out of EPA's National Exposure Research Laboratory in Las Vegas, the Consortium for Site Characterization Technology (CSCT) is one of twelve technology-specific pilots under the Environmental Technology Verification (ETV) Program. Some evaluations had been previously done under the Superfund Innovative Technology Evaluation (SITE) Program. With its broader client orientation, the recently established CSCT is now responsible for field testing technologies under controlled, yet realistic, field conditions to evaluate technology performance against vendor claims and standard or accepted methods for achieving the goals of the technologies. The results of these evaluations, conducted through third-party "verification partners," are captured in summary reports. Each report includes a four-page verification statement signed by the Director of the EPA National Exposure Research Laboratory. The main verification report details the design and implementation of each evaluation project and the basis for its conclusions.

The following technologies have been through or are currently going through the ETV/CSCT verification program:

- Cone Penetrometer/Laser Induced Fluorescence (CPT/LIF): 2 vendors/2 technologies **(reports complete)**;
- Field Portable X-Ray Fluorescence (FPXRF): 5 vendors/7 technologies **(reports complete)**;
- Field Portable Gas Chromatography/Mass Spectrometry (GC/MS): 3 vendors/3 technologies **(reports complete)**;
- Soil and soil gas sampling technologies: 6 vendors/7 technologies;
- PCB-measuring technologies: 5 vendors/7 technologies; and
- In-situ (well-head) monitoring: 7 vendors/7 technologies.

Upcoming verification projects include

- Decision Support Software (DSS);
- Field extraction methodologies;
- Groundwater sampling technologies; and
- Sediments sampling technologies.

TIO has worked with the CSCT pilot managers to promote the acceptance of verified technologies. TIO has created or employed a number of mechanisms to publicize and distribute the verification reports to potential technology users:

- A network of characterization technology advocates located in EPA's regional waste and laboratory programs;
- A relationship with the Interstate Technology Regulatory Cooperation (ITRC) Workgroup;

- The use of the Technology Innovation Office's exhibit booth to gain visibility at relevant environmental, regulatory, and professional conferences;
- Internet access to all documents through the Technology Innovation Office web site (CLU-IN) at **http://clu-in.com/char1.htm#verification**;
- Mass mailings of fliers announcing the availability of new CSCT documents;
- Announcements through e-mail and postal mail distribution of the *TechDirect* listserver and *TechTrends* newsletter; and
- Topical seminars and briefings for key user groups at the various levels of government and the private sector.

## Documenting Performance

Working with its federal partners, TIO is addressing the need for case studies to document successful applications of field analytical and geophysical technologies and techniques. Mindful of the benefits attributable to collecting this information in a uniform manner, TIO will work with the member agencies of the Roundtable to develop a guide for collecting and presenting case study information relevant to site characterization. This guide will consist of two parts: the first section will facilitate the collection and documentation of information during the actual performance of the project which will be vital to later preparation of a case study report; the second part of the guide will serve as a template for writing the case study report in a consistent format.

TIO is gathering information on intriguing projects already underway in a number of places around the United States. One such effort, recently completed through joint effort of EPA Region 1, Tufts University, and the Air Force at Hanscom AFB (in Massachusetts), is the subject of a case study, which will concisely describe the investigational tools used, the use of the field generated analytical data that addressed the site decision, and the costs. Some information about the work done at Hanscom AFB is currently available through the Clean-Up Information (CLU-IN) Internet site at **http://clu-in.com/char1.htm#regional**. Similar projects have been done by other federal and state programs, with information accessible through Internet sources. TIO will continue to work to identify these projects and disseminate their results through the preparation of additional case studies. TIO realizes it may be unaware of some projects and is actively seeking information on their existence and results.

## Promoting Technology Availability and Use

Tracking technology availability and deployment represents another critical activity in the promotion of improved technologies and processes. To address the need of site managers, consulting engineers, and others for better understanding of the tools and services available to conduct site characterization and on-site chemical analysis, TIO developed the Vendor Field

Analytical and Characterization Technologies System (Vendor FACTS). Vendor FACTS is a searchable database of innovative site characterization technologies and vendors, which is updated yearly. It is currently in its third version (Vendor FACTS 3.0), and contains 154 analytical, geophysical, chemical extraction, and sampling technologies provided by 116 technology vendors.

The product information within Vendor FACTS is provided by the vendors (without EPA endorsement), and covers applicability, performance, and current use. It is available from EPA at no charge in CD-ROM format. Alternatively, it can be downloaded from the Internet through the CLU-IN web site at **http://clu-in.com/char1.htm#selection**. Vendor FACTS allows a potential user to quickly screen technologies for a particular application, and to examine particulars such as potential media, analytes, detection limits, interferences, etc. Developers of field analytical technologies are encouraged to participate by completing a Vendor Information Form. Vendor participation is free-of-charge.

EPA is also working with the US Naval Facilities Engineering Command and the US Army Corps of Engineers to develop a *Field Analytical and Sampling Technology Matrix and Reference Guide* for field analytical and sampling/extraction technologies. In poster format, the *Matrix* will provide a tool for project managers to quickly identify technology options and compare them against their specific site problems. Composed of two parts, one for field analytical technologies and one for sampling and extraction technologies, the matrix provides simple ratings on the capabilities and limitations of a wide range of technology options. Parameters include target analytes, throughput, media types, cost, verification/evaluation experience, interferences, depth limitations, etc. The accompanying *Reference Guide* provides more detailed descriptions of how the ratings were derived and lists supporting information resources. The printed matrix will be available summer 1998. The Corps will also arrange for on-line availability at the Federal Remediation Technologies Roundtable home page at **http://www.frtr.gov**. The FRTR homepage already includes the FRTR Treatment Technologies Screening Matrix.

A new EPA report, *Field Analytical and Site Characterization Technologies: Summary of Applications*, was released by TIO in November 1997. It summarizes (in tabular format) over 200 applications of 23 field analytical and characterization technologies at actual remedial sites as reported by federal and state site managers. The report documents the way the deployed technology was used (e.g., health and safety monitoring, cleanup or compliance monitoring, site screening or characterization). In addition, each entry provides information about the site where the technology was used, the problems addressed (contaminants and media), and most importantly, the name and telephone number of a colleague who can provide insights on their experiences with a particular technology under real site conditions. TIO expects that this kind of inventory can increase the comfort level of project managers who are considering use of a particular technology for the first time by indicating where the technology has been used before.

## Promoting Expedited Assessment Tools for Leaking Underground Petroleum Storage Tanks

To support more efficient site assessment practices in this important program area, the Office of Underground Storage Tanks (OUST) has published a site assessment manual, entitled *Expedited Site Assessment Tools For Underground Storage Tank Sites: A Guide For Regulators.* Over 7,000 copies were distributed to federal and state Underground Storage Tank/Leaking Underground Storage Tank (UST/LUST) regulators. The manual includes a chapter on field analytical methods for petroleum hydrocarbons, and discusses the operating principles, capabilities, and limitations of each method to aid the reader to select appropriate applications.

To address a specific, critical program need, OUST is working with the U.S. Geological Survey (USGS) of the Department of Interior. They are jointly exploring the possibility of developing and publishing a manual on the characterization of fractured bedrock. The document would be applicable to all types of contaminant sites, not just petroleum UST releases.

## Technology Training

An initial task of the Federal Remediation Technologies Roundtable Subgroup on Site Characterization is developing a training course for federal agencies which will synthesize critical aspects of existing workshops on innovative technologies and expedited characterization processes. This new course for will not only educate federal project managers on the full range of technology options and capabilities, but more importantly, emphasize the critical role of planning to manage field work in a way that maximizes the benefits and strengths of field analytical technologies.

The Technology Innovation Office coordinates the offering of training courses through both the CERCLA Education Center (CEC) and the Northeast Hazardous Substance Research Center (NHSRC). Courses provide instruction on the use and application of innovative site characterization technologies. The CEC course targets EPA project managers (although it can be offered to other federal and state project managers) and is presented in both one-day and three-day formats. The three-day course provides hands-on training with the technologies. A modified CEC course is offered though a cooperative agreement between TIO and NHSRC and is open to the general public with a specific emphasis on reaching staff from state and local governmental agencies. It uses the condensed one-day format, but includes opportunities for students to receive some hands-on training directly from the technology vendors. Stipends are available to cover travel expenses to assist state and local project managers' attendance at one of the five offerings in 1998. These courses are not designed to produce expert operators of the equipment: the goal is to make line-level decision makers more familiar with technology options and the applicability and limitations of these options to their site-specific projects.

The Office of Solid Waste's Methods Team provides technical support and instruction related to the use and selection of analytical methods used within hazardous waste programs. The RCRA Program's Analytical Strategy Training is offered several times a year, and is also provided locally to regional EPA offices and state agencies upon special request.

OUST has organized and conducted several site assessment workshops with state regulators that have promoted the use of field analytical methods. One workshop was conducted in Chicago by the EPA Region 5 UST section, April 4-6, 1995, for Region 5 states. Another workshop was conducted in San Antonio, Texas, September 16-18, 1996, for Region 6 and 7 states. A third was held in Portland, Maine, July 15-17, 1997, for Region 1 and 2 states covering characterization in fractured bedrock. These workshops provide state personnel an opportunity to learn about field methods for the analysis of petroleum hydrocarbons and when their use is appropriate.

### EPA's Clean-up Information World Wide Web Site (CLU-IN)

As more and more information resources are developed, TIO facilitates their dissemination to decision makers and technology users. TIO maintains the CLU-IN web site (**http://clu-in.com**) to provide updates on the operation, development, and commercialization of innovative site characterization and remediation technologies. Recently published documents and databases related to these issues can be downloaded from the web site. CLU-IN also contains information about interagency and public-private partnerships, and provides links to other web sites concerned with environmental restoration and technology development.

## CONCLUSION

EPA is coordinating its internal and external efforts to encourage greater efficiency in site cleanup activities. Adequate site characterization is essential to define the nature and extent of contamination so that site decisions regarding cleanup will be done in a scientifically and legally defensible, yet cost effective, manner to achieve the ultimate goal of human health and environmental protection. The range of experience and knowledge gained over the past decade is permitting EPA to capitalize on new technologies and new ideas. To maintain the momentum of this progress, EPA must continue to recognize, coordinate, and promote the often isolated individual initiatives underway, while developing a cohesive program to advance their use. Both in terms of technology and process, significant improvements have been achieved which stand to not only increase the effectiveness of our clean-up programs, but also to save considerable resources. More and more voices within governmental, academic, and private sectors are calling for the use of thorough systematic planning, team participation, field analytical technologies and other innovations to save time and money without sacrificing data quality or the level of protectiveness required of the Agency. The challenge for EPA's clean-up programs lies in communicating and cultivating these advancements within all levels of the decision making structure.

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# RAPID SITE ASSESSMENT APPLIED TO THE FLORIDA DEPARTMENT OF ENVIRONMENTAL PROTECTION'S DRYCLEANING SOLVENT CLEANUP PROGRAM

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## ABSTRACT

Applying the rapid site assessment approach to characterize soil and groundwater contamination at drycleaning facilities and drycleaning wholesale supplier sites is drastically reducing the time and costs associated with site assessments. Rapid site assessments conducted under the Florida Department of Environmental Protection (FDEP) Drycleaning Solvent Cleanup Program (DSCP) are attaining the FDEP DSCP goal to reduce the time spent "studying" sites and to move the sites into remediation within one year.

Specific rapid assessment tools to achieve the FDEP DSCP goal are administrative, such as flexibility in scoping work and costing (e.g., unit pricing), and technical, including streamlined work plans and innovative sampling and analytical methods. Flexible scoping allows the approval of proposed scope changes to accommodate on-site conditions identified during fieldwork and facilitates more complete delineation of contamination during initial field efforts and minimizes the need for additional mobilizations. Innovative technical methods include soil gas surveys, direct-push (DP) technologies, and the use of certified mobile laboratories. Soil gas surveys serve to speed up the assessment of source areas and to focus overall assessment activities. DP technologies are used to characterize site lithology, geology, and hydrogeology and to collect soil and groundwater samples. On-site mobile laboratories provide the on-site hydrogeologist with screening data for targeted analytical suites in less than 30 minutes. Rapid collection and analysis of samples in the field provide "real-time" data for evaluating the three-dimensional distribution of chemicals of concern in soil and groundwater.

The rapid site assessment approach, which cost-effectively expedites the investigation process, can be successfully applied to other federal, state, and privately funded site assessment/remediation projects. Resources allocated for site assessment and remediation can be directed primarily into actual site remediation, rather than into conventional, lengthy, and costly site assessment.

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# INTRODUCTION

Applying the rapid site assessment approach to characterize soil and groundwater contamination at drycleaning facilities and drycleaning wholesale supplier sites is drastically reducing the time and costs associated with site assessments. Rapid site assessments conducted under the Florida Department of Environmental Protection (FDEP) Drycleaning Solvent Cleanup Program (DSCP) are attaining the FDEP DSCP goal to reduce the time spent "studying" sites and to move the sites into remediation within one year.

Specific rapid assessment tools to achieve the FDEP DSCP goal are administrative, such as flexibility in scoping work and costing (e.g., unit pricing), and technical, including streamlined work plans and innovative sampling and analytical methods. Flexible scoping allows the approval of scope changes proposed to accommodate on-site conditions identified during fieldwork and facilitates more complete delineation of contamination during initial field efforts and minimizes the need for additional mobilizations. Innovative technical methods include soil gas surveys, direct-push (DP) technologies, and the use of certified mobile laboratories. Soil gas surveys serve to speed up the assessment of source areas and to focus overall assessment activities. DP technologies are used to characterize site lithology, geology, and hydrogeology and to collect soil and groundwater samples. On-site mobile laboratories provide the on-site hydrogeologist with screening data for targeted analytical suites in less than 30 minutes. Rapid collection and analysis of samples in the field provide "real-time" data for evaluating the three-dimensional distribution of chemicals of concern in soil and groundwater.

By obtaining real-time data, senior hydrogeologists are able to make decisions that facilitate completion of site assessments during a minimum number of fieldwork phases. On-site laboratories immediately analyze samples from existing monitoring wells (where available) and from DP locations; these real-time analytical data enable senior hydrogeologists to direct fieldwork and refine the site conceptual model. Real-time data and rapid decision-making in the field mean the ability to perform work which is necessary but beyond the original scope of work while still in the field. Such work can involve additional DP sampling to delineate the vertical and horizontal extent of contamination as well as installing and sampling permanent monitoring wells. Using DP technology also greatly reduces the production of investigation-derived waste and associated disposal costs.

Rapid assessment techniques allowed field teams to characterize eight drycleaning and wholesale supply facilities in Jacksonville, Florida, within 10 weeks. Approximately 575 samples were collected using DP sampling techniques, and approximately 675 samples were analyzed by the on-site laboratories. Additionally, based on the analytical data, 37 permanent monitoring wells were installed. For seven of the eight sites, the initial scope of work was expanded 50 to greater than 100 percent. Five of the eight sites exhibited contaminant concentrations suggesting the presence of dense nonaqueous-phase liquids (DNAPLs).

As with most approaches, some limitations were encountered during the application of rapid assessment techniques, including resource coordination and physical limitations of the DP technologies. Careful planning of resources and logistics was necessary to optimize utilization of the DP unit and mobile laboratories and to prevent "down time," delays in sample collection and/or analysis. In some areas, DP sampling was limited by the refusal of advancement of DP probes by the subsurface lithology or by difficulty imposed by subsurface geologic conditions, such as "flowing sands."

The rapid site assessment approach, which cost-effectively expedites the investigation process, can be successfully applied to other federal, state, and privately funded site assessment/remediation projects. Resources allocated for site assessment and remediation can be directed primarily into actual site remediation, rather than into conventional, lengthy, and costly site assessment.

## Florida's Drycleaning Solvent Cleanup Program

In 1994, the Florida Legislature established a state-funded program to remediate properties contaminated as a result of the operations of a drycleaning facility or drycleaning wholesale supply facility (Chapter 376.3078, Florida Statutes ["the Statute"]); the Drycleaning Solvent Cleanup Program (DSCP) is administered by the FDEP. The Statute was sponsored by the drycleaning industry to address environmental, economic, and liability issues associated with drycleaning solvent contamination. The DSCP limits the liability of the owner, operator, and real property owner of drycleaning or wholesale supply facilities for remediating drycleaning solvent contamination if these parties have complied with and met the conditions stated in the Statute.

A fund has been established to pay for costs related to the assessment and remediation of drycleaning solvent-related properties. Revenue for the fund is generated by a gross receipts sales tax, a tax on tetrachloroethene (PCE) sold to or imported by a drycleaning facility, annual DSCP registration fees, and structured deductible payments. The Drycleaning Solvent Cleanup Rule (62-781, Florida Administrative Code, effective March 13, 1996 ["the Rule"]) sets forth the requirements for application to the DSCP and provides the forms to apply to the DSCP and to document contamination. The FDEP began accepting applications to the DSCP on the effective date of the DSCP, and to date has found more than 900 facilities eligible for the DSCP.

The Rule identifies the criteria that determine whether a site is eligible. The FDEP reviews the DSCP application and determines whether a site has met the requirements. A score is developed for the site by the FDEP in accordance with the statutorily prescribed scoring system. The scoring system considers various factors, including evidence of contamination at the site and the potential risks to human health and the environment. Of the more than 900 sites that have been determined eligible to date, 82 sites have been assigned to 10 state contractors for assessment and remediation, as necessary.

As drycleaning-solvent sites are typically more complex than petroleum sites and often require greater resources for assessment and remediation, the FDEP needed to develop more efficient and cost-effective methods for assessing relative risks associated with each site, for minimizing resources used in the assessment, and to focus the DSCP's limited funding on actual site remediation.

For more general DSCP information, related documents and other program information are available through the FDEP Fax-On-Demand System. Copies of the registration forms, Rule 62-781 and forms, a DSCP status update, and other information can be obtained by telefacsimile by calling (800) 789-4502. The system is periodically updated as additional information becomes available. Information also can be retrieved from the Internet at: http://www.dep.state.fl.us/waste/programs/dryclean/index.htm.

### Objectives of the FDEP Drycleaning Solvent Cleanup Program

The FDEP has selected 10 contractors (state funded) to assess and remediate eligible sites under the DSCP and other state-funded hazardous waste sites. Because of the limited funding available, the FDEP has developed numerous methods to cost-effectively address drycleaning-solvent sites. During the contractor selection process, the FDEP required each firm to present an overview of how they would administer a drycleaning solvent cleanup program, reduce costs, and meet the FDEP goal of moving from assessment to remediation within one year. The FDEP compiled the contractors' best ideas along with its own to establish the DSCP, a program that quickly and cost-effectively identifies sites that pose the greatest potential risks to human health and the environment.

The FDEP's objectives are to rapidly assess DSCP-eligible drycleaning-solvent sites, perform risk-based corrective action (RBCA) evaluations, and then decide the appropriate future action(s) for each site. To meet these objectives, the FDEP developed guidelines for its contractors that include administrative and technical methods and considerations. The intent of the guidelines is to facilitate moving sites through assessment into remediation within one year of the site's assignment to one of the 10 state-funded contractors. These guidelines include: 1) assigning sites within one or nearby geographical areas to the same contractor; 2) establishing well negotiated labor, equipment, and laboratory rates; 3) developing streamlined and flexible work plans and cost estimates; 4) completing site assessments in a minimum number of phases by using rapid assessment techniques and maintaining open communication during assessment activities; 5) establishing standard database formats for all data that are generated and submitted to the FDEP for Geographic Information Systems (GIS) application; and 6) establishing streamlined and standard contamination assessment reports (CARs), remedial action alternative evaluations, and remedial action plans (RAPs).

## ADMINISTRATIVE METHODS AND CONSIDERATIONS

Conducting rapid assessments for the FDEP DSCP was facilitated by the preparation of streamlined work plans that were concise and flexible in scope and associated costs. This was extremely important to the rapid assessment approach because the main goal was to complete the assessments in a minimum number of fieldwork phases. Work plans and cost estimates were prepared so that, during the initial phase of fieldwork, changes necessitated by conditions in the field could be agreed upon between the project and contract managers and the additional work could be conducted without schedule delays.

### Streamlined Work Plans

Preparing streamlined work plans required initial site visits and meetings with the FDEP contract managers to develop scopes of work for each site. During these meetings and the development of the work plans, specific sampling locations, resources needed for conducting the work, and key potential obstacles to the assessment (e.g., property access issues) were identified.

Typical streamlined work plans consisted of a one-page site background/description, a two-page scope of work, and three figures showing site location, site features, and proposed sampling locations. The document format minimized preparation time and associated costs and enabled reviewers of the work plans to quickly understand the background of each site and the proposed scope of work, thus facilitating the approval process.

### Unit Pricing Structure

Developing a unit cost pricing structure using established rates (either contract rates or actual price quotes from subcontractors) enabled project managers to quickly develop cost estimates to accompany the scopes of work. Contract rates included labor and per diem, rates for subcontractors (e.g., DP unit, mobile laboratory, and fixed-base laboratory), and equipment rates. Many of these rates were structured in the work plans as unit price daily rates. Unit pricing allowed quicker review and approval time for conducting work because rates were known and agreed upon prior to the preparation of the work plans.

Furthermore, unit pricing facilitated preparing change orders in the field for additional sampling points, if needed. As the main goal of rapid assessment was to complete the assessment within a minimum number of mobilizations, it was important that changes in the scopes of work were easily defined, estimated, and approved. Historically, change orders for additional fieldwork might have indicated that a contractor project manager had not scoped the work appropriately. For rapid assessment, the submittal of change orders was expected. It is important to remember that site assessments were conducted because the extent of contamination was *not* known; therefore, changes in the scopes of work and associated change orders were expected. Communication between the project and contract managers during time-critical phases of fieldwork and the completion of the required paper work facilitated the efficient performance of additional fieldwork, thereby enabling completion of the rapid assessments in a minimum number of fieldwork phases.

## TECHNICAL METHODS AND CONSIDERATIONS

### Rapid Assessment Methods - Planning and Scheduling

Completing the eight Jacksonville rapid site assessments required thorough planning and careful scheduling. Thorough planning minimized potentially iterative field mobilizations, such as might have resulted from difficulty obtaining permission to access neighboring properties.

The FDEP created a brief, standard site access form that adequately addressed most property and neighboring property access issues. During work plan development and prior to mobilization, neighboring property parcels were identified, property owners were contacted, and property access permission was acquired.

Thoughtful planning also minimized potential down time related to unknown underground utility locations, active drycleaning operations, overhead power lines, and traffic, as well as other existing site contamination, such as petroleum constituents potentially associated with neighboring gasoline stations. Acquiring background information on hydrogeology and potential contaminant sources during the work plan development was critical to the rapid assessments. This background information enabled specific targeting of horizontal and vertical sampling locations. Collecting relevant background information included researching lithology, geology, and hydrogeology in each site area to evaluate routes of potential migration and to identify confining/semiconfining units or other features such as fill, peat, and/or significant geological units. In-depth interviews with drycleaning facility representatives were conducted to identify and target potential source areas, such as floor drains, sewer lines, spills, leaks, or used filter storage areas, for assessment.

Careful scheduling minimized the number of field mobilizations and realized cost savings by using subcontractors, such as DP contractors, mobile laboratories, and drillers, on multiple site assessments within a common geographical area. For the DSCP, detailed schedules for the assessment phase of work were developed using Microsoft© Project® software. These schedules addressed mobilization to multiple sites by utilizing teams of DP and mobile laboratories. Careful scheduling also optimized other labor, equipment, and subcontracted services, such as sharing sampling technicians, sampling equipment, and surveying services among sites.

At the first scheduled site assessment during rapid assessment, DP drilling and sampling were conducted, followed by immediate sample analyses by an on-site mobile laboratory. Subsequent to completing work at the first site, the DP unit and mobile laboratory moved to the second site (in the same geographical area) without requiring additional mobilization. The drilling and installation of monitoring wells was then initiated on the first site, and so on. The DP contractor and mobile laboratory were available to mobilize to multiple sites if additional assessment was deemed necessary during the initial assessment phase.

## Rapid Assessment Tools

Rapid assessment tools have been available for several years, but their use for state-funded and Superfund assessments has been limited. The limited use of rapid assessment tools may have resulted because regulatory agencies and regulatory guidance documents have considered the use of such tools more a “screening” method than a sampling method that yields defensible and valid data. Only recently have these tools gained recognition for enabling the collection of data that are readily acceptable, and as initial tools to focus more permanent sampling locations, such as the installation of permanent monitoring wells.

**Soil Gas Screening Technology.** Soil gas screening was conducted at a limited number of the Florida DSCP sites in Jacksonville. Soil gas surveys were used prior to more quantitative assessment techniques because potential source areas and the locations of septic system drain fields were unknown. A small diameter hole was punched through the asphalt cover, if present, and a small diameter hollow soil gas probe was pushed into the soil. Once at the desired depth, the soil gas probe was retracted slightly to allow soil gas to enter the probe. A specially designed, intrinsically safe suction pump was used to create a vacuum to withdraw soil gas. After evacuating several liters of soil gas, a photoionization detector (PID), equipped with a 10.0-electronvolt lamp, measured the organic vapor content (parts per million) of the soil gas. This initial screening technique was used to identify potential source areas and to focus DP activities for quantitative assessment. Soil gas data generated at the sites strongly correlated with subsequent DP sampling data.

**Direct Push Technology.** DP technology has been available for years, but for Florida’s DSCP, it is the tool of choice for initial assessment activities. DP utilizes hydraulics to drive a small diameter rod into the subsurface to collect both soil and groundwater samples. There are a great number and variety of probes, many of which work on similar principles, and have a variety of applications. The probes are versatile, can get to "hard to reach" places, and can obtain soil and groundwater samples more quickly than conventional drilling techniques. DP has the capability to collect excellent continuous and undisturbed core samples for lithologic identification with better recovery than conventional split-spoons from drilling rigs.

The depths of sampling range from several feet below ground surface (bgs) to depths exceeding 100 feet bgs. Costs for conducting DP typically ranges between $1,000 to $1,500 per day, and the rapid growth in available contractors using DP has increased the competition and reduced the cost of conducting DP assessment.

Soil and groundwater data obtained using DP is typically used to locate permanent monitoring wells. It also appears that the environmental industry is moving toward acceptance of DP-generated data and a concomitant reduction in the number of required permanent wells. Additionally, microwells, which can yield representative data, can be installed using DP in less time and at lower cost than the installation of conventional monitoring wells. Microwell screens are pre-packed so that minimal formation disturbance occurs during installation. The validity of the analytical data obtained from DP points is further supported by the favorable comparison between chemical concentrations detected in groundwater at DP points with concentrations detected in monitoring wells installed near the DP points.

DP technology significantly reduces the amount of solid and liquid investigation-derived waste (IDW) generated during site assessments. Because formation materials are pushed to the side and not retrieved from the subsurface during DP, there is much less IDW to dispose of upon completion of the assessment. Historically, the costs for handling and disposing of IDW from site assessments ranged up to more than 30 percent of the total assessment costs. Using DP technology combined with permanent monitoring wells for the DSCP, costs associated with IDW ranged from 5 to 10 percent of the assessment costs, representing a significant reduction in costs and project management time.

**Mobile Laboratories.** Using a mobile laboratory in the field is a key ingredient in rapid and successful site assessment. Historically, the cost for an on-site mobile laboratory prohibited the use of on-site mobile laboratories for most site assessments (costs typically ranged from $1,000 per day to $1,500 per day). In addition, few mobile laboratories had acquired state certification for running standard U.S. Environmental Protection Agency (U.S. EPA) analytical methods in the field. Since the inception of the Florida DSCP, numerous mobile laboratory companies have obtained or are in the process of obtaining certification for U.S. EPA analytical Methods 8010 and 8020 from the FDEP Quality Assurance Section. Such certification has facilitated the use of mobile laboratories, thus enabling receipt of valid data *while in the field* for chlorinated and nonchlorinated volatile organic compounds (VOCs) in soil and groundwater. Although the cost of an on-site mobile laboratory may appear prohibitive, the benefit of obtaining real-time soil and groundwater data *in the field* outweighs the lower cost of using traditional fixed-base laboratories during the initial phase of an assessment. As more companies move into the mobile laboratory market and obtain state certification, competition will most likely reduce the cost of mobile laboratories further.

The advantages of using an on-site mobile laboratory include optimizing information output for plume and source area delineation, thereby guiding the placement of additional soil and groundwater sampling points and permanent monitoring wells for confirmatory and long-term sampling. The mobile laboratory is key to defining the extent of contamination with a minimum number of mobilizations. Most mobile laboratories can obtain the nondetect line for benzene, toluene, ethylbenzene, and xylenes (BTEX), PCE, and PCE breakdown products (detection limits range from 1 to 5 parts per billion).

## Emerging Rapid Site Assessment Technologies

The FDEP DSCP has conducted limited fieldwork utilizing emerging assessment technologies for site characterization, particularly to screen for DNAPL contamination. Technologies used by the FDEP include:

- **Cone penetrometer test (CPT) systems, utilizing electronic resistivity probes.** CPT technology was used on site to characterize lithology. CPT measured pressure on the tip and along the sleeve of the advancing probe, thus providing information about soil characteristics (e.g., whether sand, silt, or clay is present). Measuring electrical resistance in the soil was used to indicate whether DNAPL was present (water is a good conductor of electricity; DNAPL is not). Readings of increased electrical resistance may indicate DNAPL is present.

- **DP units equipped with laser-induced fluorescence (LIF) systems.** LIF technology was used on site to detect the presence of DNAPL in unsaturated and saturated soil. As a DP probe with an LIF system is advanced vertically, optic fibers deliver light from a multiwavelength laser excitation source to the subsurface. The fluorescence (energy emission) produced by the analytes in the formation is recorded by a spectrograph. The data can be displayed as three-dimensional fingerprints of contamination at given DP locations and depths. Selected LIF fingerprints are evaluated for characteristic patterns and are compared with fingerprints of "clean" samples spiked with known amounts of a suspected analyte.

Early results from the application of these technologies have provided positive results for the detection of the presence of DNAPLs at the DSCP test site, the Former Sages Dry Cleaner site. Data collected using both methods were confirmed through the collection of DNAPL in soil cores, which were located based on the data generated by the screening methods. These data have led to significant revisions in the conceptual site model for the Sages test site, which was originally developed using the initial DP and monitoring well sampling data. Both technologies promise to become additional effective tools for the rapid assessment of DNAPL-contaminated sites.

## Limitations of Rapid Assessment Techniques

As with most applications of innovative techniques, implementation and experience in the field identified limitations. While the rapid assessment approach led to the collection of significant amounts of valid data, additional data collection was needed to completely characterize some of the sites because of limitations inherent in equipment or of the rapid assessment approach itself. These limitations included:

- “Refusal” of advancement of DP probes by subsurface lithology (e.g., clay or consolidated sand units), particularly limited vertical delineation. In these cases, vertical delineation generally required additional conventional monitoring well installation.

- Limited groundwater sample recovery because of subsurface geologic conditions (e.g., “flowing sands”) that interfered with sample collection. Typically, adequate samples were collected, although field delays were encountered during the multiple attempts to collect the samples.

- Comprehensive review of the final data submittals identified data gaps which required resolution to complete site characterization. Additional data requirements were addressed by the strategic placement of long-term monitoring wells.

- Expanding scopes of work for additional site assessment led to delays associated with obtaining site access permission from neighboring property owners. Such delays often meant additional mobilization following acquisition of site access permission.

### Real-Time Data Interpretation and Decision Making

DP technology and mobile laboratories have been available for many years. What is unique today is that their combined utilization makes rapid assessment successful in meeting its objective: to define the horizontal and vertical extents of contamination in a minimum number of fieldwork phases. Experienced hydrogeologists and scientists evaluate and interpret real-time soil and groundwater data *in the field,* which is key to the rapid assessment decision-making process. Timely communication of real-time field data to project managers facilitates in-field decisions regarding expanded scopes of work, if necessary, and further streamlines the assessment phase.

## RAPID ASSESSMENTS AT EIGHT FDEP DRYCLEANING SOLVENT CLEANUP PROGRAM SITES

In November 1996, Levine·Fricke·Recon Inc. (LFR) was one of 10 firms contracted under the FDEP DSCP to conduct contamination assessments at drycleaning and drycleaning wholesale facilities in Florida. LFR was initially assigned 12 sites, eight of which were located in Jacksonville, Florida. Initial site visits and interviews with the drycleaning facility owners/operators were conducted, and scopes of work and cost estimates were prepared using the streamlined work plan and unit pricing approach discussed above. Site access permission was obtained by project managers prior to mobilization. Detailed schedules were prepared using Microsoft© Project®.

To complete the eight site assessments in Jacksonville, LFR’s scheduling approach used four teams of experienced hydrogeologists and scientists. The schedule was designed so that two teams used the same DP/drilling contractor and mobile laboratory; after the initial DP work was performed at a site, the DP and mobile laboratory subcontractors moved to the next site, while drilling commenced at the first site.

In January 1997, four teams commenced work using two teams of DP/drilling contractors and State-certified mobile laboratories. Within the next 10 weeks, rapid assessments were completed at all eight sites. More than 500 soil and groundwater samples were collected and analyzed; an average of approximately 72 soil and groundwater sampling points were advanced at each site.

The settings for most of the drycleaning-solvent sites were actively operating drycleaning facilities located in populated neighborhoods, strip malls, and/or shopping centers. The eight sites were ranked highly in the FDEP DSCP as most were within 0.5 mile to 1 mile of public drinking water supply wells; therefore, these sites were among the first to be assessed. Because most of the facilities assessed were active, disturbance to operations was minimized.

## Typical Scope of Work

A typical scope of work for the eight rapid assessments involved an initial two to five days of DP and mobile laboratory activities (from 8 to 20 DP sampling points), followed by the installation of three to seven permanent monitoring wells. The numbers and placement of the monitoring wells were focused by the DP/mobile laboratory soil and groundwater data.

The first fieldwork task was to evaluate site-specific lithology by collecting continuous macro cores across the site. This task identified potential confining or semiconfining units that could potentially be compromised during an invasive phase of the assessment. Soil and groundwater sampling and analysis then commenced with the DP and mobile laboratory, using an “outside-in” approach. As data were collected and analyzed, the on-site scientists tabulated and evaluated the data and created summary tables and figures to quickly help illustrate and interpret the results.

During and after evaluating and interpreting the initial data, the field hydrogeologist continually communicated the data and recommendations to the FDEP project/contract manager. The field hydrogeologist received timely approval for additional sampling points beyond the original scope of work, if applicable, to define the horizontal and vertical extents of contamination. Vertical sampling intervals using DP typically ranged from 10 to 15 feet bgs; horizontal sampling intervals typically ranged from 10 to 50 feet. For seven of the eight sites, the original scopes of work were expanded by 50 to more than 100 percent. Table 1 presents details by site illustrating the magnitude of the Jacksonville field effort.

**TABLE 1** Total numbers of DP sampling points, mobile laboratory samples, monitoring wells installed, and fieldwork days for the eight Jacksonville site assessments

| Site Name | DP Sampling Points | Mobile Laboratory Samples | Monitoring Wells Installed | Total Days of Fieldwork |
|---|---|---|---|---|
| Miller Machinery & Supply, Inc. | **96** | **119** | **5** | **17** |
| Butler Cleaners | **87** | **114** | **3** | **8** |
| Professional Cleaners | **124** | **161** | **9** | **20** |
| Herman Jackson Cleaners | **73** | **96** | **5** | **10** |
| Former Sages Dry Cleaner | **52** | **78** | **5** | **7** |
| Denim & Lace Cleaners, Inc. | **23** | **25** | **3** | **3** |
| Walgreen Store | **46** | **54** | **3** | **7** |
| Koretizing Cleaners | **50** | **56** | **4** | **7** |
| **TOTAL** | **574** | **634** | **37** | **79** |
| **AVERAGE PER SITE** | **72** | **79** | **4.5** | **10** |

The results of the initial soil and groundwater data showed that contamination at all but one site (Denim & Lace Cleaners, Inc.) was more extensive than anticipated. Most of the drycleaning facilities were located on small tracts of land. The assessment results indicated long, narrow groundwater plumes of PCE and its breakdown products had migrated off site. In addition, five of the eight sites exhibited PCE concentrations suggesting the presence of DNAPLs. Most of the scopes of work were increased to define the extent of contamination (within a minimum number of fieldwork phases). As unit prices were already established and agreed upon, it was a simple matter of agreeing to the number of additional sampling points and time to complete the additional work. After evaluation of the DP data, monitoring wells were installed, developed, and sampled, and the groundwater samples were sent to fixed-base laboratories. Fixed-base laboratory values for groundwater concentrations in monitoring wells compared favorably with concentrations detected by the mobile laboratory analyzing groundwater samples collected at the same locations using DP. It should be noted that the quality of the data from the mobile laboratory was within normal ranges and is considered valid data. Figures 1 through 4 illustrate data from the Former Sages Dry Cleaner site, one of the eight drycleaning-solvent sites assessed by LFR in Jacksonville, Florida.

Following completion of the field assessments, detailed property surveys were conducted to locate sampling points and to determine top of casing elevations for monitoring wells.

The volume of IDW was minimized through the use of DP. Furthermore, prior to demobilizing the mobile laboratory, both solid and liquid IDW were analyzed by the mobile laboratory, thus reducing the cost of analysis and disposal of IDW. The costs for treating liquid IDW also were evaluated.

After the rapid assessments were complete, a mobile treatment unit, consisting of a tray air stripper and carbon unit, was used at the Jacksonville sites to cost-effectively treat the liquid IDW. Solid IDW was characterized, manifested, and sent off site for disposal.

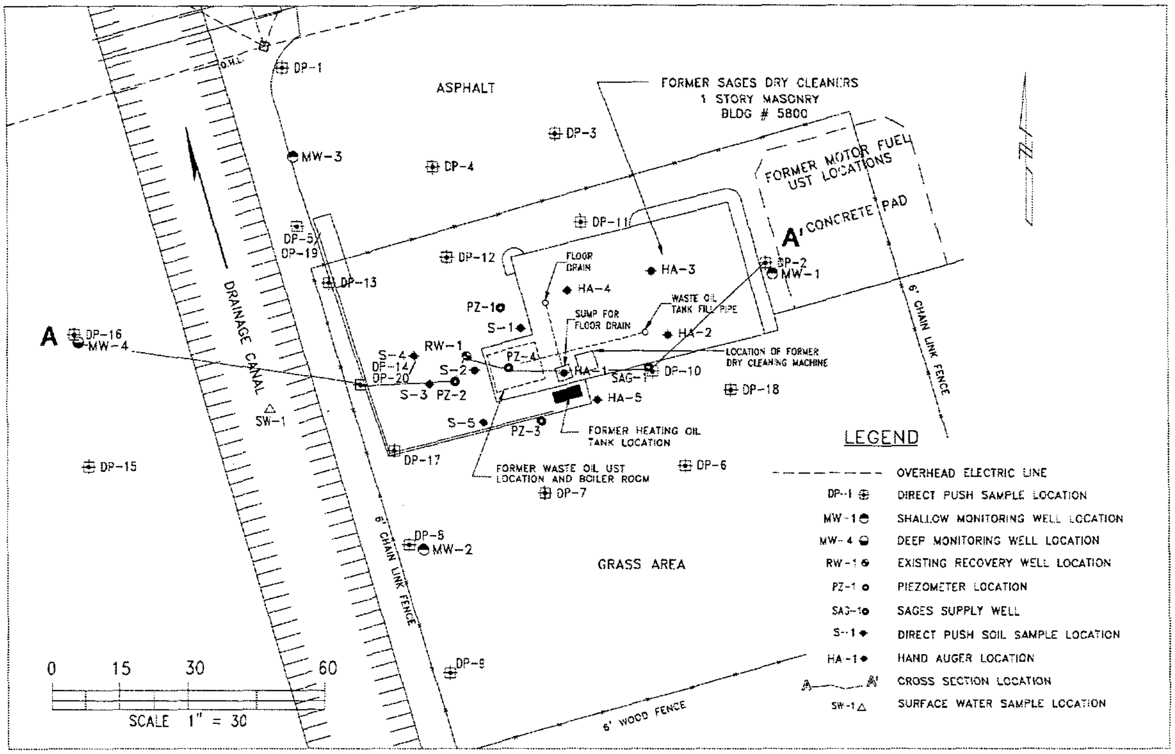

**FIGURE 1** Site Map with Sampling Locations and Geologic Cross-Section Location

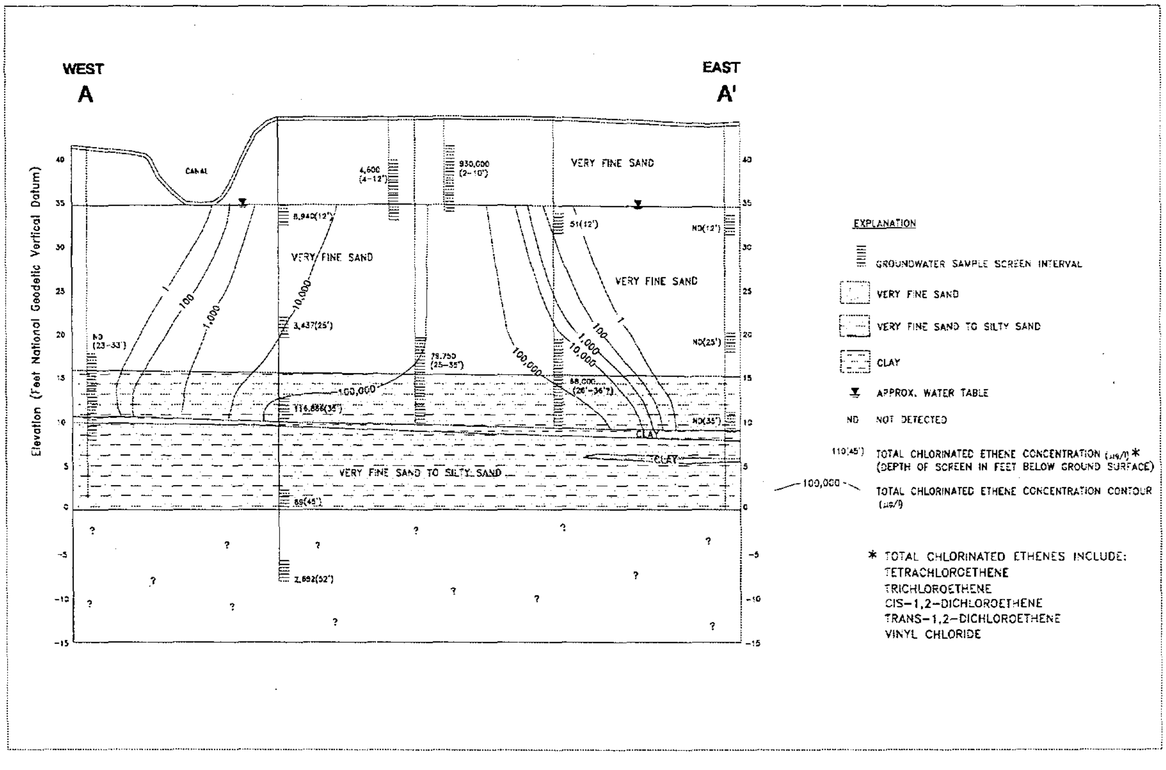

**FIGURE 2** A-A' Geologic Cross Section Showing Total Chlorinated Ethenes in Groundwater

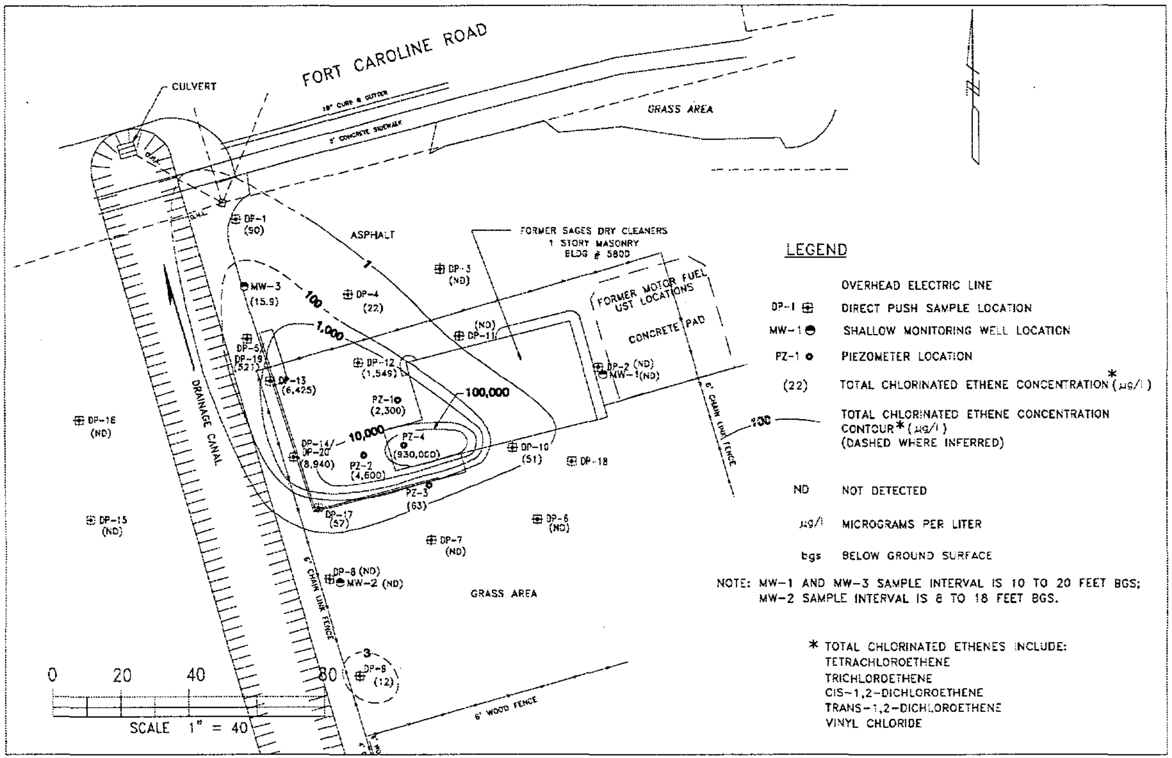

**FIGURE 3** Isosurface of Total Chlorinated Ethenes in Groundwater (10-12 feet bgs)

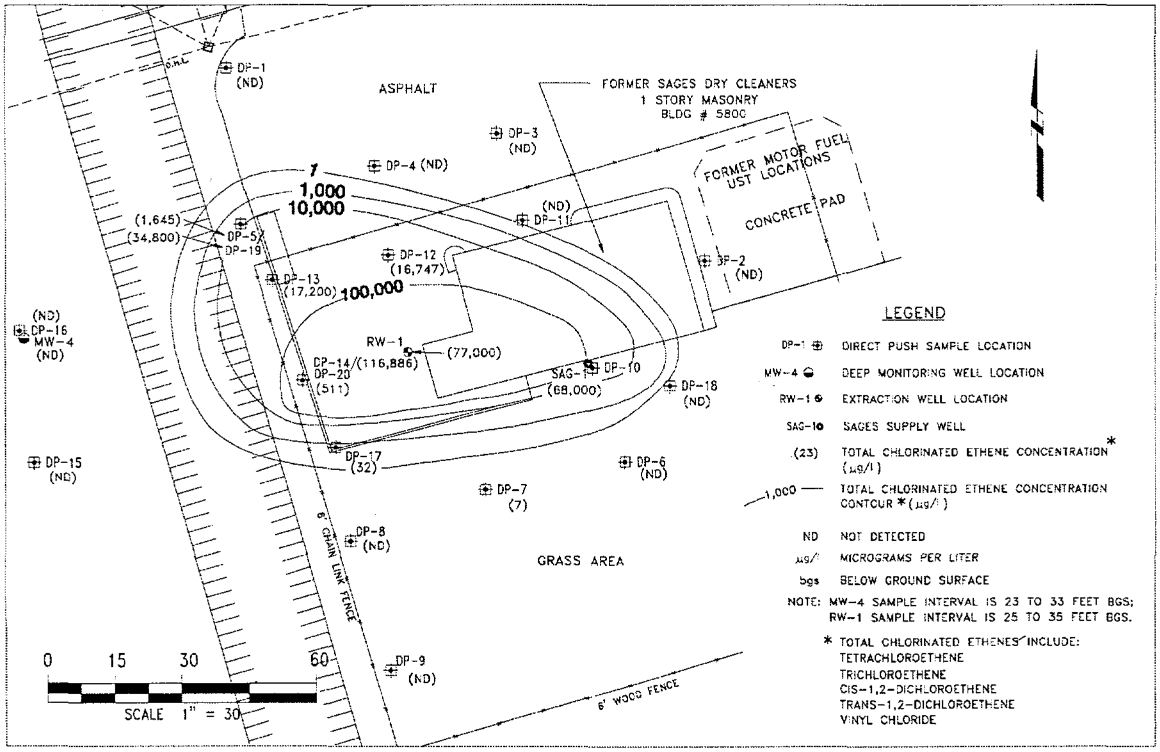

**FIGURE 4** Isosurface of Total Chlorinated Ethenes in Groundwater (33-35 feet bgs)

## Data Management and Reporting

Data collected during the assessments was loaded into a Microsoft™ Access® database. The data included soil and groundwater chemical concentrations, monitoring well construction information, sampling field parameters, water levels, and survey data. Data were electronically uploaded into the database, minimizing the time involved in data manipulation by individuals and the potential human error associated with manually transposing data into a database. Data were obtained from both the mobile and fixed-base laboratories in electronic formats that were readily entered into the database.

A CAR template was developed for the FDEP DSCP that focused on presenting data in table and figure formats to minimize the amount of text in the report body. Data from the database were electronically queried and exported to Microsoft© Excel® workbooks to construct the report data tables, thus minimizing the time to create the tables and potential human error associated with manually transcribing data into report tables. Upon notification from the FDEP that the reports were final, the database and the reports were submitted to the FDEP on CD ROM. The FDEP will include the data and the reports in the FDEP DSCP database. An average of three months was required to conduct a rapid assessment at a site and submit the draft CAR to the FDEP.

## Risk-Based Corrective Action Evaluation and Remedial Action Planning

Following final submittal of the eight DSCP Jacksonville site CARs to FDEP, risk-based corrective action (RBCA) evaluations were conducted for each of the sites to identify chemicals of concern, concentrations of the chemicals of concern in affected media (soil, groundwater, and/or surface water), potential routes of exposure relating to human health and the environment, and potential remedial goals for each site. Upon reviewing the RBCA evaluations, the FDEP will decide the future action for each site.

Remedial action will be conducted at sites where extensive soil and groundwater contamination exist that present significant potential risks to human health and the environment. Remedial action options include monitoring only, natural attenuation, soil vapor extraction, air sparging, hydraulic control and physical barriers, and innovative technologies. Innovative technologies that have been proposed include co-solvent injection and chemical oxidation. Pilot testing for proposed innovative technologies will be performed prior to full implementation of a remedial system.

## SUMMARY AND CONCLUSIONS

With limited funding and a large number of drycleaning-solvent sites in the DSCP, the FDEP has developed the aggressive goal for the DSCP of moving sites from the assessment phase into remediation within one year. The eight sites discussed in this paper were the first sites to be characterized for the FDEP under the DSCP; these eight sites were assessed during a 10-week period using rapid assessment tools and methods.

Using rapid assessment tools, geological and hydrogeological evaluation, on-site soil and groundwater chemical analyses, and experienced in-field decision making, rapid contamination site assessment was completed within a minimum number of fieldwork phases. Although initially it may appear that the rapid assessment approach is more expensive than conventional assessments (because of the costs of mobile laboratories and other rapid assessment tools), conventional site assessments often involve numerous mobilizations, which require preparation, review, and approval of separate work plans and cost estimates. In addition, the conventional process is often lengthier and more costly because it can extend the site assessment process by several months to many years. The number of soil and groundwater samples obtained during rapid site assessments is greater than the number of samples obtained using conventional assessment methods, thereby providing a more refined definition of the extent of soil and groundwater contamination.

The costs for assessing the eight drycleaning-solvent sites discussed herein ranged from approximately \$47,000 to \$130,000, with an average cost of approximately \$83,000 (costs include additional fieldwork necessary to delineate contamination beyond the limitations of the DP technology and the installation of additional long-term monitoring points).

The rapid assessments were completed using experienced on-site staff, who evaluated and interpreted real-time data and made decisions *while on site* for focusing and completing the assessment. This on-site decision-making process was integral to accomplishing the rapid site assessments within minimal mobilizations.

The rapid assessment approach used by the FDEP for the DSCP provides the following advantages:

- completing assessments within three to four months: average cost 30 to 50 percent less than conventional assessments, average time 50 percent to more than 300 percent less than conventional assessments.

- rapid assessment tools enable greater numbers of soil and groundwater sampling points than conventional assessments. More samples are collected both vertically and horizontally, providing a better three-dimensional definition of chemicals of concern in soil and groundwater.

- minimization of IDW, thus a reduction in costs associated with the disposal of IDW.

- immediate identification of potential risks to human health and the environment.

- immediate identification of the need to perform interim remedial actions.

By using the rapid assessment tools and methods discussed in this paper, the eight FDEP DSCP Jacksonville assessments were conducted more cost efficiently than if conducted using conventional assessment techniques. Time and resources for the assessment phase were reduced, and more FDEP DSCP resources were available for remediation. Meeting the aggressive FDEP DSCP goal of "assessment to remediation" within one year was facilitated by the rapid assessment approach.

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# USING GEOLOGICAL INSIGHT AND DETAILED OUTCROP OBSERVATIONS TO IMPROVE INPUT TO FLUID FLOW SIMULATIONS

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## ABSTRACT

Methods developed to study outcrop analogs of petroleum reservoirs in consolidated rocks can be adapted to build high-resolution models of soil type and hydraulic conductivity for input to groundwater flow and solute transport simulations. Because suitable outcrop analogs are lacking for many unconsolidated deposits, we propose to use closely-spaced cone penetrometer testing (CPT) data, calibrated by continuously-cored drillholes, to map detailed spatial variations in soil stratigraphy. For each soil type, a histogram can be defined for each CPT parameter (e.g.s, tip pressure, sleeve friction, pore pressure). This yields a characteristic set of histograms that can be used to infer soil type at CPT penetrations where calibration core data are unavailable. High-resolution flow simulations performed to study waterflooding in petroleum reservoirs illustrate the methodology and show the impact of fine-scale facies architecture on petroleum production performance. Similar studies can be performed for shallow groundwater systems to evaluate which fine-scale architectural features should be captured in the numerical simulators when modeling alternative methods for groundwater remediation.

## INTRODUCTION

It has long been recognized that subsurface heterogeneity associated with particular depositional settings can produce important spatial variations in hydraulic parameters. We have been studying rocks exposed in outcrop as analogs for subsurface petroleum reservoirs to understand how geological processes influence the spatial distribution of the petrophysical properties that control fluid flow. This approach is particularly valuable because it provides direct observation of the way geologic units should be correlated between wells. In addition, the permeability structure of well-characterized geological features associated with specific depositional settings can be identified. The lessons learned in these outcrop studies provide a foundation for performing similar studies in shallow groundwater flow systems found in unconsolidated deposits.

Good outcrop exposures are typically lacking in unconsolidated deposits. Thus, we propose to use closely-spaced cone penetrometer (CPT) logs, calibrated by continuously-cored drillholes, to characterize the soil stratigraphy and distribution of hydraulic properties at specific sites. Histograms generated during calibration are used to infer the soil stratigraphy at CPT locations where calibration cores are unavailable. An important element of this work involves using our best understanding of the depositional setting to help infer the details of the subsurface stratigraphy at the site. Our ultimate goal is to construct geologically-plausible, 3-D permeability structures that allow us to preserve the most important features of the system in groundwater flow and solute transport models. High-resolution fluid simulations help us to evaluate which features should be included in site-scale models.

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This paper illustrates the integrated approach that the petroleum industry has prompted us to use at two sites in consolidated sandstone. Elements of this approach can be directly applied in building the hydraulic conductivity structures needed to model groundwater flow and solute transport at contaminated sites found in shallow groundwater systems.

## OUTCROP TO SIMULATION IN THE FERRON SANDSTONE

Examples are drawn from two recently completed projects to show how we integrate outcrop-based lithofacies architecture with detailed petrophysical testing as a foundation for assigning permeability values in high-resolution fluid flow models. The Coyote Basin project targets a small volume of fluvial deposits that might fill a typical gridblock used in a full-field petroleum reservoir simulation. A complete description of the Coyote Basin project is provided by McMechan and Soegaard, 1996 and 1997). In contrast, the Ivie Creek project targets heterogeneities at the interwell scale. A more complete description of the Ivie Creek project is provided by Chidsey (1997).

### Coyote Basin Project

The Coyote Basin project provides detailed, quantitative insight into the 3-D petrophysical structure of fluvial channel-belt deposits in the Cretaceous Ferron Sandstone of central Utah. Integrated, field, laboratory and numerical studies have been performed within a volume of rock (Figure 1) that approximates the size of a small grid block in a full-field reservoir simulation model (20 m by 40 m in plan, 15 m deep). The key objective of the study is to understand the value of including the permeability characteristics of detailed stratigraphic features in fluid flow models. An important result of the study is to use the detailed permeability measurements, integrated with the fluvial stratigraphy mapped at the site, to derive a characteristic equivalent hydraulic conductivity tensor for the target volume.

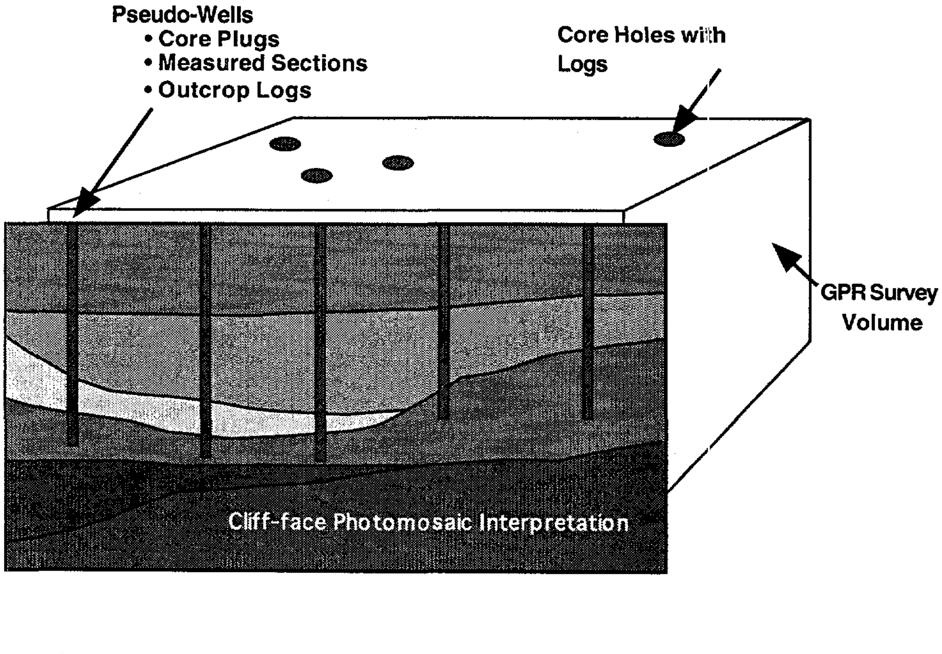

**FIGURE 1.** Schematic of integrated data used to develop a detailed 3-D petrophysical model at the Coyote Basin study site.

A unique aspect of this study is the way that a large quantity and wide variety of data collected at the site are integrated to infer the permeability structure of the target volume (Figure 1). This uncommonly complete data set includes:

- detailed outcrop measured sections
- detailed sedimentological logs of split, continuous drillcore
- photomosaic panels of cliff-face exposures
- high-resolution, 3-D ground penetrating radar
- gamma-ray profiles on both outcrop and continuous drillcore
- detailed petrographic studies
- over 1,000 permeability measurements
- detailed geostatistical models of permeability within the study volume

Two-dimensional, two-phase (oil and water) numerical simulations of water injection were performed using a single 2-D vertical slice extracted from the 3-D permeability model constructed for the site. Figure 2a shows the permeability structure obtained by combining the lithofacies architecture derived from outcrop and GPR mapping with geostatistical models constrained by the detailed permeability measurements. Figure 2b shows the computed distribution of oil remaining in the model volume after one year of water flooding from right to left.

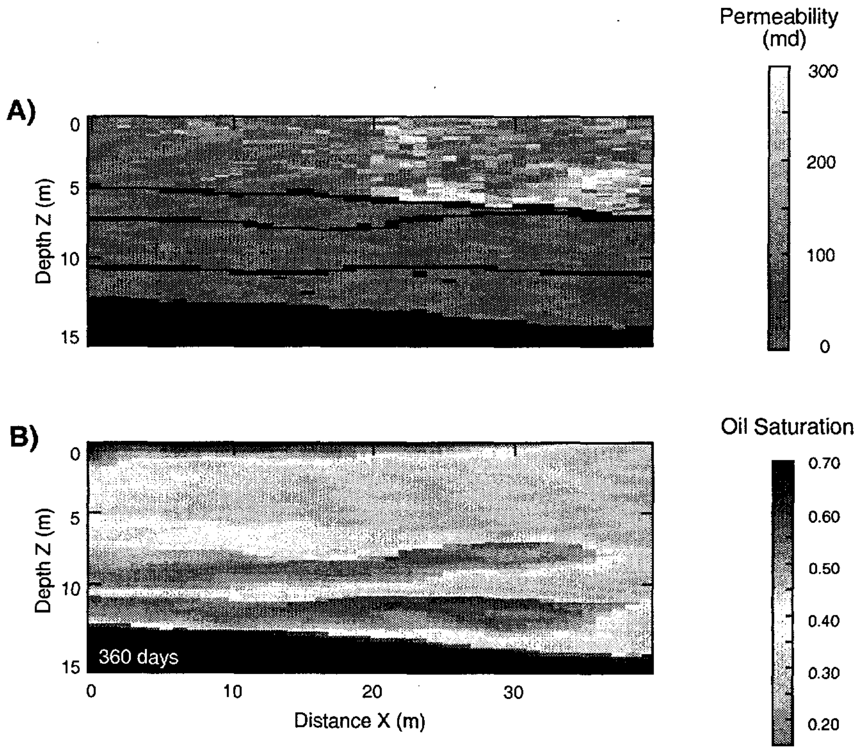

**FIGURE 2.** Computed permeability structure and waterflood simulation results at Coyote Basin, UT: a) one vertical, 2-D slice extracted from a 3-D, geostatistically-derived permeability model obtained by integrating detailed stratigraphy and permeability measurements, and b) oil saturation after one year of water flooding from right to left.

Figures 2a and 2b show that the preferred pathway for water flow is through the upper, higher-permeability unit. It is also apparent that the low permeability, shaley bounding layers (black blocks are 0.1 md) restrict water flow such that significant volumes of oil remain in place. This result is clearly analogous to the situation where water is used in an attempt to flush LNAPLs from a contaminated aquifer.

### Ivie Creek Project

In contrast to the small volume studied at Coyote Basin (40 m by 20 m in plan, 15 m deep), the Ivie Creek project uses outcrop data collected from within a much larger volume (600 m by 600 m in plan, 20 m deep). At Coyote Basin we examined components of specific architectural elements found at the site (e.g., bounding layers and different channel facies). Although the goals of both projects are similar, the Ivie Creek site provides insight into the way that characteristic permeability structures are associated with complete architectural features. Thus, this case study includes complete views of extensive, discontinuous bounding layers and discrete sandy bodies typically found in delta-front depositional settings (Figure 3). One important difference between the two studies is that surface geophysical surveys are not available to help infer the detailed 3-D architecture of the Ivie Creek site.

The outcrop architecture at Ivie Creek (Figure 3) consists of juxtaposed variants of a single architectural element, the clinoform, and indicates prograding, shallow marine deposition of a fluvial-dominated delta-front system. The sandstone bedsets within each sigmoidal-shaped clinoform record an episode of deposition, followed by partial erosion. Depositional episodes were likely related to variations in the sediment load carried by the distributary channel(s) feeding the delta front, and by upstream channel switching. Clinoforms are inclined seaward, arranged en echelon, and are usually separated from each other by a thin (< 0.3 m thick), discontinuous mudstone and siltstone bounding layer. The resulting architecture provides a sound spatial framework for distributing permeability and porosity within a numerical model of the outcropping cliff face.

The impact of the primary architectural elements on fluid flow is illustrated using waterflood simulations similar to those described above for the Coyote Basin project. It is important to note that the high resolution of the permeability structure cannot be incorporated in full-field reservoir simulations. An important contribution of this project is to provide a basis for testing different methods that might be used to compute average properties for the larger gridblocks that must be used in full-field reservoir simulators. Figure 3 shows that the injected water tends to preferentially invade the upper, higher-permeability zone of the model domain. The obvious tendency for the water to override the underlying oil is enhanced where the bounding layers are absent in the upper part of the model domain. These 'holes' in the bounding layers are most likely to occur in the higher energy regimes of the depostional system found on the upper slopes of each clinoform body.

## DEFINING PERMEABILITY STRUCTURE USING CPT DATA IN LIEU OF OUTCROP OBSERVATIONS

Outcrop studies have largely been aimed at studying the consolidated rocks that are analogous to rocks found in deep petroleum reservoirs and groundwater aquifers. The relatively small number of depositional systems represented by these reservoirs and aquifers requires studying only a small subset of the rock types found in the subsurface. Thus, an outcrop representative of a particular reservoir or aquifer can generally be found somewhere in the world. Outcrop analogs for the much wider range of shallow unconsolidated deposits that host contaminated groundwater are less easily found, although efforts to remediate groundwater

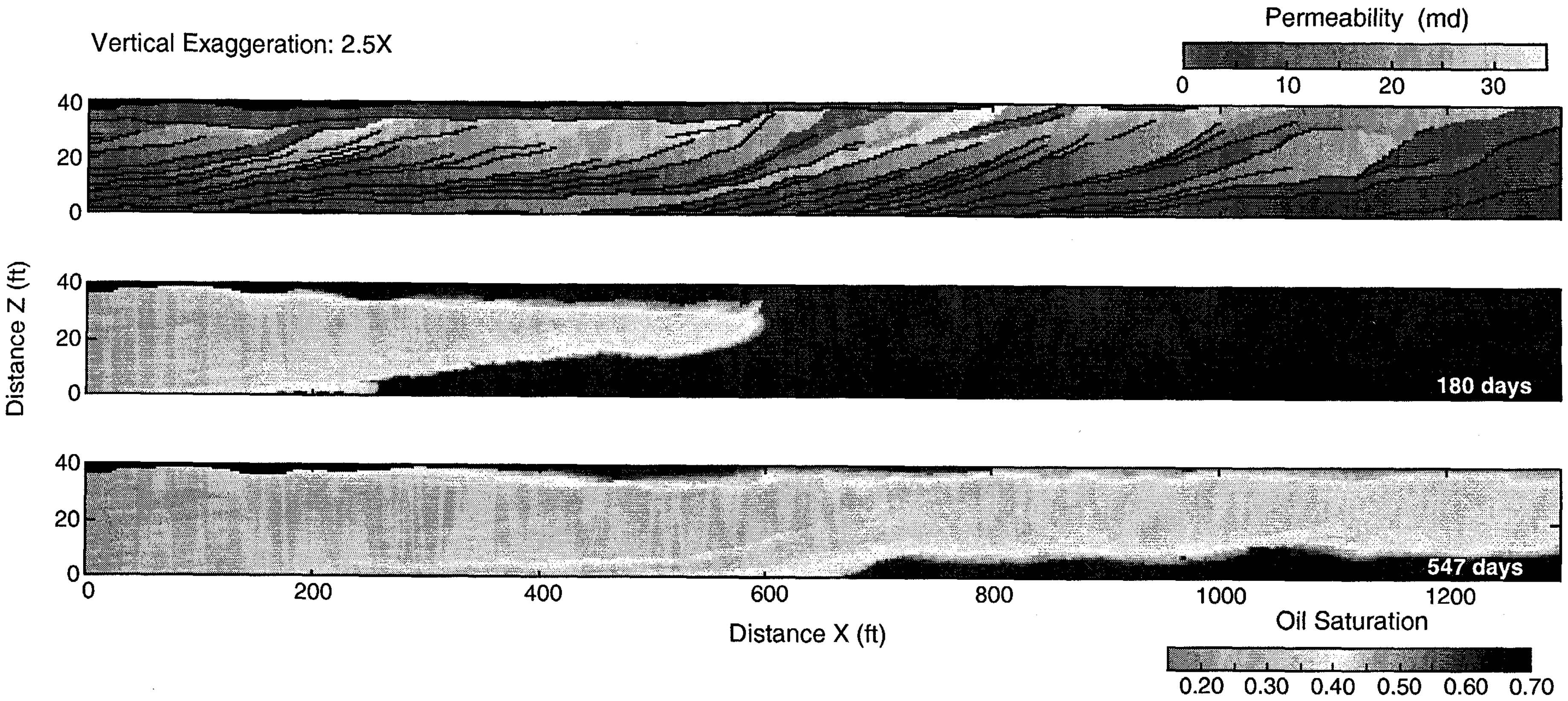

**FIGURE 3.** Permeability model with discontinuous shaly bounding layers between sandstone units and computed oil saturation at 180 and 547 days after the start of water injection along the left-hand side of the modeling domain.

contamination could benefit from the increased understanding of permeability heterogeneity that outcrop analog studies provide. Thus, we propose to augment the sparse outcrop exposures available for unconsolidated deposits found in specific geologic environments by making extensive use of cone penetration testing (CPT) data.

Cone penetration testing involves pushing a cylindrical cone vertically into the ground at a constant rate of penetration (Robertson and Campanella, 1988). Continuous measurements of cone resistance ($Q_t$), side friction resistance ($F_s$), and pore water pressure ($U$) during penetration yield detailed logs of the variability in each parameter as a function of depth (Figure 4). The CPT method does not yield samples for directly determining the stratigraphic significance of changes observed in plots of $Q_t$, $F_s$, and $U$. Thus, inferring stratigraphy and permeability structure from CPT data requires site-specific calibration of the logs by comparison to a suite of continuous cores obtained adjacent to the CPT data. A hypothetical stratigraphic log that might be used for calibrating the CPT data is included in Figure 4.

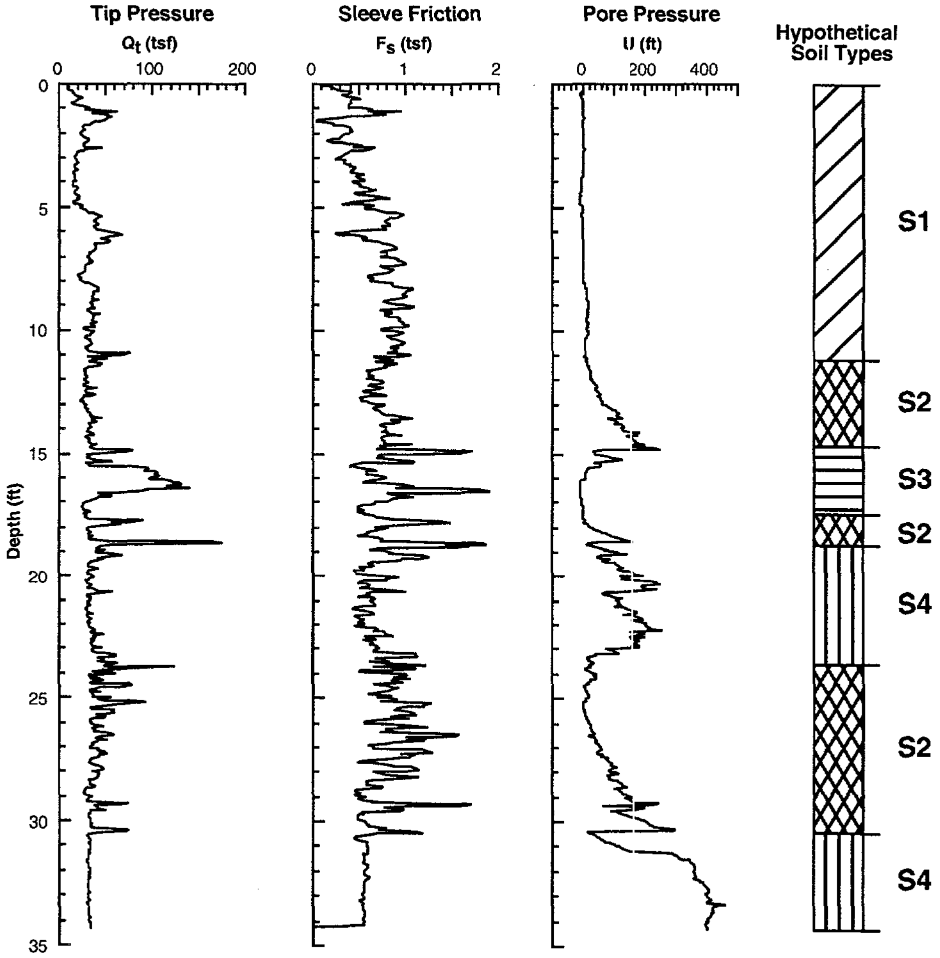

**FIGURE 4.** Typical CPT parameter logs obtained by cone penetration testing (Montgomery Watson, unpublished data) compared to a hypothetical soil type log that would be derived from continuous core sampling in an adjacent drillhole.

Commercial CPT operators usually provide an interpreted stratigraphic log based on generalized empirical correlations between CPT measurements and soil type (Robertson and Campanella, 1988). In practice, stratigraphic interpretation is often based on the these interpreted logs. We contend, however, that it is preferable to perform stratigraphic interpretations using characteristic log signatures that can be correlated between CPT holes before making stratigraphic interpretations. Calibration cores collected after a preliminary CPT stratigraphy is defined provide an efficient way to tie correlated CPT units to soil type, and then to develop a final stratigraphic interpretation for the 3-D distribution of soil type. Because the CPT method is relatively inexpensive, the lateral continuity of different soil types can be resolved by strategic placement of closely-spaced CPT locations.

Our approach to correlating the CPT data is similar to that used in defining permeability structures in the Ferron Sandstone. Thus, a detailed set of parameter data (in this case ($Q_t$, $F_s$, and $U$ ) is used to assign a soil type to each grid block within a discretized 3-D volume. This approach can be augmented using surface geophysical surveys (e.g., ground penetrating radar or high-resolution 3-D seismic) tied to the CPT data and continuous core samples to map major stratigraphic units. The CPT parameters are interpolated within each major stratigraphic unit using the geostatistical approach described in the previous section.

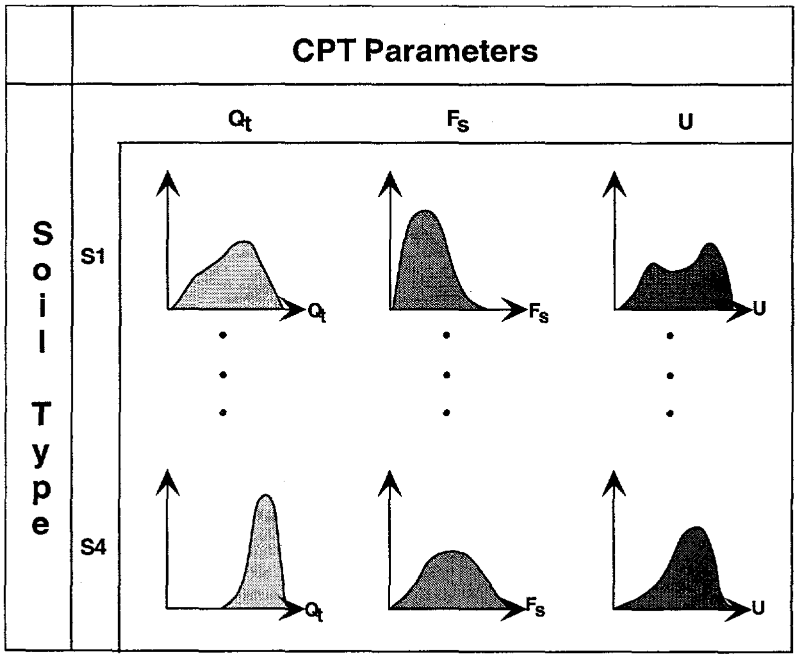

**FIGURE 5.** Hypothetical histograms showing how each CPT parameter might vary soil type.

Calibrating the CPT stratigraphic interpretation is complicated by the fact that each soil type found at a site is unlikely to exhibit a unique combination of CPT properties. Thus, uncertainties inherent in identifying specific soil types must be accounted for when converting the CPT stratigraphy to soil type stratigraphy. The first step in developing the soil type stratigraphy involves using histograms to identify how each CPT parameter varies within a specific soil type (Figure 5). Although the various histograms will overlap, the goal is to find a set of histograms comprising the three CPT parameters ( $Q_t$, $F_s$, and $U$ ) for each soil type logged in the continuous core samples. The most likely soil type for each gridblock is identified using the characteristic histogram sets defined in the calibration process (Figure 6). Once the hydraulic properties of each soil type are characterized using in situ and laboratory tests, the 3-D soil type distribution established using this approach supplies the basis for assigning hydraulic conductivity values in groundwater flow models.

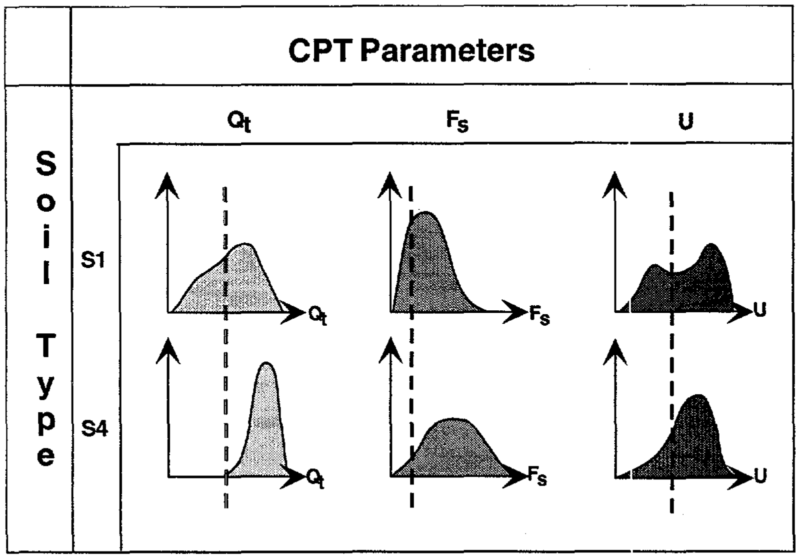

**FIGURE 6.** Inferring soil type from the CPT parameter histogram sets for each soil type (Figure 5). Although significant overlap might occur for any given parameter, a combined inspection of all parameters suggests that the set of hypothetical CPT data defined at a specified depth (dashed lines) can be identified as soil type S1.

## SUMMARY

Experience in the petroleum industry shows that outcrop analogs can provide important insight into the oil production characteristics of consolidated rocks found in a variety of depositional settings. We propose to apply a modified form of the outcrop analog methodology to achieve similar improvements in understanding how different depositional settings might influence fluid flow and solute transport in site-specific, shallow groundwater systems. Given the lack of outcrop analogs for many unconsolidated deposits we plan to use detailed CPT logs, calibrated with continuous core samples, to obtain the 3-D distribution of soil types found in specific geological settings. Combining the inferred soil type distribution with *in situ* and laboratory hydraulic conductivity testing provides the input needed for high-resolution groundwater flow and solute transport models. Although our integrated approach does not depend upon data obtained from high-resolution surface geophysical surveys, when available such data can greatly increase our confidence in inferring 3-D permeability structures.

*Acknowledgments:* The Coyote Basin and Ivie Creek projects were both jointly funded by the U.S. DOE (Contract Nos. DE-FG03-96ER14596 and DE-AC22-93BC14896) and several corporate sponsors. We are indebted to our collaborators at the Utah Geological Survey, University of Utah, and the University of Texas at Dallas that contributed to the various data sets that form the foundation for our modeling studies. Cone penetrometer data obtained from Hill AFB were graciously provided by Montgomery Watson, Salt Lake City, UT.

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# AN INTEGRATED APPROACH TO WETLANDS CHARACTERIZATION IN DETERMINING HYDROLOGIC FUNCTIONS

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## ABSTRACT

The development of the southern Rocky Mountains wetland classification scheme, which incorporates both the HGM methods of Brinson (1993), and the Conceptualization and Characterization of Kolm (1993); Kolm et al. (1996); and Kolm and van der Heijde (1996) is described in a step-wise, integrated approach. Surface characterization, subsurface characterization, ground-water system characterization, and determination of wetland class and subclass are the major steps which are included in this approach. Surface characterization allows the wetland scientist to delineate a wetland. This information is incorporated into the functional assessment and used for interpretative aspects of steps 2 through 4. Subsurface characterization is partially based on the surface characterization and is used for interpretative aspects of steps 3 and 4. The ground-water system characterization (step 3) is based upon the surface and subsurface characterizations. This ability to hypothesize the ground-water system provides the necessary link between the wetland and the regional landscape, and allows for the incorporation of aspects of the system beyond the boundaries of the wetland. Finally, the wetland class and subclass can be determined based upon steps 1 through 3. Using this approach, the Pennsylvania Mine wetland, near Dillon, Colorado was characterized and wetland variables and functions were identified.

## INTRODUCTION

### General Background

Wetland functions are the physical, chemical, and biological processes that characterize wetland ecosystems. Included among these functions are the storage of surface waters during flooding events and the removal of chemicals from the ground-water system through sorption onto organic materials. Since 1975, several functional assessment techniques have been developed in order to identify wetland functions and determine the degree to which the wetlands are functioning. In general, these techniques have not been applicable to a variety of wetland types, and have not provided an areal basis for comparing wetland functions (National Research Council 1995). The Hydrogeomorphic Wetland Classification (HGM) was developed by Brinson (1993) to correct for these deficiencies.

HGM allows for the classification of functionally similar wetlands based on 1) geomorphic setting; 2) water source and transport; and 3) hydrodynamics. The HGM approach assumes that the maintenance of the wetland and related ecosystem is primarily a function of a combination of physical and chemical factors. The measurement of these physical and chemical factors, therefore, provides an avenue for the investigator and the regulator to understand the nature and function of wetlands and to evaluate the relative values of each wetland. Although HGM is currently being developed nationwide under the leadership of the US Army Corps of Engineers, Waterways Experiment Station, HGM is subject to some of the same limitations

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which have been apparent with previous functional assessment methods. Among these limitations are the difficulty of incorporating a landscape perspective into the assessment, the low level of understanding of physical functions as compared to biological functions, and the lack of wetland studies in the western United States (National Research Council 1995).

### Purpose of Research

In order to develop an HGM assessment methodology specific to the wetlands in the southern Rocky Mountains that addresses some of these limitations, it was recommended that the logic and some aspects of the conceptualization and characterization methodology described by Kolm (1993), Kolm et al. (1996), and Kolm and van der Heijde (1996), be combined with the hydrogeomorphic parameters and wetland functions defined by Brinson (1993). In addition to the development of this HGM assessment methodology, the goals of the research were to supplement current knowledge of the functioning of wetlands in the western United States, and to identify the physical and geochemical functions on which future research should be focused.

### Methods

During the 1997 field season, five wetlands in Colorado were investigated. The study was designed to measure the influence of ground-water and surface water on the hydrologic regime of each wetland, and the influence of the hydrologic regime on the biogeochemical functions of each wetland. As a initial step, data were collected and the wetlands were characterized with conceptualization and characterization. Upon completion of this conceptualization and characterization, field data were collected for each wetland. Included in the hydrologic field data were ground-water head levels and surface water characteristics. Chemical data included field measurements of pH, Eh, and conductivity. Water samples were analyzed in the laboratory for total and dissolved iron, zinc, chloride, nitrate, and sulfate content.

Based upon the results of this research, a step-wise, integrated approach for wetland hydrologic function classification was developed. This southern Rocky Mountains wetland classification scheme, which incorporates both the HGM methods of Brinson (1993), and the Conceptualization and Characterization of Kolm (1993); Kolm et al. (1996); and Kolm and van der Heijde (1996) is described in a step-wise, integrated approach involving both surface and subsurface characterization and analysis. This approach is designed hierarchically for wetland identification, wetland function delineation, and, ultimately, wetland type.

## STEP-WISE, INTEGRATED HYDROGEOMORPHIC APPROACH FOR WETLAND HYDROLOGIC FUNCTION CLASSIFICATION

In the following approach and classification scheme, the ground- and surface water flow systems and dynamics can be determined. This information, in conjunction with geomorphic settings, can be used to determine the wetland process, and wetland class and subclass. In addition, this classification scheme provides the framework or structure for wetland functional identification and analysis. Table 1 provides guidance for the use of the classification scheme. The table can be used as a checklist of which variables or indicators are present on site. In determining which variables are present, the wetland functions that may be present are also identified with Table 1. Table 2 provides a definition of the functions identified on Table 1. In

**TABLE 1** Step-Wise Integrated Hydrogeomorphic Approach for Wetland Hydrologic Classification

| System Unit | Indicator/Characterization Variable | | | Hydrologic Function | PM* |
|---|---|---|---|---|---|
| Step 1: Surface Characterization | A. Vegetation | 1. | Hydrophyte | ET, GWmove | X |
| | | 2. | Non-hydrophyte | | |
| | B. Soil | 1. | Peat | GWmove, GWinter, Gwstorelt, SWstoredynSWstorelt | X |
| | | 2. | Mineral | GWstoredyn | |
| | C. Surface Water | 1. | Springs/seeps | SWin, GWoutss | X |
| | | 2. | Overland flow | | ▨ |
| | | 2a. | Source = springs/seeps | SWout, GWoutss | X |
| | | 2b. | Source = flooding | SWstoredyn, ED, SWin | |
| | | 3. | Channel flow | | ▨ |
| | | 3a. | Channel Enters Wetland | SWin | |
| | | 3b. | Gaining Stream in or on the Boundary of Wetland | GWoutr | X |
| | | 3c. | Losing Stream in or on the Boundary of Wetland | GWstorelt, ED | |
| | | 3d. | Channel Exits Wetland | GWoutr, SWout | |
| | | 4. | Still water | GWoutss, SWstorelt, Gwinter | X |
| | D. Climate | 1. | Evaporation | ET | X |
| | | 2. | Annual Precipitation | | ▨ |
| | | 2a. | Snowpack | ATMin | X |
| | | 2b. | Rain | ATMin | X |
| | E. Topography | 1. | Locally (on site) | | ▨ |
| | | 1a. | Low Gradient (<2%) | GWmove, GWstoredyn, SWstorelt, SWstoredyn, ED | X |
| | | 1b. | High Gradient (>2%) | GWmove | |
| | | 1c. | Slope Direction | GWmove | ▨ |
| | | 1d. | Microtopography (hummocky) | SWstoredyn, SWstorelt, ED, GWstoredyn | X |
| | | 2. | Locally (boundary conditions) | | ▨ |
| | | 2a. | Low Gradient (less than or equal to on-site gradient) | GWmove | |
| | | 2b. | High Gradient (greater then on-site gradient) | GWinter, GWmove | X |
| | | 2c. | Slope Direction Into Wetland | GWinter, GWmove | X |
| | | 2d. | Slope Direction Away From Wetland | GWmove, GWoutr | X |
| | F. Animals | 1. | Beaver Activity | SWstorelt, ED, SWstoredyn | |

* Variables and Functions Present at Pennsylvania Mine Wetland

**TABLE 1** cont. Step-Wise Integrated Hydrogeomorphic Approach for Wetland Hydrologic Classification

| System Unit | Indicator | | | Characterization Variable | Hydrologic Function | PM* |
|---|---|---|---|---|---|---|
| Step 2: Subsurface Characterization | A. Geomorphic Deposits/ Hydrogeomorphology | 1. | Periglacial | 3-D Structure of System, Hydraulic Conductivity, Storativity, Saturated Thickness, Transmissivity | GWstorlt, GWstordyn, GWmove, GWinter, SWstorlt, SWstordyn, ED | ▨ |
| | | 1a. | Stone Nets, Stone Stripes, Patterned Ground | | | |
| | | 1b. | Lakes- "depressional" | | | |
| | | 2. | Glacial | | | ▨ |
| | | 2a. | Morraine (lateral, terminal and recessional) | | | X |
| | | 2b. | Morraine Lacustrine Deposits | | | |
| | | 2c. | Till | | | |
| | | 2d. | Erosional lakes (tarns) | | | |
| | | 3. | Mass Wasting | | | ▨ |
| | | 3a. | Colluvium | | | X |
| | | 3b. | Lacustrine deposits within colluvium | | | |
| | | 4. | Fluvial | | | ▨ |
| | | 4a. | Terraces, Abandoned Floodplains, Outwash Plains | | | |
| | | 4b. | Modern floodplain | | | |
| | | 4d. | Lacustrine (oxbow lakes) | | | |
| | B. Geology/ Hydrogeology | 1. | Fracture Flow | 3-D Structure of System, Hydraulic Conductivity, Storativity, Saturated Thickness, Transmissivity, | GWstorlt, GWstordyn, GWmove, GWinter, SWstorlt, SWstordyn, ED | ▨ |
| | | 1a. | Stratified Igneous Extrusive Rocks | | | |
| | | 1b. | Metamorphic and Igneous Intrusive Rocks | | | X |
| | | 1c. | Crystalline Limestone Rocks (With or Without Karst) | | | |
| | | 2. | Matrix Flow | | | ▨ |
| | | 2a. | Stratified Sandstones (With Fracture Flow) | | | |
| | | 2b. | Fault Gauge | | | |
| | | 3. | Confining Units | | | ▨ |
| | | 3a. | Shales | | | |
| | | 3b. | VolcanicAshes | | | |
| | C. Geologic Structure/ Hydrostructure | 1. | Fracture Zones | 3-D Structure of System, Hydraulic Conductivity, Storativity, Saturated Thickness, Transmissivity | GWstorlt, GWstordyn, GWmove, GWinter, SWstorlt, SWstordyn, ED | X |
| | | 2. | Faults (Normal and Reverse) | | | X |
| | | 3. | Folds | | | |
| | | 4. | Igneous Contact Zones | | | X |
| Step 3: Ground Water System Characterization | A. GW Movement (Direction) And Boundary Conditions | 1. | Horizontal | Head or Potentiometric Surface | GWstorlt, GWstordyn, GWmove, GWinter, SWstorlt, SWstordyn, ED | ▨ |
| | | 1a. | To River or Channel | | | X |
| | | 1b. | From River or Channel | | | |
| | | 1c. | To and From River (seasonally) | | | |
| | | 1d. | To and From River (spatially) | | | |
| | | 1e. | From Bedrock Source | | | X |
| | | 2. | Vertical | | | ▨ |
| | | 2a. | Up | | | |
| | | 2b. | Down | | | |
| | | 2c. | Up and Down (seasonally) | | | X |
| | | 2d. | Up and Down (spatially) | | | |

* Variables and Functions Present at Pennsylvania Mine Wetland

addition to the tables, maps may be created to identify the location of each of the variables which will aid in the identification and interpretation of the spatial distribution of the wetland hydrologic functions.

**TABLE 2** Definition of Hydrologic Functions Identified in Southern Rocky Mountain Wetlands

| Function Abbreviation | Function Name | Function definition |
|---|---|---|
| ET | Evapotranspiration | The removal of water from the terrestrial environment to the atmosphere. |
| GWinter | GW interception | The interception of ground-water, typically by a low K layer. |
| GWoutss | GW out springs/seeps | The removal of water from the ground-water system to the surface water system via springs and seeps. May result in water remaining on site. |
| GWoutr | GW out river | The removal of water from the ground-water system to the surface water system (results in a gaining stretch of river or stream). Results in movement of water off site. |
| GWstorelt | GW storage-long term | Storage of water into regional system, or in subsurface of wetland. |
| GWstoredyn | GW storage-dynamic | Storage of water in subsurface of wetland during flooding events. |
| GWmove | GW movement (moderation of) | A change in the direction and velocity of ground-water. |
| SWstoredyn | SW storage-dynamic | Short term storage of surface water. e.g. during flooding events. |
| SWstorelt | SW storage-long term | Storage of surface water for long periods of time. Water is stored because recharge to a ground-water system is retarded by a low hydraulic conductivity layer, or is retained by microtopography or dam like structures. |
| SWin | SW in | Surface water enters wetland as a channel. |
| SWout | SW out | Surface water exits wetland as a channel. |
| ATMin | Atmosphere in | Input to wetland from atmosphere. |
| ED | Energy Dissipation | Degree to which wetland can dissipate energy. |

## Step 1: Surface Characterization

The purpose of the surface characterization step is to determine or reaffirm if, by definition, the area being assessed is a wetland. In addition, the wetland functions pertaining to hydrologic sinks and sources within the system are identified. Surface characterization consists of evaluating the appropriate vegetation, soils, surface water, climate, topography, and animals associated with the wetland. The anthropogenic aspects of the evaluation are to be included in these categories.

Step 1a) Vegetation observed on-site and in the surrounding area is used to determine the presence of a near-surface water table (in some cases, depth to water table may be approximated) and can indicate water quality (e.g. low vrs. high salinity). Where hydrophytes are present, wetlands may be present, and the wetland function of evapotranspiration of water from the water table is observed (Table 1). Evapotranspiration is a ground-water system loss or sink. In addition, during the growing season, the plant functions as a pumping well and draws water toward it in a radial-like manner. In this respect, the hydrophytes are part of the wetland function of ground-water movement.

Step 1b) Soils observed on-site and in the surrounding area are used, in conjunction with the vegetation analysis, to determine the presence and horizontal distribution of peat vrs. mineral soils. Vertical peat distribution, if required, is determined by other direct (cores, etc.) or indirect (geophysics) measurements.

Step 1c) Surface water observed on-site and in the surrounding area is used in conjunction with the vegetation map to determine the location of springs and seeps, types of overland flow, type and distribution of channeled flow, and the presence of still water. Surface water flow, inundation, velocity, and other parameters may be determined by direct measurements if required. Where surface water occurs, the area may be classified as a wetland, and the wetland functions identified on Table 1 may be observed.

Step 1d) Climate data observed on-site and in the surrounding area is used in conjunction with the vegetation and surface water data and analysis to determine the type and distribution of precipitation and evaporation. Precipitation, such as daily or annual rainfall and snow pack, and evaporation may be measured directly if required.

Step 1e) The topography observed on-site and in the surrounding area is used to determine the microtopography of the site, the topographic slope gradient and slope direction of the site, and the topographic slope gradient and slope direction of the areas surrounding the site. Topographic slope gradients, slope directions, and microtopography may be determined by direct measurements or with topographic maps.

In the southern Rocky Mountains, microtopography will most likely be geomorphologically and/or anthropogenically derived, for example meander scrolls in a fluvial environment, hummocky terrain in moraine or mass wasting topography, and excavations where anthropogenic activity has occurred. Typically, the wetland topography is of low slope gradient resulting in low-gradient ground-water movement. The direction of slope is variable, but usually reflects a river or mass wasting process. The topography of the area surrounding the wetland is typically high slope gradient and the direction of the slope is usually towards the wetland. This indicates that ground-water, if available, will be moving into the wetland from a high gradient system and that the surrounding area may be a source for long-term ground-water input into the wetland system. In addition, most of the southern Rocky Mountain wetlands have moderate to low slope gradients on one of the boundary conditions where the wetlands connect to nearby streams or topographically low areas. This indicates that ground-water, if available, will be moving from the wetland to the river or surrounding areas.

Step 1f) Animal, specifically beaver, activity observed on-site and in the surrounding area is used to determine the hydrologic changes in either the ground-water flow or chemistry (e.g., water table changes), or surface water flow or chemistry. Where beaver dams have been constructed, the wetland functions identified on Table 1 are observed.

## Step 2: Subsurface Characterization

The purpose of the subsurface characterization step is to further understand the spatial and temporal nature of the three-dimensional structure of the wetland system, and to understand the material properties with regards to fluid flow and chemical transport in the ground-water system that supports the wetland. In addition, the wetland functions pertaining to ground-water storage-long term, ground-water storage-dynamic, and ground-water movement are determined, and functions pertaining to ground-water interception, ground-water out river, ground-water out springs/seeps, surface water storage-long term, surface water storage-dynamic, and energy dissipation are refined. Subsurface characterization consists of evaluating the appropriate geomorphic deposits, geology, and hydrogeology associated with the wetland being evaluated (Table 1). The anthropogenic aspects of the evaluation are to be included in these categories.

Step 2a) The type and distribution (three-dimensional nature) of geomorphologic deposits and landform features observed on-site and in the surrounding area of the wetland are determined in conjunction with the vegetation, soils, and topography. The stratigraphic nature of these deposits, if required, is determined by other direct (e.g. cores) or indirect (e.g. geophysics.) measurements.

The physical and chemical characteristics of the geomorphologic deposits, such as sorting or gradation, texture, and mineralogical composition, can be used to interpret hydrogeological and hydrochemical properties and the three-dimensional structure of the wetland. The depth or thickness of geomorphologic deposits will be variable due to the various processes and time of formation. In the southern Rocky Mountains, these deposits and landforms may be of periglacial, glacial, fluvial, lacustrine, or mass wasting origin.

Step 2b) The three-dimensional geologic framework observed on-site and in the surrounding area of the wetland is determined in conjunction with the surface and geomorphologic analysis. The stratigraphic and lithologic nature of these rocks, and the geologic structure can be determined by direct (e.g. mapping, and cores) or indirect (e.g. geophysics) measurements. If a wetland has been identified in the surface characterization step, based upon the presence of the appropriate hydric soils, hydrophytes, and/or surface water, then the geologic bedrock and structure can be interpreted to derive the hydrogeology necessary for the wetland functions of ground-water movement, ground-water storage-long term, and ground-water storage-dynamic (Table 1). In addition, the distribution of geologic lithology and structure can be interpreted for microtopography, and be part of the wetland functions of surface water storage-long term, surface water storage-dynamic, and energy dissipation.

The physical and chemical characteristics of the bedrock materials, such as sorting or gradation, texture, and mineralogical composition, can be used to interpret hydrogeological and hydrochemical properties, and the three-dimensional structure of the wetland. The depth or thickness of geologic units will be variable due to the various processes and time of formation. In the southern Rocky Mountains, most types of lithologic materials exist, including crystalline metamorphic and intrusive igneous rocks, and stratified sedimentary (including karst) and volcanic rocks. In addition, faults and fracture zones (derived by direct mapping or indirectly by a lineament analysis) are commonly observed. The bedrock geology and geologic structure will be interpreted in the next step to show the areas within and around the wetland where the ground-water movement, ground-water interception, ground-water out, and ground-water storage functions occur with respect to the ground-water saturated zone, and to show information regarding the microtopography and surface water system storage (Table 1).

Step 2c) Hydrogeologic characterization is then performed to assess the important ground-water system features of the geologic and geomorphologic framework including aquifer permeability, type, homogeneity and heterogeneity, and isotropy and anisotropy. Hydrostratigraphic and hydrostructural units are determined and attributes, such as saturated thickness, hydraulic conductivity, storativity or specific yield, mode of flow (e.g. matrix or fracture flow), and geologic and topographic continuity, are evaluated. The hydrogeologic properties of the bedrock and unconsolidated deposits can be determined by direct (e.g. aquifer and slug tests) or indirect (e.g. gravel texture, sorting) measurements.

The three-dimensional hydrogeologic framework should be characterized for the wetland and surrounding area. The physical characteristics of the hydrogeologic units, such as hydraulic conductivity, specific yield or storage, and saturated thickness, can be used to interpret the overall ground-water flow system with regards to the three-dimensional structure of the wetland. In the southern Rocky Mountains, most types of hydrogeologic units and characteristic flow properties exist, including crystalline metamorphic and intrusive igneous rocks with fracture flow properties, crystalline limestone rock with or without karst properties, stratified sedimentary units such as sandstones that may have both matrix and fracture flow properties, stratified volcanic rocks such as tuffs and breccias, that may have fracture flow properties, and stratified shales or volcanic ashes that have very low permeability and porosity and function as ground-water system confining units. In addition, most types of hydrostructural units and characteristic flow properties exist, including normal and reverse faults, regional and local-scale fracture zones, folding, and igneous contact zones. Ground-water movement will be influenced by these features, for example by enhanced flow regimes seen in fracture zones, or by restricted flow when two hydrologically disparate units are moved together. The hydrogeologic units will be interpreted in the next step to show the areas within and around the wetland where the ground-water movement, ground-water interception, and ground-water storage functions occur with respect to the ground-water saturated zone, and to show information regarding the surface water system storage.

### Step 3: Ground -Water System Characterization

The ground-water system of the wetland is now characterized using the hydrogeologic framework and attributes, and the surface characterization. This procedure involves the determination of type, amount, and distribution of recharge; type, amount, and distribution of discharge; flow path vectors; type and distribution of wetland boundary conditions; and potentiometric surfaces of the wetland aquifer units. The type, amount, and distribution of recharge to and discharge from a wetland ground-water unit can be determined by direct (e.g. rain gages, lysimeters, spring measurements, evapotranspiration, or wells) or indirect (e.g. vegetation analysis, or soil textures) measurements. Flow path vectors, wetland boundary conditions, and potentiometric surface are determined by the interpretation of the recharge, discharge, and hydrogeologic data, and the interpretation of data gathered by direct measurements, such as head in a water well. The ground-water system analysis is used to derive wetland functions of ground-water interception, ground-water movement, ground-water storage-long term, and ground-water storage-dynamic (Table 1). These functions represent ground-water system transport and storage. In addition, the ground-water system can be interpreted for the wetland functions of surface water storage-long term, surface water storage-dynamic, and energy dissipation.

The three-dimensional ground-water system should be mapped and characterized for the wetland units and surrounding areas. The recharge, discharge, flow paths, boundary conditions, and potentiometric surface of each wetland aquifer unit can be used to interpret the overall ground-water flow system with regards to the three-dimensional structure of the wetland. In the southern Rocky Mountains, two types of ground-water flow paths are observed: predominantly horizontal and predominantly vertical. The critical horizontal flow paths are from the wetland to a river, from a river to the wetland, both to and from a river (spatially separated) with respect to the wetland, and from a bedrock source to the wetland. A fifth category of horizontal flow includes those wetlands that have flow paths to and from a river that vary seasonally with the river elevations and inundation cycles. The critical vertical flow paths are from deeper parts of the wetland through low hydraulic conductivity (K) material (usually peat) to the surface, from the surface of the wetland through low K material to deeper parts of the wetland, or both up and down through the low K material depending on head distribution. A fourth category of vertical flow includes those wetlands that have both up and down flow paths based on seasonal variation through low hydraulic conductivity material. These flow path categories have significant implications regarding both hydrological and geochemical functions.

### Step 4: Determine Class of Wetland System Based on Ground-Water System Assessment

In the southern Rocky Mountains, the two HGM classes of wetland systems observed, based on this ground-water system assessment, are slope and riverine.

Slope wetland systems are defined as wetlands with return flow from ground-water being the dominant water source and dominant hydrodynamics being horizontally unidirectional (Brinson et al. 1995). The primary functions of slope wetland systems in the southern Rocky Mountains, as derived from the ground-water system assessment, are ground-water out, ground-water movement, ground-water interception, and ground-water storage-long term. There are two subclasses of slope wetland systems that are observed in the southern Rocky Mountains: peat-dominated and mineral-soil/geomorphic deposits/bedrock-dominated.

Riverine wetland systems are defined as wetlands with the dominant water source being overbank flow from a channel, and dominant hydrodynamics being horizontally unidirectional (Brinson et al. 1993). The primary functions of riverine wetland systems in the southern Rocky Mountains, as derived from the ground-water system assessment, are ground-water outr, ground-water movement, ground-water storage-dynamic, and ground-water storage-long term. In addition, ground-water system assessment is helpful for determining the functions of surface water storage dynamic, surface water in, and energy dissipation. There may be subclasses of riverine wetland systems in the southern Rocky Mountains based on wetland structure and hydrology. For example, most riverine wetlands are associated with modern alluvium deposited on bedrock. If the bedrock has a large hydraulic conductivity, such as a fractured sandstone, the function of the wetland is to further enhance ground-water storage-long term, ground-water movement, and ground-water out If the bedrock has a small hydraulic conductivity or if the bedrock system has an upward gradient, then these same functions are diminished. However, the reference sites necessary to delineate these subclasses were not studied.

## CASE STUDY: THE PENNSYLVANIA MINE WETLAND

### Peat-dominated slope wetland subclass

The Pennsylvania Mine wetland, investigated in this study, is at an elevation ranging from 10,025 ft to 10,880 ft on the western side of the Continental Divide. The wetland is located at 39°36'00" latitude and 105°48'30" longitude and is approximately 60 miles south west of

Denver, Colorado. The Pennsylvania Mine, an abandoned mine which is a source of metals to the wetland, is located at the base of a mountain near the boundaries of the wetland and is at an elevation of 11,000 ft; the Pennsylvania Mine wetland is located on the floor of the glaciated valley and is adjacent to the southern edge of Peru Creek (Figure 1). Based upon Steps 1 through 3 of the step-wise integrated hydrogeomorphic approach, this wetland was classified as a slope wetland, subclass: peat-dominated.

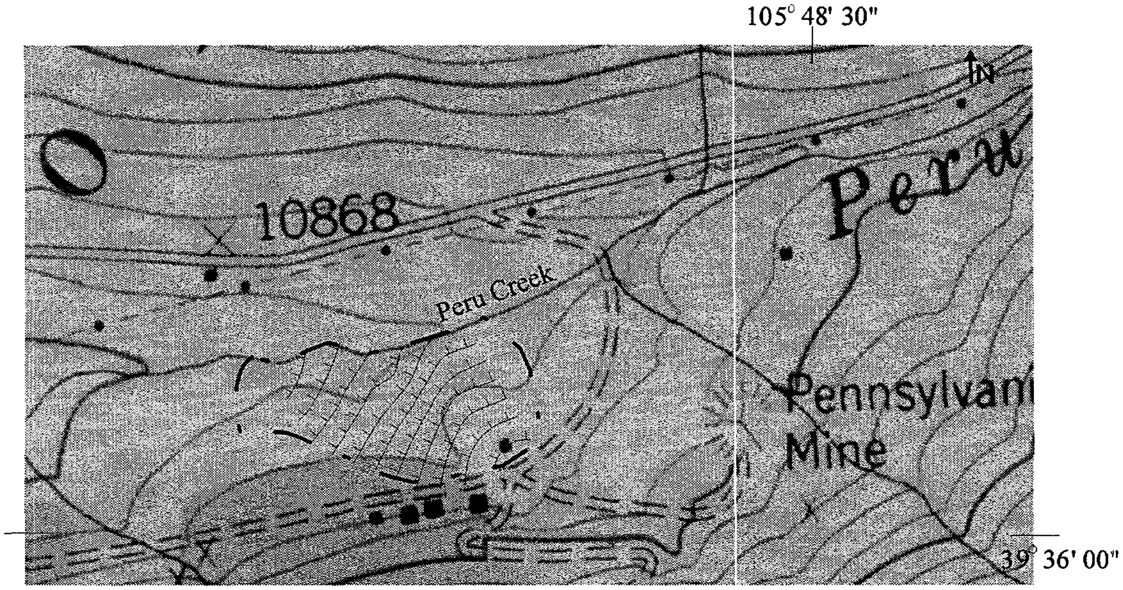

**FIGURE 1** Potentiometric Surface in Peat Layer of the Pennsylvania Mine Wetland on 6/19/97. Contour Lines Represent Four Foot Change in Potentiometric Surface. Hachures Indicate Downhill Direction. Ground-Water Flow Direction is at Right Angles to Potentiometric Surface. Wetland Boundary Indicated by Dashed Line

## Surface Characterization

Step 1a) Vegetation data was obtained from Huskie (1987) and was field checked during on-site visits. The data and field work revealed that hydrophytes were observed to be continuous along the south side of Peru creek and intermittent along the north and west side. *Salix spp.* are the dominant species along the creek. The continuous presence of hydrophytes indicates that there is some continuity of ground-water levels along the creek. Hydrophytes are located south of Peru Creek and north of the site access road. Included in these wetland plants are *Deschampsia cespitosa* (tufted hairgrass), *Carex aquatilis* (sedge), and *Betula glandulosa* (bog birch). According to Huskie (1987), *D. cespitosa* is indicative of poorly drained soils and occurs where winter snow depths are greater than 2.5 feet. Tufted hairgrass has been determined by several researchers be tolerant of heavy metals (Coulaud and NcNeilly 1992; Von Frenckell-Insam and Hutchinson 1993a; Von Frenckell-Insam and Hutchinson 1993b). *C. aquatilis* are a successional species to *D. cespitosa* and generally found on deep accumulations of peat. Soil saturation has been found to range from standing water to deep water table conditions when *C. aquatilis* is present (Huskie 1987). The soils on which *B. glandulosa* are generally found have large accumulations of organic matter. When *B. glandulosa* is present, standing water in the spring and water tables near the soil surface throughout the summer are common (Fire Effects

Information System 1998). These observations indicate that ground-water movement is governed locally by the vegetation (Table 1).

Step 1b) Peat is observed in the Peru Creek wetland. The spatial distribution (lateral and vertical extent) of the peat was estimated from the wells hand-augered in and from published data (Huskie 1987).

Step 1c) Peru Creek is a perennial stream topographically located on the downward side of the wetland. According to the data presented by Huskie (1987), the stretch of the Creek bordering the wetland site is gaining. This indicates that ground-water enters the surface water system at the wetland boundaries, and that the wetland function of ground-water out river occurs.

The second body of surface water present throughout the summer season was the surface water inundation of the wetland. Still water and overland flow across the eastern section of the wetland was noted. This surface water was stagnant in places due to the microtopography of the wetland, but was, in general, flowing towards Peru Creek. The source of the overland flow and still water was ground-water springs/seeps.

Anthropogenic surface water features include settling ponds associated with the mine and channeled trenches along the side of the wetland. Water is present year round in both of these features. An inspection of these ponds and trenches indicated that they leak and, therefore, contribute to surface water inputs into the wetland. Ground-water was noted to daylight near the entrance to the ponds. These anthropogenic features contribute to the wetland functions of ground-water storage-long term and ground-water interception. In addition, these features may provide transport mechanisms for metals and sulfates to enter the wetland.

Step 1d) Precipitation data was collected from the Dillon 1E weather station # 052281 (elevation: 9080 ft.) and was accessed through the National Weather Service Western region home page at http://wrcc.sage.dri.edu. It is expected that the values for precipitation will be higher and temperature will be lower at the Peru Creek site due to the differences in elevation. The average annual precipitation over a 90 year period is 16.36"/yr as rain and 131.3"/yr as snowfall at Dillon 1E. Total precipitation (snow and rain) can be estimated to be 29.49"/yr Fetter (1988). Historical data indicates two peak climatic events. The first is due to snow melt from April to early June which results in increased inputs to surface and ground-water systems. The second event is due to monsoonal rains and occurs from August through September. With the average temperature ranging from 16.36° F to 51.8°F, snowfall occurs every month of the year except July and August. The majority of precipitation is in the form of snow from November to April at Dillon 1E.

Step 1e) A 1:24:000 topographic map of the Montezuma, CO quadrangle (USGS 1958) was used, in conjunction with field observations, to determine slope gradient, slope elevation, microtopography, drainage locations, patterns, and density. The site elevation ranged from approximately 10,880 ft on the southeast portion of the wetland to approximately 10,025 ft at Peru Creek at the northwest corner of the site. The mountains immediately adjacent to the wetland reach up to 12,890 ft in elevation. The site is divided into two topographic regions. Along the valley floor, where the wetland is located, the slope gradient is 0-2% generally toward the stream indicating that water is recharged and that soil (including peat) formation is a dominant geomorphic process. There is also microtopography that stores water on the wetland surface. The mountainous terrain surrounding the site slopes towards the wetland and river, and the slope gradients are greater than 2%. If this terrain has a ground-water system associated with it, the water will move towards and into the wetland system. Therefore, the wetland functions of ground-water interception, ground-water movement, and ground-water out river occur (Table 1).

Step 1f) There was no apparent recent activity by beaver at the Peru Creek site. The main alteration of surface water activity was due to human activity (primarily mining related).

## Subsurface Characterization

Step 2a) The geomorphic deposits observed on-site include glacial moraines, colluvium, and weathering/pedogenic materials (primarily mineral soil and peat). Currently, the glacial materials are moving down slope under mass wasting processes to form modern colluvial deposits. The wetland is actually formed in a topographically flat area on top of colluvial deposits. The geomorphic material of peat is observed to be lying on top of the colluvium.

Step 2b) A 1:31,680 Geologic map (Neuerburg and Botinelly 1972) was used, in conjunction with field observations, to determine structural geologic features, bedrock geology, and mineralization locations and type. The hydrothermally altered Idaho Springs formation is the dominant bedrock geology underneath the wetland site. A zone of alteration is located along the southeastern corner of the site. In addition, an igneous contact zone forms the western boundary in the bedrock underneath the wetland.

Step 2c) The three dimensional structure of the wetland is believed to be composed of three hydrogeologic layers that are all water-bearing. The Idaho Springs Formation bedrock, with fracture flow predominating, is the bottom layer of the wetland. A thin colluvial layer, composed primarily of cobbles, overlies the crystalline bedrock. Peat overlies the colluvial hydrogeologic unit and is the visible surface layer.

Estimates of hydraulic conductivity range from $10^{-3}$ to $10^{-5}$ cm/sec in the peat layer, $10^{2}$ to $10^{-2}$ cm/sec in the unconsolidated colluvial layer, and from $10^{-2}$ to $10^{-6}$ cm/sec in the bedrock layer (Huskie 1987; Domenico and Schwartz 1990). The colluvial deposits have the greatest hydraulic conductivity, and are expected to allow water to easily enter (porosity range from 2-36%), and to easily pass horizontally through via matrix flow.

Storativity was estimated for the colluvial gravels to be from 23 to 28 percent, and for the bedrock to be 10 percent. By comparison, the peat layer will have relatively high storativity and is estimated at 44 percent. Peat is water-bearing, but the water is retained by the unit, and movement is slow. The majority of water movement through peat is expected to be vertical; water is removed from the system by evapotranspiration and/or replaced by ground water from below and/or precipitation infiltrating from above. The hydrothermally altered Idaho Springs formation is chiefly composed of clays. The storativity of this formation is expected to be significantly lower and porosity higher than the colluvial deposits. This geologic unit, where present, will be water-bearing, but the yield is estimated to be low. However, the chemistry associated with this unit may significantly affect the chemistry observed in the wetland.

A final hydrogeologic unit, and a source of chemical contamination to the wetland, is mine tailings piles which are found on site. Based upon the chemical data, some of these tailings are believed to be buried within the wetland. Additionally, some of these tailings are on the surface of the wetland and are mostly unsaturated with respect to ground-water. However, infiltration of atmospheric water through these surface piles will alter both ground- and surface water quality.

## Ground-Water System Characterization

Step 3) Water levels were measured from shallow wells, including wells located in both colluvium and peat, on 6/12/97 (snow melt), 6/19/97 (snow melt), 8/4/97 (post-snow melt), 9/13/97 (monsoon), and 10/18/97 (post-monsoon). These water levels were analyzed for potentiometric surfaces for each separate hydrogeologic unit (colluvium and peat), and seasonal and spatial comparisons were made. This analysis was used to confirm the proposed hydrologic functions.

Using the Ground-Water System Characterization (Step 3), as presented in this paper, the ground-water system of the Peru Creek wetland was conceptualized to be composed of three components: the bedrock system, the colluvial system, and the peat system (Figure 2). Regional ground-water support for this wetland is derived from the crystalline bedrock system. The recharge to this system is from infiltration of precipitation in the upland mountain ridges and valley sides. The ground-water flow paths in this system are from topographically high areas to the valley bottoms and streams in the topographically low areas. The Peru Creek wetland is located between the regional recharge and discharge zones. Therefore, the bedrock ground-water system will discharge water on a long term basis into the colluvial system supporting the wetland.

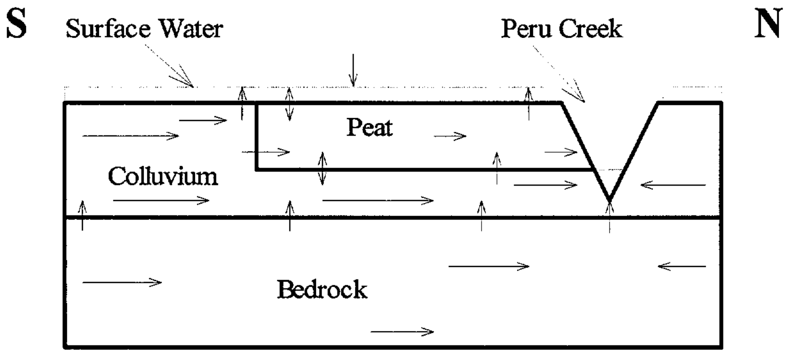

**FIGURE 2** Conceptualization of Ground-water Flow in the Pennsylvania Mine Wetland.

The peat ground-water system is recharged by infiltration of precipitation and/or surface water inundation on the wetland surface, and by discharge from the colluvial system into the peat system (Figure 2). In general, the potentiometric surface interpreted from the heads observed in the peat show that the general flow direction is nearly horizontal from the topographically upgradient area of the wetland to Peru Creek (Figure 1). However, the low hydraulic conductivity of the peat, and the agreement of the peat heads with the surface water elevations indicate that vertical flow upward from the peat system into the surface water is the dominant process.

The colluvial ground-water system is recharged by infiltration of precipitation and/or surface water inundation on the wetland surface, and by discharge from the bedrock system into the colluvial system (Figure 2). In general, the potentiometric surface interpreted from the heads observed in the colluvium show that the general flow direction is nearly horizontal from the topographically upgradient area to Peru Creek. In addition, the heads in the colluvium are generally greater that those in the peat indicating that the colluvial system discharges water vertically into the peat system (Figure 3a). However, an analysis of seasonal effects show that during times of surface water inundation, the reverse is true in part of the upgradient area of the wetland and that in the downgradient areas of the wetland the heads in the colluvium and peat are nearly equal (Figure 3b). This indicates that ground-water from the peat system can vertically recharge the colluvial system during that time period in those parts of the wetland where the head in the peat system is greater than the head of the colluvial system. In those parts of the wetland where the heads are equal, the two systems are behaving as one and are affected by surface water.

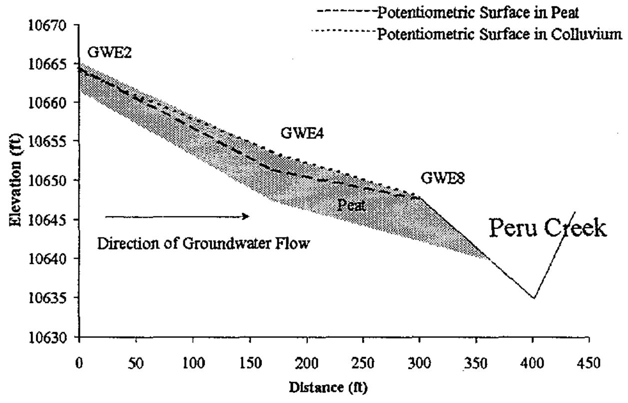

**FIGURE 3a** Cross Section of Pennsylvania Mine Wetland on 6/19/97

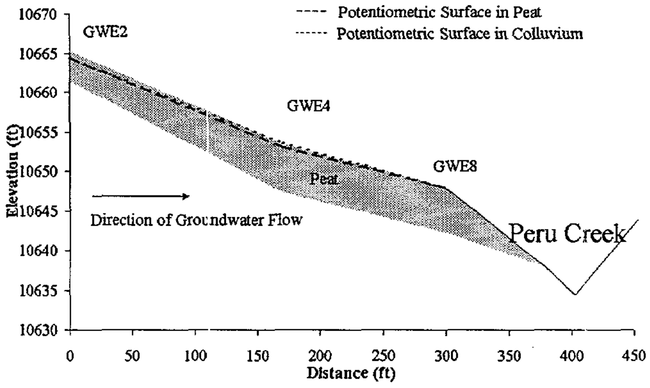

**FIGURE 3b** Cross Section of Pennsylvania Mine Wetland on 8/4/97

In summary, ground-water movement was determined to move mostly horizontally through the colluvium from the bedrock source to the river, vertically through the peat from the colluvium to the surface water inundating the wetland surface, and seasonally to and from the peat to the colluvium based on surface water inundation levels in the upgradient part of the wetland. Ground-water from the bedrock aquifer recharges the surficial units regardless of season (ground-water movement vertically up). The analysis confirms that the ground-water functions of ground-water movement, ground-water storage-long term, ground-water storage-dynamic, ground-water interception and surface water storage-dynamic occur in this wetland.

## DISCUSSION

### Future Work

Future work should be designed to determine how the hydrologic variables identified in Table 1 should be measured and combined. This determination should be based on field research conducted on wetlands in the southern Rocky Mountains. In keeping with HGM methods, this would allow for a comparison of the degree to which wetlands function. In addition, a wetland functional assessment of geochemical functions should be developed in a similar manner as the hydrologic functional assessment presented in Table 1.

Based upon the research conducted on the southern Rocky Mountain wetlands, the geochemistry of the systems is hypothesized to be controlled by hydrologic regime, wetland structure, and biologic cycles. However, these processes are inter-related; this makes a determination of which single factor is controlling wetland biogeochemical cycles a difficult task. It is our belief, however, that these proposed controls over wetland biogeochemistry, in conjunction with field research, can be used to preliminarily identify wetland geochemical variables and functions.

## CONCLUSION

In conclusion, the development of this wetland functional assessment has provided the framework for wetland researchers and delineators to identify ground-water flows with minimal on-site effort. In addition, the presence or absence of variables identified on Table 1 can be determined within hours. For these reasons, it is recommended that this step-wise, integrated approach be incorporated into the development of future HGM regional assessments by the Assessment Procedure Development Team in defining the wetland function, and in determining the variable indices for each function.

### Acknowledgments

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# APPLICATION OF THE CONE PENETROMETER AS AN INNOVATIVE TECHNOLOGY TOOL IN NATURAL ATTENUATION RESEARCH

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## ABSTRACT

As part of the natural attenuation study of explosives, the Cone Penetrometer (CPT), has been used to provide data for a multi-objective project conducted at two contaminated sites. The CPT, used in geotechnical work since 1931, determined the geohydrologic characteristics and lateral and vertical extent of plumes at a Gulf Coastal Plain site at the Louisiana Army Ammunition Plant (LAAP), Minden, Louisiana and a Glacial Till environment of deposition at the Joliet Army Ammunition Plant (JAAP), Joliet Illinois. The ground water modeling system (GMS) and its three-dimensional ground water model FEMWATER, was used to simulate flow and mass transport of TNT, RDX and related chemicals at the sites. Initial modeling runs for LAAP indicate that the TNT and RDX plumes are static and possibly slowly diminishing.

## INTRODUCTION

### Physiography

The Louisiana Army Ammunition Plant ( LAAP) lies within the Western Gulf Coastal Plain physiographic province. Two major landforms, dissected uplands and rolling prairie, are found within LAAP. Minor landforms include abandoned channels, typically filled with clay, which were deposited by ancient courses of the ancestral Red River. Relief at LAAP is moderate with elevations varying from about 130 feet mean sea level (MSL) near Dorcheat Bayou to 80 feet MSL at Clarke Bayou.

The Joliet Army Ammunition Plant (JAAP) is located within the northern portion of the Central Lowlands physiographic province. This province is characterized by relatively flat topography and low relief. The most prominent topographic feature of JAAP is a fifty feet high glacial escarpment that trends north-south across the installation. The installation is drained by four streams; Grant Creek, Prairie Creek, Jordan Creek and Spoil Bank Creek. The L1 (Site L1, Group 61) area is drained by Prairie Creek which flows east to west across the southern portion of the site.

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## Regional Geology

Regionally, LAAP lies within the North Louisiana Syncline. This syncline, a subsurface structural feature, lies on the eastern limb of the Sabine Uplift and was formed by deformation of sediments during tectonic activity, which began approximately 225 million years ago (Paleozoic Era). The LAAP region is bounded to the east by the Monroe Uplift and to the west and north by the Sabine Uplift. Smaller local uplifts exist in the area and significantly modify the local structural geology (i.e., formation dip) and a groundwater flow regime in the vicinity.

Regionally, JAAP is located on a large structural high called the Kankakee Arch. This feature is located between the Michigan Basin to the northeast and the Illinois Basin to the south. Faulting in the area includes the Sandwich Fault Zone, which trends northwest-southeast through the eastern portion of JAAP. Structural contour maps indicate vertical displacement of the fault increases with depth and may locally affect groundwater flow.

## Site Function and Evolution

LAAP is a government owned, contractors operated facility located 22 miles east of Shreveport, Louisiana (Figures 1 and 2). The primary mission of the 14,974 acre plant was to load, assemble and package ammunition items, manufacture ammunition metal parts and provide associated support functions for ammunition production. Eight ammunition lines and one ammunition nitrate graining plant were constructed by the Silas Mason Company between July 1941 and May 1942. Production ceased in August 1945 at the conclusion of World War II. The plant was then placed on standby status in September 1945 and in November of 1945 the Federal Government relieved Silas Mason Company of responsibilities for the plant operations. In February 1951 with the outbreak of the Korean Conflict Remington Rand Corporation reactivated LAAP under contractual agreement with the federal government. Ammunition production was suspended in October 1957 and again the facility was placed on standby status. The federal government again reactivated the facility in September 1962 and contracted with Sperry Rand Corporation to operate the munitions production in support of the Vietnam Conflict. In 1974 Thiokol Corporation took over the facility operations when Sperry Rand Corporation relinquished its contract. Thiokol Corporation maintained the facility until the summer of 1996 when most operations at the plant ceased. As of August of 1997, five contractors were bidding to resume very limited production of black powder products at a single load line (Y line).

JAAP is a government owned, contractor-operated installation maintained in non producing conditions. The plant was constructed in the early 1940's in Will County, Illinois about 17 miles south of Joliet, and was used extensively during WWII. In August of 1945, all production of explosives of explosives was halted, the sulfuric acid and ammonium nitrate plants were leased out and the remaining productions' facilities were placed in layaway status. The explosive manufacturing area was reactivated between 1953 and 1957 during the Korean War and again between 1965 and 1969 for the Vietnam conflict. After 1969, production gradually decreased until is being stopped in 1977. Currently, various tracks of land in the 30,000 acre site are being returned to the Department of Interior as part of the National Tall Grasslands program. Additional tracts of

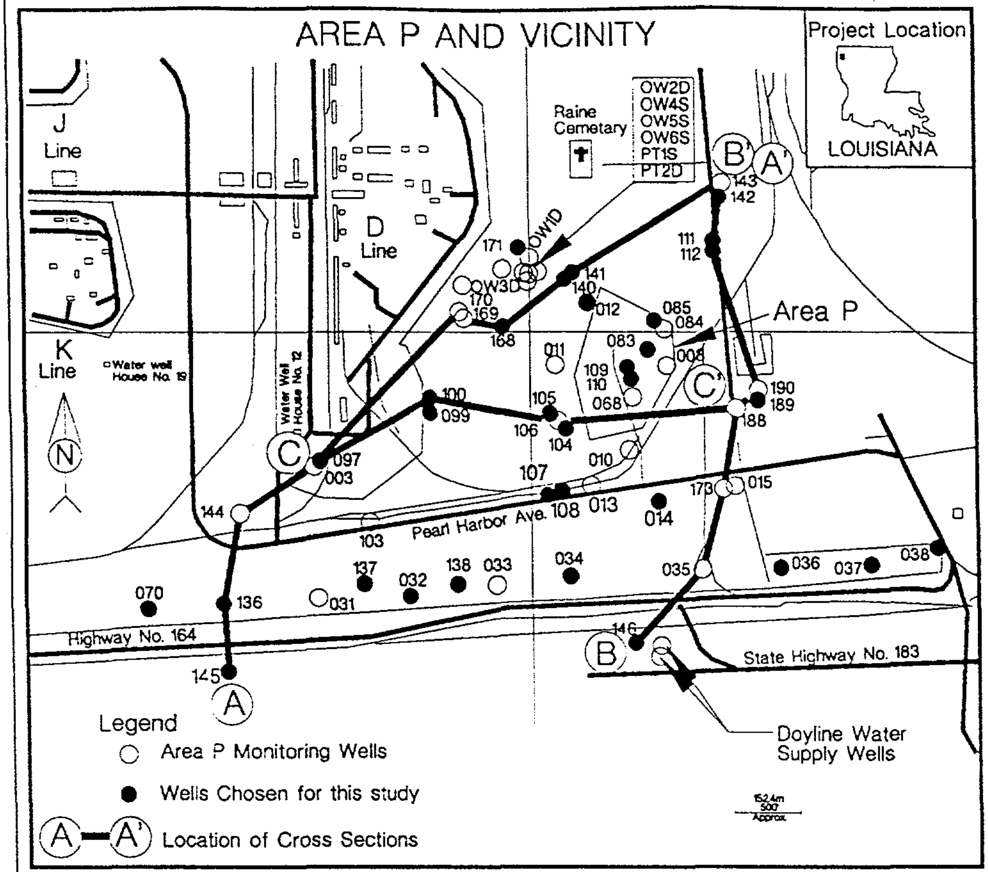

Figure 1. Louisiana Army Ammunition Plant - Area P and Vicinity.

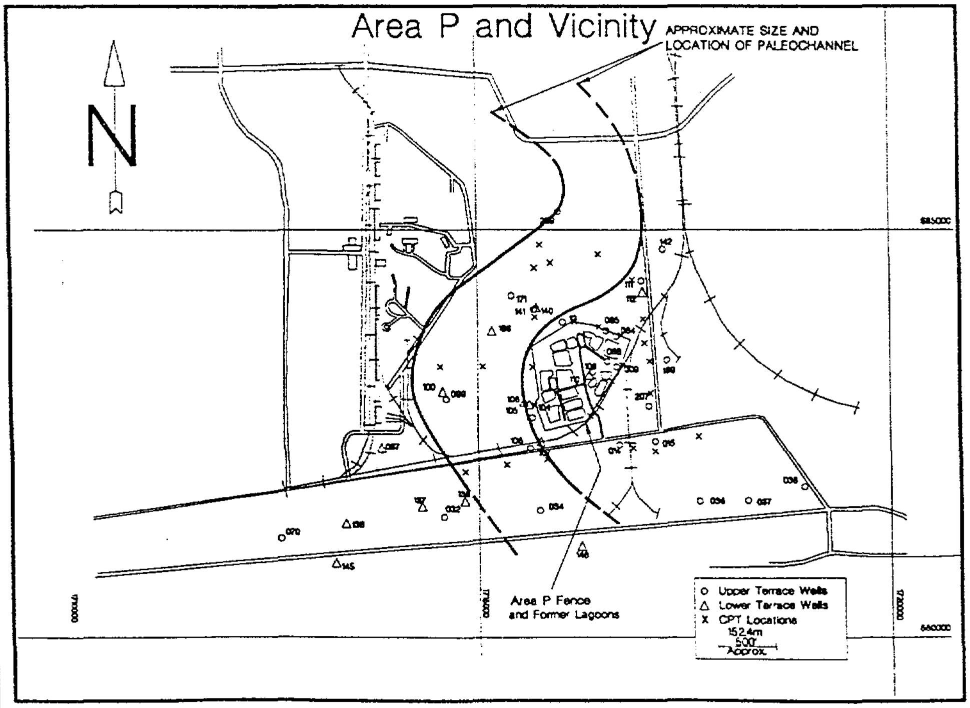

Figure 2. Location of former Area P Lagoons.

land are being returned to farming use. During the Installation Assessment and Installation Restoration Surveys, site conditions indicated the potential for contamination from past operations. Subsequent studies identified contamination in the ground water, surface water, soil and sediment at the LAP areas. The LAP area was placed on the National Priority List (NPL) and designated a Superfund site. In April of 1989, the LAP area of JAAP was placed on the Final NPL list. As part of a Remedial Investigation report by Dames and Moore (1993), some 35 specific study sites were identified in the LAP area.

## HISTORICAL CONTAMINANT DATA

### Site Geology

Historical geological reports (Louisiana Department of Conservation 1954, U.S. Geological Survey 1983, USACE Ft. Worth District 1984 and 1987; Engineering Technologies Associates (ETA) 1991; Science Applications International Corporation 1994; International Technology 1997) and cone penetrometer data gathered for the natural attenuation demonstration project (Pennington et. al., 1998) indicated that the shallow aquifers underlying LAAP consist of Pleistocene age terrace deposits unconformably overlying the Cane River Formation (Figures 3 through 5 ). The Terrace deposits in Area P are subdivided into the Lower Terrace consisting of fine sands and a trace of gravels, and the Upper Terrace consisting of very fine grained silts, clays and silty clays. An intermediate clay unit is present at some locations, is not uniform over the entire site, and is totally absent at many locations. However, the unit does serve as a limited aquitard as evidenced by the Paleochannel defined by the cone penetrometer (Figures 3 and 5). Collectively, these Pleistocene age units are a fining upwards sequence deposited during a waning glacial episode. The Eocene age, Cane River Formation consists primarily of clay or clay sufficiently indurated to be classified as a claystone. The Cane River Formation is not an aquifer beneath Area P, and is, therefore, considered the confining layer for modeling the site.

Ground water in the Upper Terrace aquifer generally exists under water-table (unconfined) conditions at depths varying from approximately 5 to 25 feet below sea level (BSL). The Lower Terrace aquifer, while not present in all areas, typically occurs from 25 feet BSL to the top of the Cane River, which is about 50 feet BSL. The Lower Terrace aquifer also tends to produce more water than the Upper Terrace deposits. Although none of the Terrace deposits supply water to production wells on the installation, some domestic wells in Haughton, Princeton, Dixie Inn, Minden, Sibley and Doyline are completed in the Terrace deposits. Ground water quality modeling conducted for Area P indicated that contaminants (explosives) migration in the Upper Terrace generally traveled downwards with little horizontal spreading (ETA 1991). Further, the modeling and water level measurements indicated that the regional groundwater flow in the Upper Terrace aquifer was southwest. Water level data collected for the Natural Attenuation demonstration project (Pennington, et. Al., 1998) indicated that the direction of ground water movement is in different directions in the Upper versus the Lower Terrace aquifers. The rate and direction of ground water movement are also influenced by the Paleochannel located on the western edge of Area P.

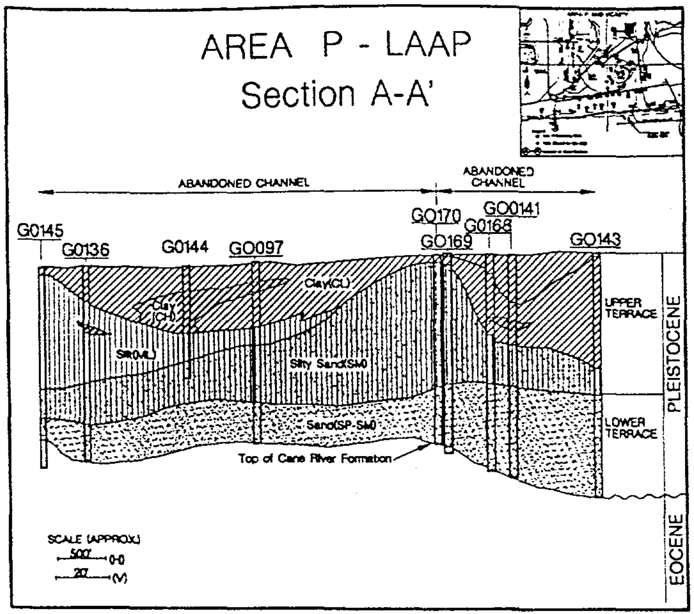

Figure 3. Area P Geologic Cross Section A-A'.

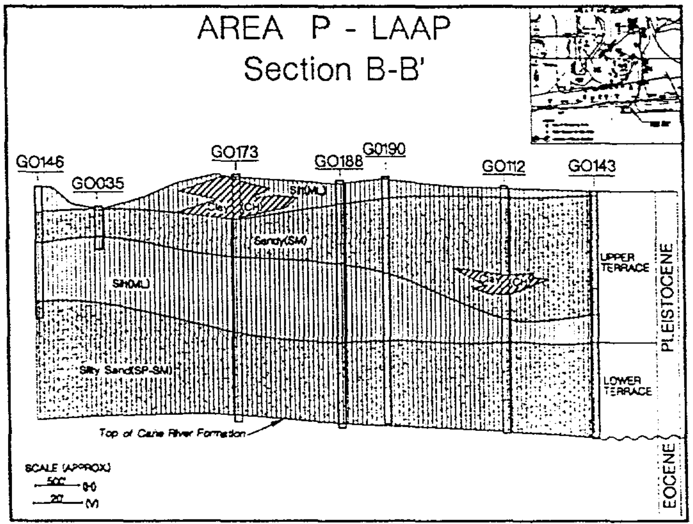

Figure 4. Area P Geologic Cross Section B-B'.

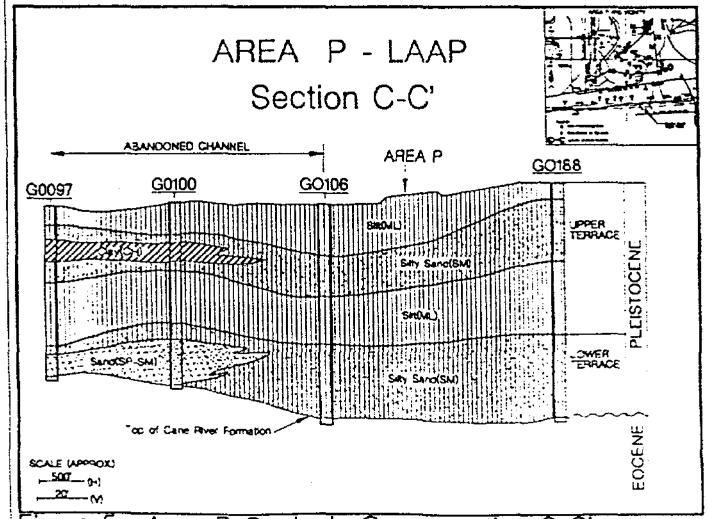

Figure 5. Area P Geologic Cross section C-C'.

The surficial soils at JAAP, Site L1, consist of glacial materials composed of very fine grained silts and clays and varying amounts of cobbles and boulders (Figures 6 through 7). These materials were deposited as outwash deposits during the waning stages of continental glaciation. The glacial materials lie unconformably on bedrock which consists of tan to greenish gray thinly bedded Silurian age dolomitic sandstone (Figure 8). This Sandstone is highly fractured and weathered near its contact with the overlying glacial deposits and has solution features in the upper portion of the section. In general the fractures and degree of weathering in the sandstone decrease with depth. Cone Penetrometer studies conducted in the summer of 1997 indicated a persistent clay layer (of glacial origins) underlies most of the L1 Site. The clay typically was first encountered at about 1.5 to 2.5 feet below ground level and generally was about 5 to 10 feet thick.

Ground water levels at LAAP are highest in late winter and lowest in the fall, which typical. Seasonal variations were slight, since low permeability precludes rapid movement or recharge. The direction of ground water movement is to the southwest in the lower Terrace and to the east possibly towards Dorcheat Bayou, in the upper Terrace.

Water level data from JAAP collected from May 1997 through January of 1998 and Dames and Moore (1993) indicates the shallow ground water in the glacial materials (overburden) and the Silurian age bedrock at L1 flows towards Prairie Creek. The hydraulic gradients vary from 0.03 for the glacial materials to 0.0007 for the bedrock. The water levels in the up dip areas of the site are about one meter higher than those near Prairie Creek, thereby suggesting a downward flow into the bedrock. Water levels from well completed near Prairie Creek suggest little downward movement and indicate ground water flows horizontally along permeable zones until it discharges into Prairie Creek.

Hydraulic conductivities for the L1 site are generally very low. A hydraulic conductivity of 9.2 x 10-6 cm/sec was reported for well MW-131 by Donohue & Associates, (1982). This well is completed in glacial till (overburden of Dames and Moore 1993) and conductivities for these materials are typically low. Conductivities in the bedrock are much higher. These higher conductivities are attributed to solution features in the upper portions of the bedrock. Using slug test data, Dames and More (1993) calculated a hydraulic conductivity of 4.9 x 10-4 cm/sec for the bedrock. Using these conductivities Dames and Moore (1993) estimated ground water flow velocities in the bedrock to be 35 feet/year and 16 feet/year for the glacial till. The approximate direction of ground water movement is to the southwest in the deep wells and southeast in the shallow wells.

## Cone Penetrometer Sampling Events

A Cone Penetrometer and Hydropunch sampling event was conducted at LAAP to support the Natural Attenuation research effort between September 9 and 29, 1996 (Figure 2). Soil samples were collected from 24 locations along eight transects. Penetrations were through the entire Upper and Lower Terrace sections. Generally, the penetrations were about 50 feet deep and reached total depth in the Cane River Formation. The locations were selected on the basis of ground water sampling data collected monthly during the previous six months. Additional data collected at the

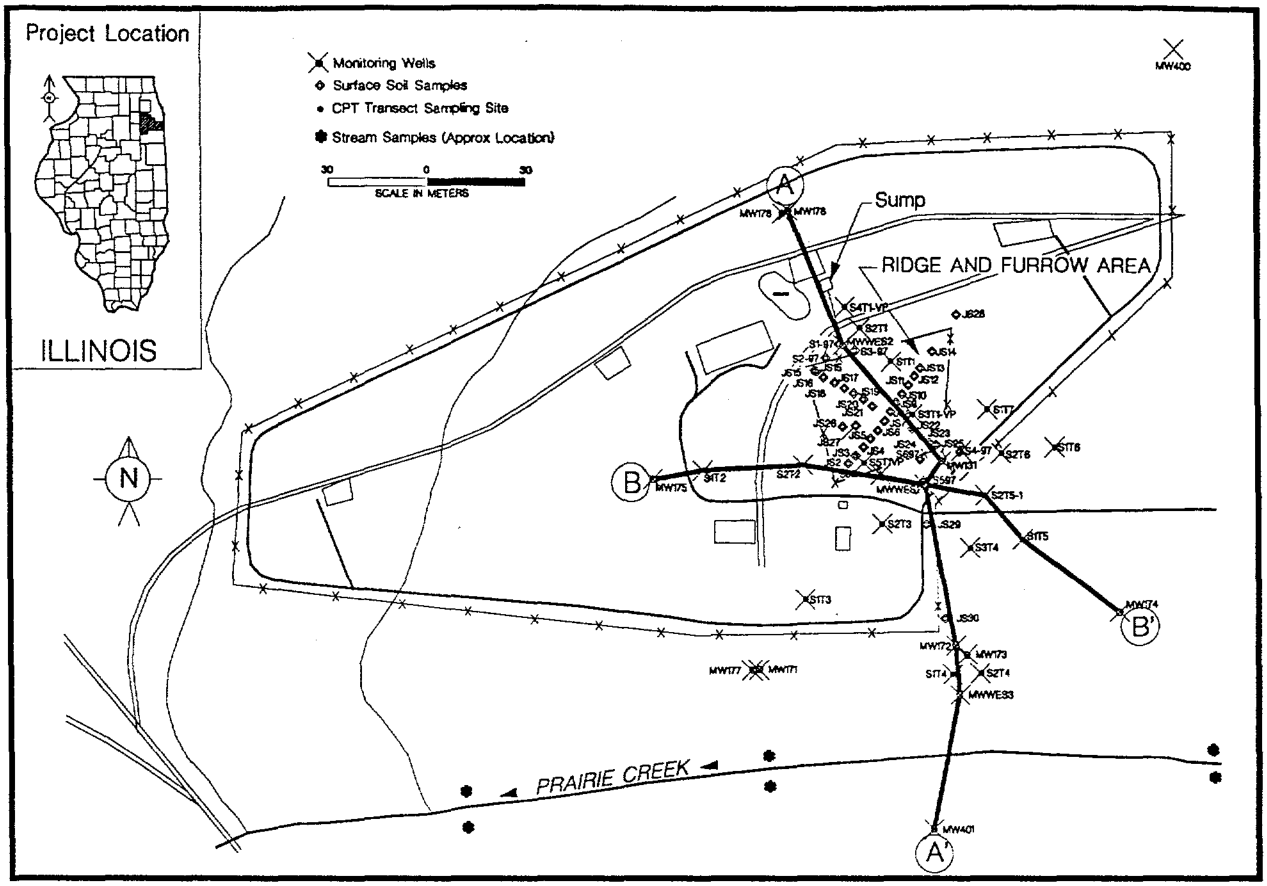

Figure 6. Locations of cross sections A-A' and B-B' at Site L1.

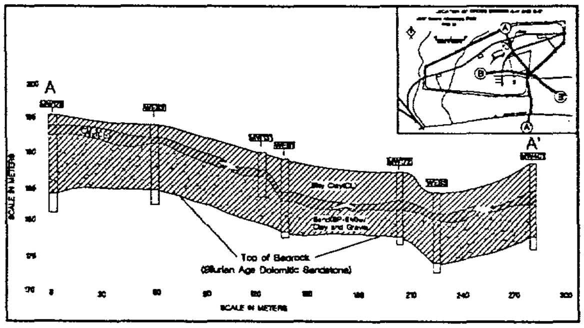

Figure 7. Cross Section A-A' illustrating general north to south subsurface lithology.

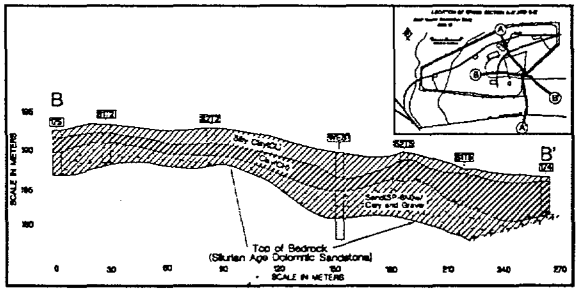

Figure 8. Cross Section B-B' illustrating general west to east subsurface lithology.

site (USACE, 1984) was utilized to stratify the various lithologies at Area P and assist in the location of the sampling sites for the 1996 events. TNT and RDX concentrations from previous ground water sampling were contoured to identify "hot spots" and potential source areas. Transects were located to assure sampling along a line extending from the zone of highest concentrations to a zone of zero concentration in all four cardinal directions from the source (original lagoons). A thin vertical slice of the soil obtained in the split spoon was removed and analyzed in the field for explosives (Jenkins, T.F., 1990). The remainder of the sample was retained for laboratory confirmation of explosives and additional research. Vertical profiles of soil were collected at five locations. Depending upon the depth of the CPT hole, samples from varying depths were collected at each location. These soil samples were used to measure vertical variations in permeability for the ground water model and for other research.

Analysis of existing geological information indicated the existence of a Pleistocene-aged paleochannel on the western edge of Area P (Figure 2). This paleochannel was first observed as a meander scar (abandoned channel ), visible in some of the earliest aerial photographs of the site. The dimensions of the paleochannel were defined by the CPT sampling in 1996. The paleochannel is at least 200 feet wide (400 feet at some locations), and 25 to 30 feet deep. The hydrogeologic effect of this feature is that the low permeability clays and silty clays in the paleochannel act as an aquitard that locally separates the Upper and Lower Terrace aquifers, thereby steering the contaminants to the Lower Terrace, which in this area, has higher permeability.

As part of the innovative technology approach to this research effort, a series of Cone Penetrometer punches were conducted at the JAAP, L1 Site in the summer of 1997 (Figure 6 ). The CPT work was conducted as a series of seven radial transects from monitoring well (MW 131). This well consistently had the highest concentrations of TNT and RDX in all rounds of sampling. At least two sites were punched to bedrock along these transects, with the objectives of further defining the geology of the L1 site , to delineate the contamination plume as defined in the Dames and Moore Phase I RI report, and to collect soil samples for the Stable Isotope and Biomarkers work. CPT stratigraphic data indicated a clay layer about 5 to 10 feet thick underlies most of the site. Further, analysis of soil samples collected at the various sites along the transects indicated most contamination was concentrated on top of the Clay layer as defined by the CPT and appeared to be restricted mainly in the Ridge and Furrow area.

Previous geohydrologic data largely from Remedial Investigations (RI) reports were used to determine the location for the CPT sampling transects at both sites. The transects were designed to sample along a line of highest explosive concentrations to a zone of zero or non-detectable concentrations in all four directions. The LAAP sampling event was conducted in September of 1996. Soil samples were collected from 24 locations along eight transects. Generally, the cone holes were about 50 feet deep and reached total depth (refusal) in the Tertiary Age, Cain River Formation. The location for the CPT transects were selected after review of existing RI data and ground water sampling data collected monthly during the first six months of the study. TNT and RDX concentrations from the first six months of data were contoured to determine "hot spots" and further refine the location of the LAAP CPT transects. The JAAP sampling event was conducted in June of 1997. Soil samples were collected from fourteen locations along seven transects. The CPT holes were about 20 feet deep, reaching refusal in the Silurian Age, Henry Formation. The locations for the JAAP's CPT transects were selected after ground water sampling for two months and a review of existing RI data. The JAAP transects were positioned to sample in a radial pattern out from Monitoring well MW-131. Well MW-131 had the highest concentrations of TNT and RDX and as at LAAP, the sampling preceded from areas of highest concentrations to area of zero concentrations (or non- detection values) in all four directions. This study has shown that the CPT is an effective tool for sampling both soil and water in varying geologic environments of deposition. CPT technology provides a cost-effective means of providing real-time data concerning the stratigraphy, resistivity and ground water contamination of a given site. Major advantages of the CPT include no soil cuttings, it eliminates the placement of unnecessary monitoring wells, permits ground water sampling from multiple aquifers and includes a self-contained decontamination system. The CPT transects coupled with vertical profile sampling, defined the lateral and vertical definition of the plume. Samples in excess of 300 grams were routinely recovered and furnished the lithologic data for the numerical modeling effort. The ground water modeling system (GMS) and its three-dimensional ground water model FEMWATER, was used to simulate flow and mass transport of TNT, RDX and related chemicals at the sites. Initial modeling runs for LAAP indicate that the TNT and RDX plumes are static and possibly slowly diminishing.

## NUMERICAL MODELING

Numerical modeling is the most cost effective means for the quantitative evaluation of multiple natural processes represented as a set of mathematical expressions, consistent with site-specific conceptualizations. The complex and incompletely understood processes involved in the natural attenuation of explosives require the computational power and flexibility of a numerical simulator. Defense of natural attenuation as a feasible remediation alternative under the scrutiny of regulatory entities necessitates the rigor afforded by numerical modeling.

The main objective of the modeling was to compliment the field monitoring and data collection for better demonstration and graphic representation of natural attenuation of explosives at LAAP and JAAP sites. The model application of JAAP is presented here; for model application of LAAP, the reader is referred to Pennington et al. (1998). The modeling effort focuses on conceptualization of the site hydrogeology and reduction of explosives by processes such as immobilization/ degradation, and first order decay.

The Department of Defense Groundwater Modeling System (GMS) (1966) with its subsurface model, FEMWATER (Lin et al. 1997), was selected for the modeling element of this study. GMS is a comprehensive computer graphical system. The GMS includes numerical tools to facilitate site characterization, site conceptualization, mesh and grid generation, geostatistical computations, and visualizations.

Subsurface conditions of Site L1 (JAAP, Figure 9) have been interpreted from the information provided in Dames and Moore, Inc. (1993) and cone penetrometer data collected by WES during 1997-1998. The descriptions given in the Dames and Moore report are based on review of lithologic logs of wells installed during the Phase 1 Remedial Investigation (Dames and Moore, Inc. 1993b) and previous hydrogeologic investigations.

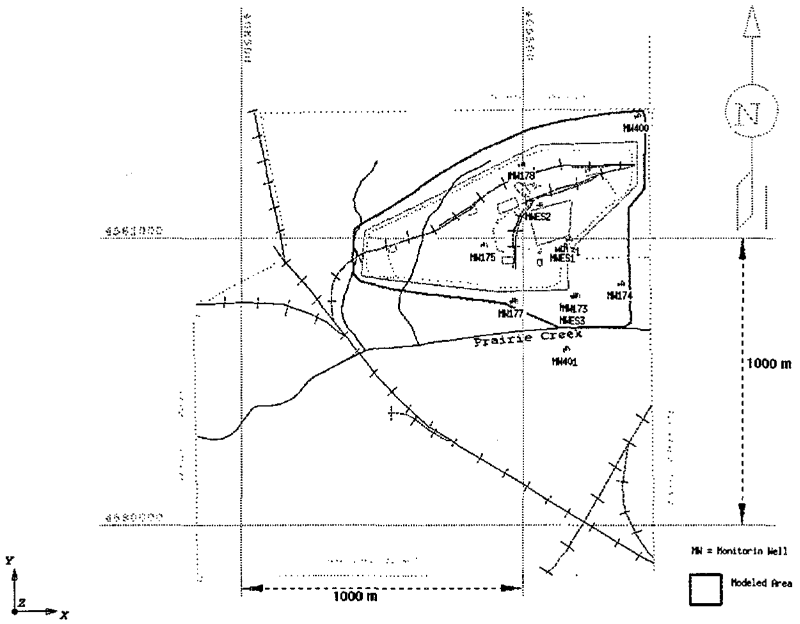

FIGURE 9. Schematic map of Site L1, Group 61 and surroundings (JAAP)

## Conceptual Model

Conceptual model is a powerful approach for abstracting and simplifying natural phenomena. To develop conceptual models for LAAP and JAAP sites, existing and new hydrogeological data including borehole geologic data (CPT data; Figure 10), hydraulic conductivity data and flow boundary conditions were used. Table 1 shows the hydraulic conductivity data of Site L1 (JAAP) used in the model.

The source of flow recharge at Site L1 was assumed to be from rainfall. Average annual precipitation is 32-35 inches. About 10-12 % of the annual precipitation is estimated to reach the groundwater reservoir in Illinois (Suter et al. 1959).

**TABLE 1** Hydraulic conductivity of the modeling layers

| **Layer No. from above (Figure 5-5)** | **cm $sec^{-1}$** | **ft $day^{-1}$** | **m $day^{-1}$** | **Material** |
|---|---|---|---|---|
| Layer 1 | 9.2E-06 | 0.026 | 0.008 | organic clay and silt |
| Layer 2 | 1.70E-03 | 4.82 | 1.469 | yellowish-brown clay and silt |
| Layer 3 | 1.7E-03 | 4.82 | 1.469 | clayey sand |
| Layer 4 | 4.90E-04 | 1.39 | 0.4234 | clayey gravel |

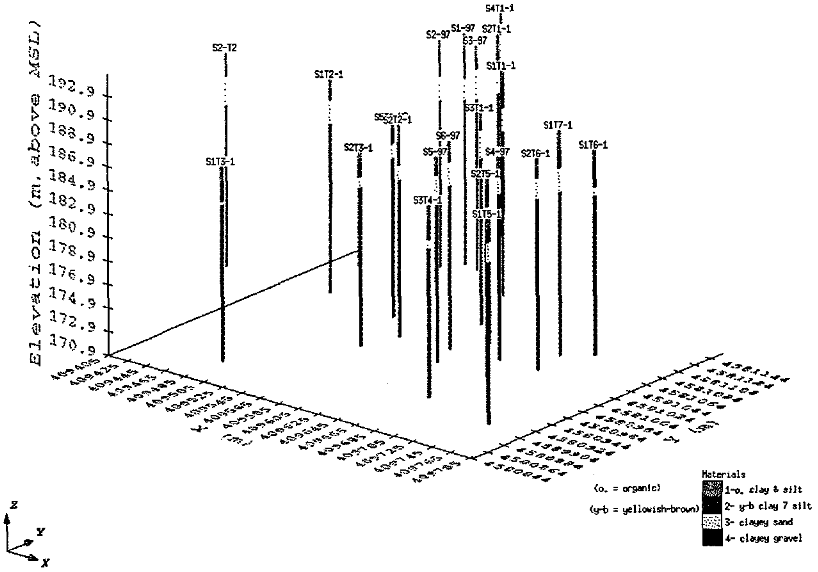

FIGURE 10. Cone Penetrometer data used in conceptualization of the Site L1 (JAAP)

## Code Description

FEMWATER (Lin et al. 1997) is a three-dimensional finite element numerical code, which may be used to model flow and mass transport through saturated-unsaturated media. FEMWATER is an enhanced version of two models, 3DFEMWATER (flow) and 3DLEWASTE (transport). FEMWATER is integrated into GMS. GMS is a state-of-the-art graphical computer interfaces program. The flow equations in FEMWATER are based on the continuity and Darcy flow equations. The model application is limited by the assumptions applied to these equations. FEMWATER also can be used for density-dependent problems.

FEMWATER simulates the primary processes affecting dissolved-phase contaminant distributions in groundwater including advection, dispersion, sorption, and decay caused by chemical reactions and/or biological transformation. FEMWATER uses the first-order decay as lumped biochemical decay.

## Model Construction

FEMWATER requires basic hydrogeologic and chemical data for simulations. These basic data include hydraulic conductivity, porosity, hydraulic gradient, initial and boundary conditions, distribution (partition) coefficients, and decay rates. The distribution coefficient, $K_{d,}$ relates the sorbate and solute for linear isotherms. Distribution coefficients for explosives have been determined (Pennington et al. 1998).

The modeling domain is defined in three dimensions (Figure 11). In plane view, the domain is bounded by Road 1 North, Chicago Road, and part of Prairie Creek (Figure 9). In the vertical direction, the modeling domain includes the shallow deposit of clay and silt, and the weathered bedrock (Figure 10).

The retardation factor is a function of both contaminant property ($K_d$) and soil ($\rho_B$,$\phi$,$S_w$) properties. The retardation factor provides a general indication of mobility of the contaminant in the soil. Tables 2 and 3 provides information on TNT and RDX adsorption coefficients and TNT, TNB and RDX first-order decay rates, respectively (Pennington et al. 1998). The decay rates given in Table 5-5 were determined from the laboratory batch studies on the Louisaina Army Ammunition Plant (LAAP) soils. The decay rate used in the model were $10^{-5}$ 1/day for TNT and TNB and $8.13\times10^{-6}$ 1/day for RDX, which were considerably lower than the batch rates. These decay rates were used based on the model calibration and fact that the field decay rates are normally lower than the batch rates.

**TABLE 2** Explosives adsorption coefficients ( $K_d$,L/Kg) for LAAP aquifer soils and regression coefficient ( $r^2$)

| | **ML Soil** | | **SP-SM Soil** | | **CL Soil** | | **SM Soil** | |
|---|---|---|---|---|---|---|---|---|
| **Contaminant** | $K_d$ | $r^2$ | $K_d$ | $r^2$ | $K_d$ | $r^2$ | $K_d$ | $r^2$ |
| TNT | 0.086 | 0.73 | 0.20 | 0.81 | 0.37 | 0.94 | 0.20 | 0.77 |
| RDX | 0.21 | 0.95 | 0.33 | 0.97 | 0.33 | 0.33 | 0.33 | 0.95 |

**TABLE 3** Explosives first order decay coefficient ( $K^{-1}$,hrs $^{-1}$) on LAAP aquifer soils and regression coefficient ( $r^2$)

| | **ML (Sandy Silt)** | | **SP-SM (Sandy Silt)** | | **CL (Lean Clay)** | | **SM (Silty Sand)** | |
|---|---|---|---|---|---|---|---|---|
| **Contaminant** | $K^{-1}$ | $r^2$ | $K^{-1}$ | $r^2$ | $K^{-1}$ | $r^2$ | $K^{-1}$ | $r^2$ |
| TNT | 0.0006 | 0.70 | 0.0006 | 0.83 | 0.0014 | 0.72 | 0.0007 | 0.78 |
| RDX | NS* | 0.06 | NS* | 0.0001 | 0.0003 | 0.39 | 0.00009 | 0.27 |
| TNB | 0.0006 | 0.83 | 0.0006 | 0.63 | 0.0027 | 0.74 | 0.0005 | 0.38 |

* NS = Not Significant

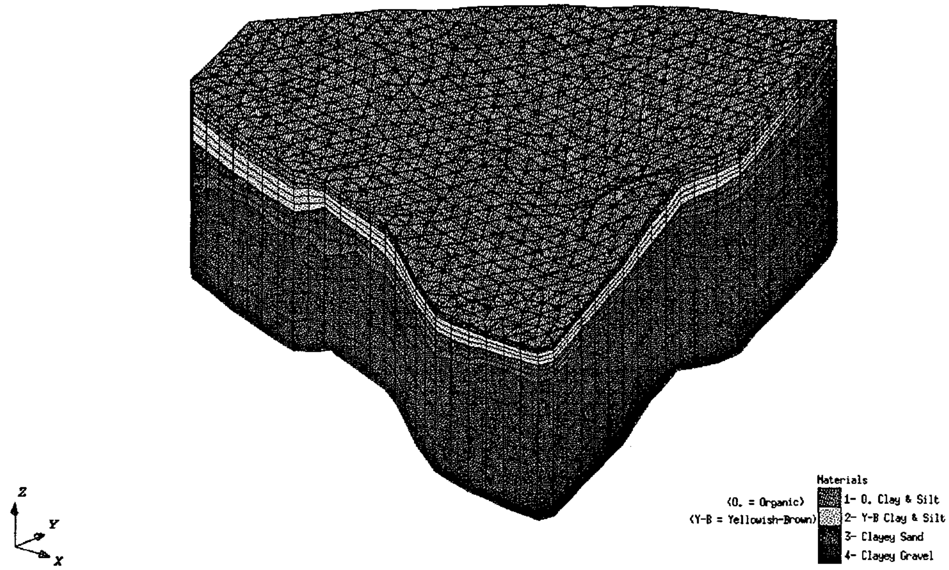

FIGURE 11. Three-dimensional mesh system used in FEMWATER for Site L1 (JAAP)

## Model Limitations

Major assumptions and limitations of FEMWATER include the following: (1) single constituent transport, thus inter-solute reactions can not be simulated, (2) abiotic and microbial degradation is treated with a first-order decay model, (3) adsorption coefficient and decay rates can be assigned for different subsurface materials; however, rate constants do not change during simulation time, (4) contaminant sorption is instantaneous and reversible and the adsorbed phase is in local equilibrium.

Some of the above assumptions may not be applicable to certain field problems. For this application, the above assumptions were applicable by simplifying some site characteristics required for the modeling without deviating much from actual site conditions. For more details, the reader is referred to FEMWATER model theory documentation (Lin et al. 1997).

## Contaminants and Initial Distributions

The modeling domain (JAAP) included the ridge-and-furrow system area. The modeling focused on the major contaminants, TNT and RDX.

Initial conditions of flow and chemical concentration play a major role in the model outcomes. Different numerical techniques available in GMS were compared to establish a realistic initial flow and mass concentration distributions at the site. The initial flow and concentration distribution of TNT and RDX were determined using monitoring well data collected in May 1997. The GMS was used to interpolate/extrapolate the data for all points of the numerical mesh system.

## Calibration

As described earlier, application of FEMWATER requires knowledge of the spatial distribution of hydraulic conductivity, porosity, boundary conditions, recharge rates, and contaminant concentration. The measurements of hydraulic conductivity are usually too few to fully characterize the heterogeneity of the aquifer and often involve errors and uncertainties. As a result, numerical flow models are often calibrated by adjusting values of hydraulic conductivity, boundary conditions, and recharge rates and their distribution so that a reasonable match between the simulated and measured hydraulic head is achieved in spite of possible measurement errors. The transport model is also calibrated by adjusting adsorption rates, decay rates, and dispersion parameters to obtain reasonable match between the observed and simulated concentration distribution.

The calibration process is often carried out by manual trial and error, which was the approach employed here. GMS version 2.0 used in this application has an option called Gages, which was used to compare simulated and measured results. This option has been replaced in GMS version 2.1 by a new option called Map Module. Figure 12 illustrates locations of gages (monitoring wells) used in the model calibration. Recently, automatic calibration (inverse) process has been investigated.

Figure 13 shows a comparison between the measured and simulated total head at the selected gage. The difference between the measured and simulated heads at these wells range from zero to about 0.5 meters which are reasonable in view of site heterogeneity. However, at a few locations the difference between measured and simulated are a few meters. The geologic deposits at the site vary from clays and silt deposits to gravelly sands in the outwash plain, which indicates a very heterogeneous system. The accuracy of the modeling results depends upon availability of detailed hydrogeologic data, particularly sufficient data of the hydraulic conductivity of discrete locations in the subsurface. In this application, only limited data were available, which made the calibration of head and concentration difficult. The results presented here, although with limited calibrations, reproduced the general trends and are acceptable within the model assumptions. The general trend of flow head (m) and velocity (m/day) distribution (Figure 14) showing that the horizontal groundwater flow is towards the Prairie Creek. With more data and calibration the differences between the observed and simulated results could be further reduced.

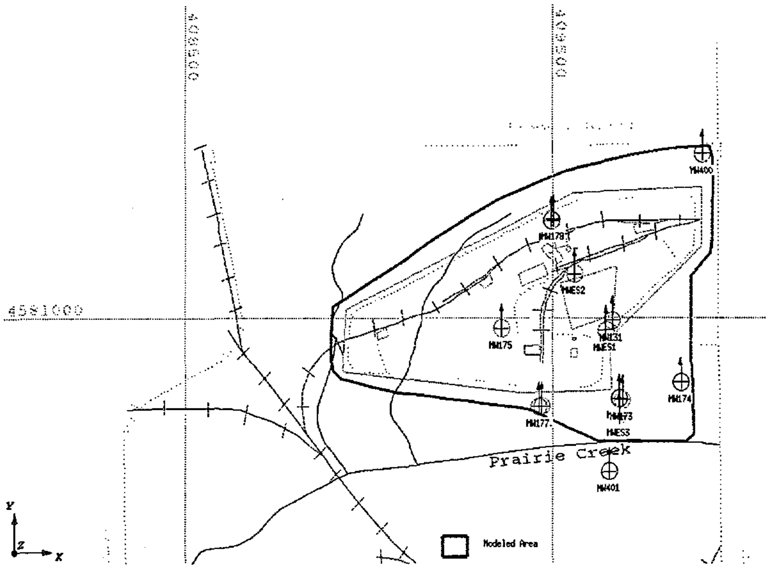

Figure 12. Location of monitoring wells (gages in GMS 2.0) screened in different aquifer layers

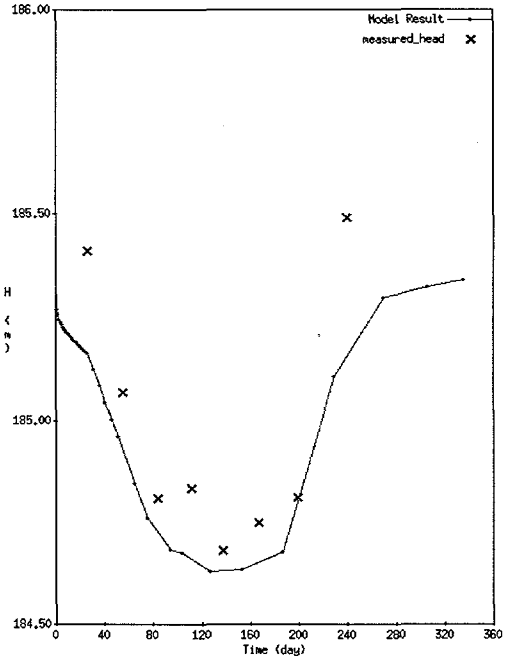

Figure 13. Comparison between measured, x, and simulated head, ---, (m, above MS) in MW177 tapped in the bedrock aquifer

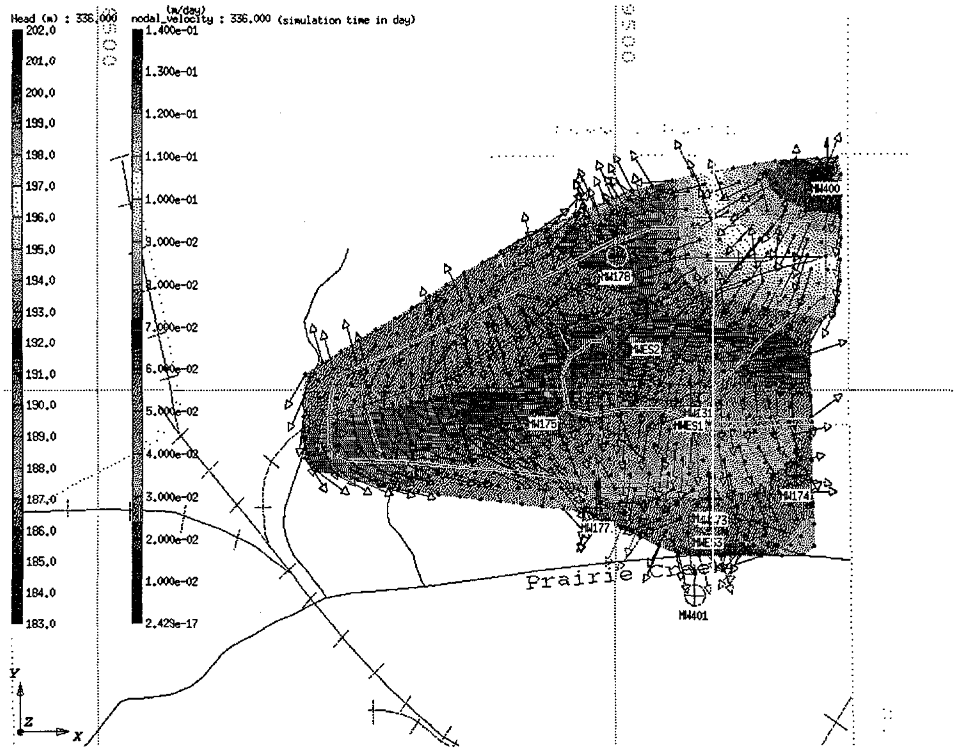

Figure 14. Simulated distribution of total head (m) and velocity at Site L1 (JAAP)

## Predictive Simulations

Prediction requires calculating future flow and transport conditioned on available historical data. The future boundary and other required model conditions are a mathematical statement of certain hypotheses, based on past experiences. The results presented here are based on the following assumptions: 1) no additional source of contamination is added into the site, 2) infiltration rate stays constant throughout the simulations, 3) flow boundary conditions recur every year, 4) no recharge or discharge through pumping occurs during the simulations. The predicated results should be updated and adjusted as new data become available. Jorgensen (1981) illustrates an iterative way in which a model predication may be improved as new information is obtained.

When comparing the simulation for twenty years to the initial conditions (May 1997), the TNT and RDX plumes are virtually static to diminishing (Figures 15 through 18). The reduction of TNT plume concentration is slightly higher than the RDX.

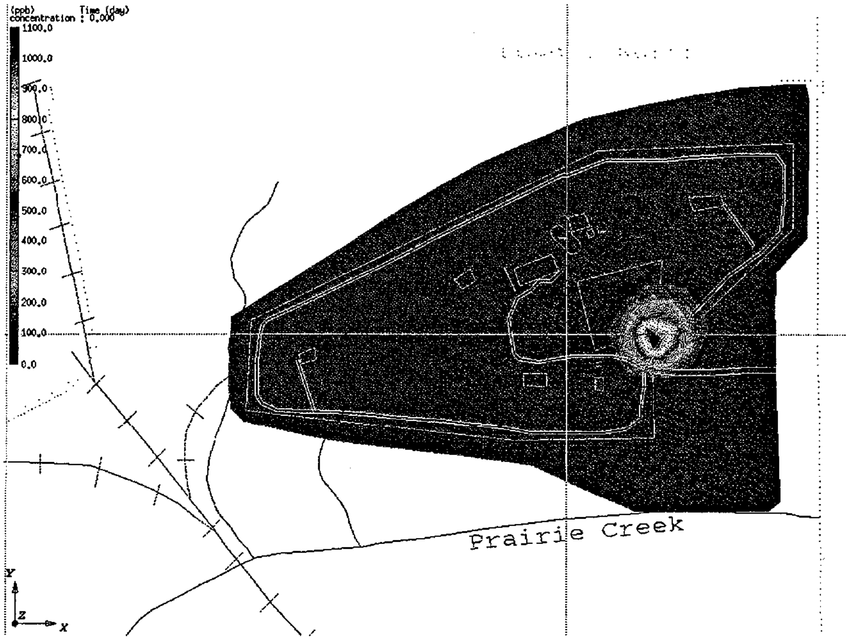

Figure 15. Initial (May 1997) distribution of TNT concentration at Site L1 (JAAP)

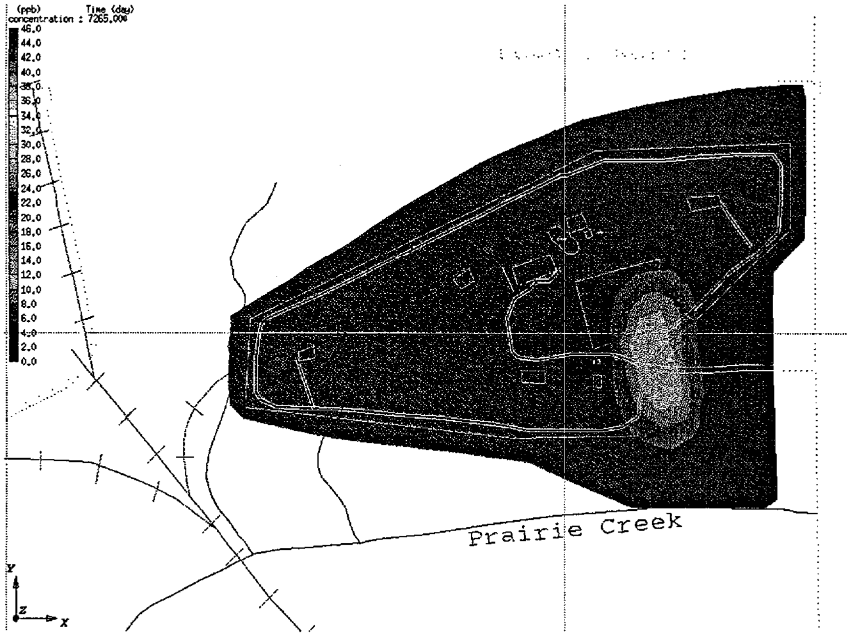

FIGURE 16. Predicted distribution of TNT plume after 20 years

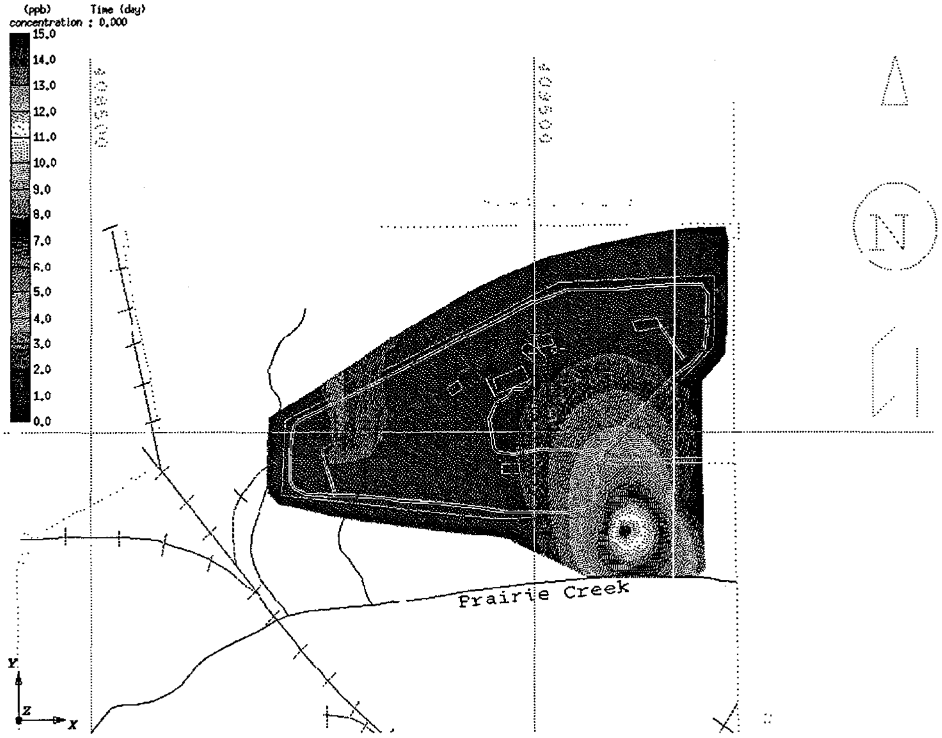

FIGURE 17. Initial (May 1997) distribution of RDX concentration

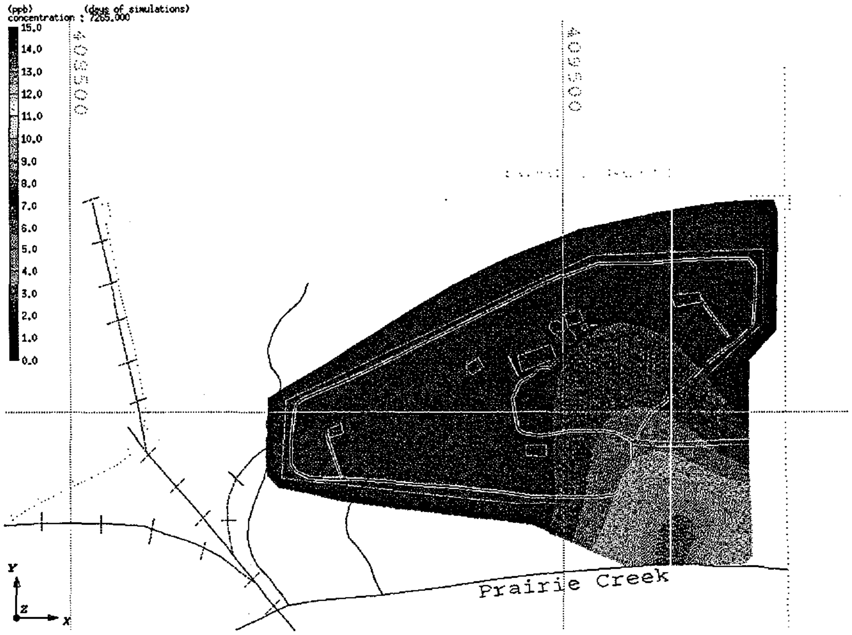

FIGURE 18. Predicted distribution of RDX concentration after 20 years

## SUMMARY AND CONCLUSION

CPT is a cost-effective means of providing real-time ground water contamination data. Important additional data that can be obtained simultaneously are stratigraphy and resistivity. Resistivity can be directly related to subsurface soil/aquifer material characteristics such as particle size distribution. These data are especially relevant for modeling of the site. Major advantages of the CPT include the generation of very little investigative derived waste (IDW). Because the CPT uses no drilling fluids (drilling mud) and pushes into the soil rather than drilling, no drill cuttings (soils) or drilling mud is generated. The CPT can also eliminate the placement of unnecessary monitoring wells, permit ground water sampling from multiple aquifers, includes a self-contained decontamination system and provides a mechanism for repeated sampling at a given location . Collection of CPT samples along transects and within vertical profiles can define the lateral and vertical extent of the contaminant plume(s). Soil samples up to approximately 300 grams are routinely recovered with the split spoon sampler. The samples furnished lithological data for the numerical modeling and samples for additional research.

Disadvantages of CPT sampling are the great size and weight of the truck ( i.e. 50,000 pounds), which can create handling and maneuvering problems in soft or muddy soils. Further, the limitation of current sampling tools is that only unconsolidated materials can be sampled . Existing site data can be used for more efficient placement of CPT sampling points and monitoring wells. CPT transects (oriented in all four directions) may be sufficient if a reasonable amount of geologic and analytical data exists. If only a small amount of data are available, CPT transects oriented radially from a "hot spot", or known source is advisable. Sample spacing is also dependent upon the available data, but typically can be several hundred feet or much more if sufficient data exist. At LAAP, the initial spacing was about 600 feet, with additional penetrations as needed. Once the plume is defined in all four directions, profile samples can be collected at strategic sites. This data coupled with the line or transect samples can effectively define the horizontal and vertical extent of the explosive plume.

The CPT also provided samples for microbiological studies and stratigraphic analysis of lithologies for the numerical modeling effort at both sites. Numerical modeling was initiated to support the natural attenuation research effort at both LAAP and JAAP. The main objective of the modeling work was to assist field monitoring and data collection for a better demonstration and graphic representation of natural attenuation of explosives. The effort focused on characterization of the site's geohydrology and the reduction of explosives by processes such as immobilization/degradation and first order decay. To facilitate the use of the existing ground water models, a comprehensive graphic package call the Ground Water Modeling System (GMS) has been developed.

The subsurface at Site L1 consists of two aquifer systems; the shallow overburden aquifer and the deep dolomite bedrock aquifer. The bedrock aquifer has fractures and solution cavities (Dames and Moore, Inc. 1993). Flow through conduits does not obey Darcy's Law, upon which the model was based. Groundwater flow through fractured media can be much faster and follows preferential pathways compared to flow in porous media. The calculations presented here are based on the assumption that the bedrock behaves as a porous medium.

The geologic deposits at the site vary from clays and silt deposits to gravelly sands in the outwash plain, which indicates a very heterogeneous system. The accuracy of the modeling results depends upon availability of detailed hydrogeologic data, particularly sufficient data of the hydraulic conductivity of discrete locations in the subsurface.

The measured and simulated flow data indicate slow subsurface flow at Site L1 due to the low permeability media and hydraulic gradients. The groundwater flows toward Prairie Creek. The shallow groundwater discharges into Prairie Creek.

The simulated concentrations of TNT and RDX indicate static and diminishing plumes. The reduction rate of RDX plume is lower than the rates for TNT plume.

The results presented here are bounded within the assumptions and limitations of the selected model. The model approximately simulated the general behavior of flow and the plume at the site. The predicated results should be adjusted and the calibration processes should be repeated as new data become available.

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# DESIGNING
# AN EFFECTIVE GROUND WATER MONITORING SYSTEM IN GLACIAL SETTINGS

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## ABSTRACT

Choosing a suitable groundwater monitoring zone in a sequence of glacial deposits is often complicated by the difficulty in determining which sand-and-gravel bodies are discontinuous and which are sufficiently continuous to constitute a preferential contaminant pathway. Upland glacial settings in the Midwestern United States are typically underlain by a sequence of fine-grained glacial sediments deposited by successive glacial advances. Stratified sand and gravels may occur at various stratigraphic positions within this fine-grained succession, depending on the history of glacial advances and on the resultant changes in depositional environments. Laterally extensive sand-and-gravel units, which constitute rational groundwater monitoring zones, are most likely to occur *between* the deposits of different glacial advances because this is the setting where widespread outwash deposition can take place; other sand-and-gravel units within the sequence tend to be discontinuous. The key to determining a suitable groundwater monitoring zone thus depends on the ability to determine the boundary between different glacial advances in these successions of primarily fine-grained deposits. Unfortunately, use of the Unified Soil Classification System (USCS) as the means for classifying and differentiating fine-grained units in glacial settings is often inadequate because different fine-grained stratigraphic units typically classify as the same in the USCS. Other properties must be recognized and described to provide suitable information for recognizing and correlating fine-grained glacial stratigraphic units, including sedimentary structure and secondary weathering zone properties. In certain situations, it may be important to select a drilling method that provides adequate sample recovery and high quality samples. This paper presents the results of two case studies, one in central Illinois, and one in northeastern Illinois, where correct understanding of groundwater flow conditions and selection of a site groundwater monitoring zone depended on identifying stratigraphic units in a succession of fine-grained glacial deposits.

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## INTRODUCTION

Glacial depositional environments are among the most complex in nature, involving deposition from ice and water in various subglacial, englacial, supraglacial, and proglacial environments (e.g., Menzies, ed., 1995). Couple this complexity of a single ice advance, with the facts that many sites are underlain by a succession from *multiple* glacial advances and that post-depositional weathering may have affected different parts of the succession, and successful site hydrogeologic characterization can be an extremely daunting task. Determination of potential contaminant pathways, i.e., whether a particular sand body within the succession is an isolated lens or a continuous monitorable unit beneath a site can only be satisfactorily determined by recognizing and understanding stratigraphic units within the sequence.

## ADVANCES IN IMPROVING HYDROGEOLOGIC SITE CHARACTERIZATION

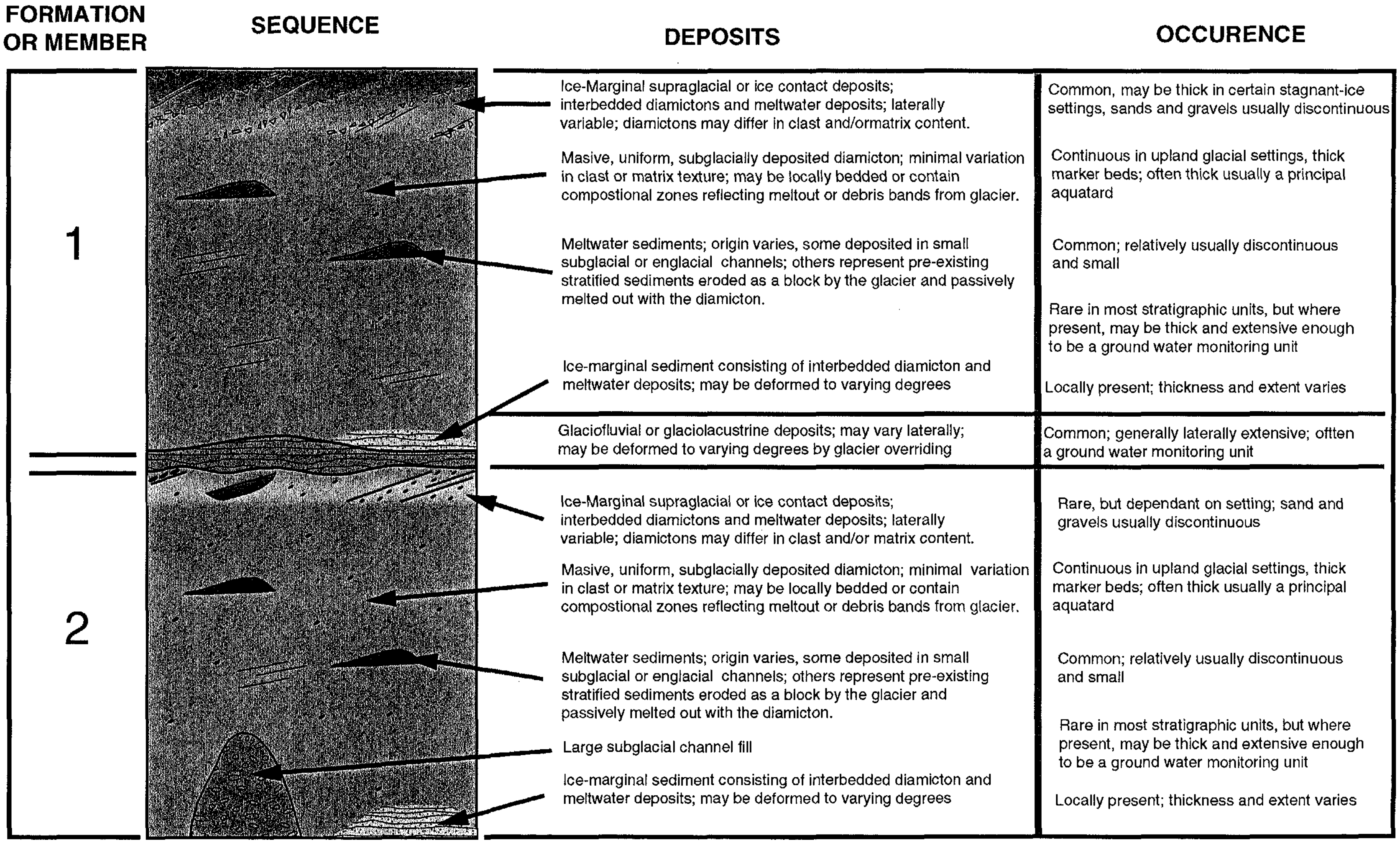
The Unified Soil Classification System (USCS) has been of limited success in adequately characterizing site hydrogeology because different fine-grained stratigraphic units commonly have similar USCS classifications and consequently, differentiation can often not be made on the basis of USCS classification alone. Adequate descriptions for recognizing glacial stratigraphic units need additional information to supplement the USCS, including description of sediment type and structure and description of secondary weathering properties.

### Soil Classification vs. Stratigraphic Differentiation

The standard practice in the environmental industry today is to use the USCS soil classification as the basis for stratigraphic differentiation and correlation. Certainly standard sediment descriptions using the USCS provide information about particle-size and plasticity-related properties, however, critical information for differentiating and correlating stratigraphic units is often not possible using the USCS alone. For example, nearly all of the fine-grained deposits in northeastern Illinois, including loess, most of the till members and formations, and many of the lacustrine deposits, classify as Lean Clay (CL) in the USCS, despite the fact that they differ in origin, lateral variability, associated sediment types, and in geotechnical properties such as particle-size distribution, soil density, consolidation, unconfined compressive strength, shear strength, and hydraulic conductivity (Kelleher, 1997). It cannot be over emphasized that *soil classification* using the USCS is not the same as *stratigraphic differentiation* of the deposits.

### Developing the Site Stratigraphic Framework

Development of the site stratigraphic framework in glaciated upland settings can be improved by recognition of the "key beds" that occur within the glacial sequence and then relating the other deposits in the sequence to these bed. The key beds are the relatively uniform subglacial diamicton deposits which occur in the sequence (Figure 1).



| FORMATION OR MEMBER | DEPOSITS | OCCURENCE |
|---|---|---|
| 1 | Ice-Marginal supraglacial or ice contact deposits; interbedded diamictons and meltwater deposits; laterally variable; diamictons may differ in clast and/ormatrix content. | Common, may be thick in certain stagnant-ice settings, sands and gravels usually discontinuous |
| | Masive, uniform, subglacially deposited diamicton; minimal variation in clast or matrix texture; may be locally bedded or contain compostional zones reflecting meltout or debris bands from glacier. | Continuous in upland glacial settings, thick marker beds; often thick usually a principal aquatard |
| | Meltwater sediments; origin varies, some deposited in small subglacial or englacial channels; others represent pre-existing stratified sediments eroded as a block by the glacier and passively melted out with the diamicton. | Common; relatively usually discontinuous and small |
| | | Rare in most stratigraphic units, but where present, may be thick and extensive enough to be a ground water monitoring unit |
| | Ice-marginal sediment consisting of interbedded diamicton and meltwater deposits; may be deformed to varying degrees | Locally present; thickness and extent varies |
| | Glaciofluvial or glaciolacustrine deposits; may vary laterally; may be deformed to varying degrees by glacier overriding | Common; generally laterally extensive; oftten a ground water monitoring unit |
| 2 | Ice-Marginal supraglacial or ice contact deposits; interbedded diamictons and meltwater deposits; laterally variable; diamictons may differ in clast and/or matrix content. | Rare, but dependant on setting; sand and gravels usually discontinuous |
| | Masive, uniform, subglacially deposited diamicton; minimal variation in clast or matrix texture; may be locally bedded or contain compostional zones reflecting meltout or debris bands from glacier. | Continuous in upland glacial settings, thick marker beds; often thick usually a principal aquatard |
| | Meltwater sediments; origin varies, some deposited in small subglacial or englacial channels; others represent pre-existing stratified sediments eroded as a block by the glacier and passively melted out with the diamicton. | Common; relatively usually discontinuous and small |
| | Large subglacial channel fill | Rare in most stratigraphic units, but where present, may be thick and extensive enough to be a ground water monitoring unit |
| | Ice-marginal sediment consisting of interbedded diamicton and meltwater deposits; may be deformed to varying degrees | Locally present; thickness and extent varies |

FIGURE 1 Hypothetical components of a succession from two glacial advances in the Midwest (Kemmis, 1997).

Glacial stratigraphic units in the Midwestern United States are usually well defined by the state geological surveys and published information is often readily available. It should be noted that Midwestern glacial stratigraphy is primarily defined by the relatively homogeneous diamicton units that are mappable over a widespread area. Localized variability within these diamicton units is usually related to variation caused by changing depositional environments.

Figure 1 shows the hypothetical components of a succession from two glacial advances in the Midwest. This succession is dominated by fine-grained diamicton deposits. Glacial stratigraphic units within this succession may often be differentiated in the field on the basis of changes in the texture of massive diamicton facies and changes in weathering zones. Deposits of different environments within these units can be often be recognized by evaluating sedimentary structures and sedimentary assemblages. Stratified sediment *within* a diamicton unit rarely has significant lateral extent unless it fills a relatively large channel, and most lenses or interbeds are discontinuous. Laterally extensive stratified sediment, which may be a potential contaminant pathway and constitute a viable groundwater monitoring zone, is most likely to be encountered between the deposits of successive glacial advances where proglacial outwash or lacustrine environments were possible. The following two case studies illustrate the importance of accurately determining site stratigraphy in the hydrogeologic characterization of a sequence of fine-grained glacial deposits.

## CASE STUDY 1
## CENTRAL ILLINOIS SITE

To be useful for most hydrogeologic site investigations, the USCS needs to be supplemented with description of the properties necessary to identify site stratigraphic units and depositional environments, including primary sedimentary structure, stratigraphic contact relationships, and weathering zones (oxidation state and carbonate status). Figure 2 shows an example from central Illinois of a site underlain by a succession of pre-Illinoian, Illinoian, and Wisconsinan sediments. The initial site characterization and unit correlation were made using the USCS alone. Figure 3 depicts the stratigraphy of the same site based on a later field investigation that included description of sediment structure, stratigraphic contact relationships, and weathering zones (oxidation state and carbonate status). Some partially saturated sand lenses (not shown) occur within the two thick stratigraphic units classified as lean clays, CL, on Figure 3 (the Radnor and underlying Vandalia Till Members, respectively).

Previous reports that based site stratigraphic correlation on USCS soil classifications did not adequately characterize the sand lenses within the confining unit. As a result, an erroneous potentiometric surface map was constructed using the mistaken assumption that the sand lenses were continuous and in direct hydraulic connection. It was later determined, based on stratigraphic and hydrogeologic information from the later field investigation, that the sand lenses occurred *within* the lean clay diamicton units, and were discontinuous and encapsulated within Radnor or Vandalia Till Members, thus explaining the erroneous potentiometric surface map. Successful site characterization thus depended on accurate determination of site-stratigraphic units using greater information than that provided by USCS classification alone, and resulted in assessment of the isolated or continuous nature of the buried sand bodies in the fine-grained glacial diamicton succession, preparation of accurate potentiometric surface maps, and construction of accurate site cross sections.

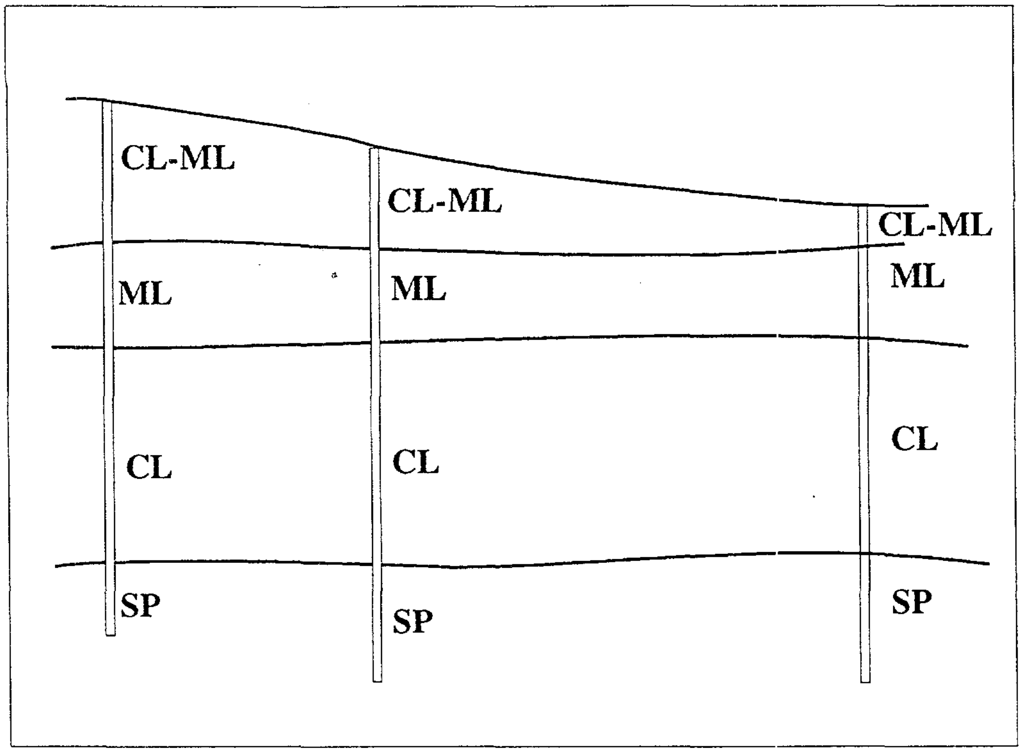


FIGURE 2 Example from central Illinois of initial site characterization using the USCS as the basis for unit correlation.

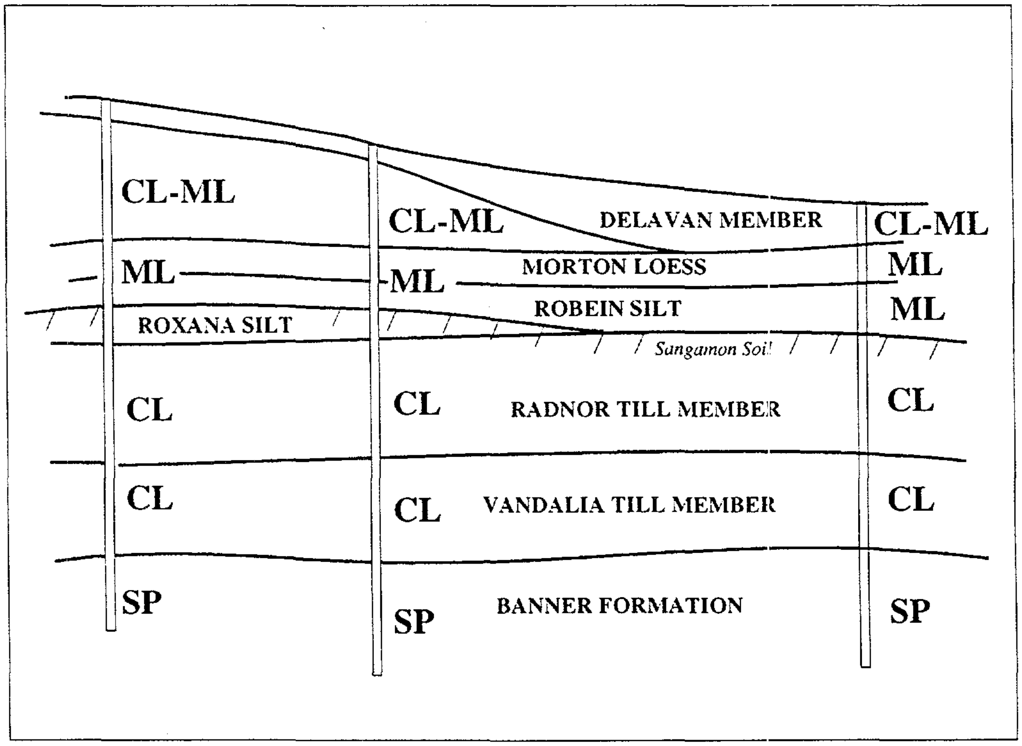


FIGURE 3 Same site based on a later field investigation that differentiated stratigraphic units. Some partially saturated sand lenses (not shown) occur *within* the two till stratigraphic units.

# CASE STUDY 2
# FERMI NATIONAL ACCELERATOR LABORATORY, NORTHEASTERN ILLINOIS

The importance of differentiating fine-grained glacial stratigraphic units in site hydrogeolgic characterization can be illustrated from an investigation at the Fermi National Accelerator Laboratory facility. The site had previously been characterized as being underlain by a thick clayey glacial till about 65 feet thick which overlay Silurian-age bedrock. Piezometers had been installed in "sand-and-gravel" deposits within the glacial till sequence that occurred at approximately the same elevation. Many of these piezometers were dry or of such low yield as to be useless as groundwater monitoring wells. The objective of later study was to refine the pre-existing stratigraphic and hydrogeologic framework of the glacial deposits, re-evaluate a sand-and-gravel unit that was reportedly non-water yielding, and install ground water monitoring wells. The tasks used to achieve these objectives included:

- Using rotasonic drilling and sampling techniques to obtain high quality samples.
- Comprehensively describing the Quaternary deposits to identify each glacial stratigraphic unit.
- Installation of shallow piezometers in the glacial deposits and deep piezometers in the Silurian-age bedrock.
- Determination of the horizontal hydraulic conductivity (by variable head testing) of screened units beneath the site and vertical hydraulic conductivities by laboratory permeability testing.
- Determination of the confining potential of the glacial deposits and the vertical hydraulic gradient between the glacial deposits and the Silurian-age bedrock aquifer.
- Determination of the ground water flow direction and velocity in the uppermost aquifer at the site, the Silurian-age dolomite.
- Installation of down gradient ground water monitoring wells.

The site was determined to be underlain by a succession of fine-grained deposits which differ in lithologic, textural, and hydrogeologic properties. A thin loess, the Peoria Silt, mantles approximately 60 feet of Lemont Formation glacial deposits that consists of two members, the Yorkville and the underlying Batestown members. The Yorkville Member may be subdivided into a vertical succession of four informal facies related to separate glacial advances. The uppermost unit is a ice-marginal facies that is successively underlain by sheet-like diamicton units informally referred to as Facies A, B, and C. The ice-marginal facies, deposited as the glacier retreated from the area, consists of fine-grained stratified diamicton and interbedded sorted sediments (silt, sand, and gravel lenses). Yorkville Member Facies A, B, and C are all massive, uniform, diamictons that classify as lean clays (CL) in the USCS, but are interpreted to be subglacial tills deposited by 3 successive glacial advances across the area. Facies A is a fine-grained lean clay with few small pebbles which contrasts with underlying Facies B that is a very gravelly lean clay. Facies C differs in being a thick, very clay-rich lean clay.

The Yorkville Member stratigraphic units are underlain by the Batestown Member, a very gravelly lean clay or sandy lean clay which is typically about 8 feet thick and directly overlies bedrock.

Based on stratigraphic and hydrogeologic information from this field investigation, the geologic framework was refined which provided information about the low-yielding "sand and gravel" unit, determine the confining potential of the glacial deposits and understanding the distribution of vertical hydraulic conductivity values.

Rotary sonic drilling techniques were very effective for characterizing these glacial stratigraphic units because the relatively large diameter continuous cores (4.5 inches) yielded high recovery rates. Two of the fine-grained diamicton stratigraphic units, Facies B of the Yorkville Member and the Batestown Member, contained clasts that were commonly greater than 3 inches in diameter. Poor sample recovery and split spoon refusal in previous studies probably resulted because of the large clast size in these units and the erroneous reporting of "sand-and-gravel" deposits in what actually were non-water yielding gravelly lean clays. This study again illustrates the importance of adequate stratigraphic characterization for understanding site hydrogeology in fine-grained glacial sequences.

## SUMMARY

Successful site characterization of fine-grained glacial successions depends on accurate evaluation of site stratigraphic units and depositional environments. The Unified Soil Classification System is satisfactory for classifying sediments, but is usually inadequate for differentiating the stratigraphic units that are critical for characterizing site hydrogeology. USCS descriptions need to be supplemented with additional information, including sedimentary structure, stratigraphic contact relationships, and weathering zone information (oxidation state and carbonate status).

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# INTEGRATED APPLICATION OF FORENSIC GEOCHEMISTRY

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## ABSTRACT

Forensic geochemistry is the knowledgeable application of information regarding chemical speciation, reactions, relationships, and fate and transport characteristics to resolve or gain insight into questions related to the presence of contaminants in the natural environment. It is often employed in support of litigation or in resolving disputes between multiple parties. It is also used to help guide the collection and interpretation of site investigation data. The three main arenas of forensic geochemistry are 1) fingerprinting releases, 2) dating releases, and 3) documenting natural attenuation processes. Though success has been varied, usage of forensic geochemistry techniques is expected to increase in importance for petroleum hydrocarbons and chlorinated halogenated hydrocarbons as demonstrated by the case histories provided.

## INTRODUCTION

In evaluating a contaminated site many questions may need to be addressed. Answers to these questions not only help guide the investigation but they often play a major role in securing closure for sites as well as settling disputes that may arise. Some of the basic questions are:

- Whose release is it?
- What compounds constitute the release?
- What is the source?
- When did it happen?
- Where is the source?
- How did it get here?
- Is it going away?

The answer to many aspects of these questions can be found in the application of forensic investigative techniques to the chemical and geochemical nature of the contaminant and the impacted site.

### What is forensic chemistry/geochemistry?

Forensic geochemistry is the application of knowledge of chemical speciation, reactions, relationships and fate and transport characteristics to resolve or gain insight into questions related to the presence of contaminants in the natural environment.

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Forensic geochemistry is used in three major activities:

- Fingerprinting of releases
- Age-dating of releases, and
- Documenting natural attenuation and/or biodegradation

## Fingerprinting

Fingerprinting, as it is often called, deals with establishing a unique identifying signature or "fingerprint" of a chemical compound or a mixture of compounds that can be used to identify and distinguish it from other compounds or constituents that may be present. Fingerprinting can take many forms and involve a number of different techniques. Of primary importance is ensuring that the most appropriate analytical method is used. Most methods typically used for screening purposes do not provide the detail needed to unambiguously characterize the true nature of a release. These methods often report results as a total of a certain type or class of compounds such as total petroleum hydrocarbons (TPH), or total volatile organic compounds (VOC). Sufficient analytical information must be obtained and provided to permit one to identify the specific component, or association of components to uniquely characterize the release.

## Age-dating

Age dating a release through the use of forensic geochemistry typically can involve any one or a combination of techniques. The presence or absence of a compound known only to exist or be used within a certain time period can be used to date a release as having occurred either prior to or after that time period. Isotopic dating of elements present can also be used help date a release or identify releases of different sources. Typical isotopes used include carbon, lead, and chloride. Finally, understanding degradation behavior of compounds as well as their transport characteristics can be used to assess the amount of time a compound has been present in the environment if the source area and current distribution of the compound are sufficiently assessed and identified.

## Documentation of natural attenuation

Recognition that many hazardous compounds degrade into less harmless byproducts or naturally bind to or incorporate into native materials in such a way that they no longer pose any threat to the environment has lead to the increasing acceptance of natural attenuation as an acceptable remedial alternative for impacted sites. Critical to this acceptance is the ability to document that the natural processes are indeed taking place and that the hazardous compounds are in fact being transformed, degraded, attenuated or in any other way removed from posing a threat to the environment.

# FINGERPRINTING

## Petroleum Hydrocarbons- Fuels

Perhaps the simplest form of fingerprinting is used in the identification of petroleum fuel products. The analytical technique that is most widely used in assessing petroleum hydrocarbon contaminated sites is gas chromatography (GC). To fingerprint a petroleum product using GC one can look at and characterize the distribution of the different n-alkanes, or straight-chained hydrocarbons. Because different fuel products may have the same general range of petroleum hydrocarbon but in different proportions, quantifying the amount of petroleum hydrocarbons present within a specific range of carbon-chain lengths is insufficient to identify the type of product present. For example, the typical hydrocarbon ranged used to quantify the amount of 'gasoline' that may be present is C4 to C12. This range of hydrocarbons however also includes kerosene, stoddard solvent, some jet fuels, and the lower range of some diesel fuels. Without examining the actual distribution of the hydrocarbons present one could not be certain what was the true nature of the product. However, by examining the hydrocarbon distribution one can determine the fuel type.

The composition of natural crude oils may vary significantly since crude is generated in many different areas and under many different conditions, however crude oils produced from one region will tend to have certain characteristics that are different from oils produced elsewhere. Many of these characteristics can still be recognized in various refined products, such as diesels and lubricating oils, and be used to distinguish between sources. The most notable characteristics used to differentiate between crude sources are the distribution and ratios of specific petroleum components. These components include paraffins, isopariffins, aromatics, naphthalenes, and olefins. In addition, stable isotope rations for carbon and hydrogen as well as trace metal content, can sometimes be used to distinguish between sources.

Non-petroleum constituents contained in petroleum products can also provide important information. The most notable additives used historically and presently are lead, lead scavengers, anti-knock compounds such as ethylene dibromide (EDB) and ethylene dichloride (EDC), and oxygenates such as methanol, ethanol and methyl tertiary-butyl ether (MTBE). These additives if analyzed for and detected are useful in refining our knowledge of a release. For example, the detection of EDB at a site contaminated by gasoline aids in identifying the release as involving leaded gasoline, and therefore most likely an older release. On the other hand, if MTBE were detected, the release would have to be more recent. Other additives such as dyes and proprietary compounds are not as useful as most dyes breakdown and change color while proprietary compounds can be quite difficult to get.

### *Case 1- Petroleum Fuels*

To illustrate the use of fingerprinting of hydrocarbons in identifying multiple types of co-mingled hydrocarbons and the associated sources, we'll examine an actual case involving a typical corner gasoline station. This gasoline station had been in operation for over 50 years, had multiple owners, and multiple underground storage tanks (UST) and pipeline configurations. Over the course of the history of this site, the USTs had stored leaded gasoline, unleaded gasoline, diesel, as well as waste oil. The two original fuel USTs, dating from the 1940s, contained leaded gasoline. The original operator abandoned these tanks in place in the early 1970s by first pumping them empty and then filling them with sand. The new operator installed new tanks and distribution lines to handle unleaded gasoline and diesel. The station remained in operation until 1992 when it closed and the property was put up for sale.

Initial soil and groundwater investigations conducted at the site identified contamination in the vicinity of the waste oil tank using EPA method 418.1 IR, and both gasoline and diesel contamination near the USTs and along the distribution lines using EPA Method 8015 mod-California (GC). Samples were also tested for organic lead to determine if any of the gasoline was leaded. No organic lead was detected. Groundwater was detected approximately 35 feet below ground surface and was found to be impacted by both gasoline and diesel range hydrocarbons.

A second round of sampling was conducted which found that the waste oil contamination detected near the waste oil tank extended over the entire site at a depth of 20 feet bgs. In addition significant gasoline contamination was found along the distribution pipelines that extended near the abandoned leaded gasoline tanks, though no organic lead. Based on these findings the current owner, who operated the waste oil tank and maintained the unleaded fuel was designated as being responsible. The previous owner was not implicated on the basis of organic lead not being detected.

As part of the lawsuit that ensued, a forensic approach was taken in the analysis of samples. First, samples of the petroleum impacted soil were analyzed using ASTM Procedure 2887 – simulated distillation, which generates a full hydrocarbon spectrum. Secondly, samples of the sand from the abandoned tanks as well as soil and groundwater samples were also fingerprinted for TPH using a full GC scan and analyzed for EBC and EDC.

Results of the simulated distillation determined that the waste oil contamination as well as some of the TPH in groundwater was actually natural crude oil. Review of the local geology uncovered some natural seeps less than a mile away. Sand from the abandoned tanks was found to have high volatile aromatic levels, and EDC. Groundwater samples from the monitoring well closest to the old abandoned tanks also contained EDC, however groundwater away form the tank area, though impacted with BTEX contained no EDC.

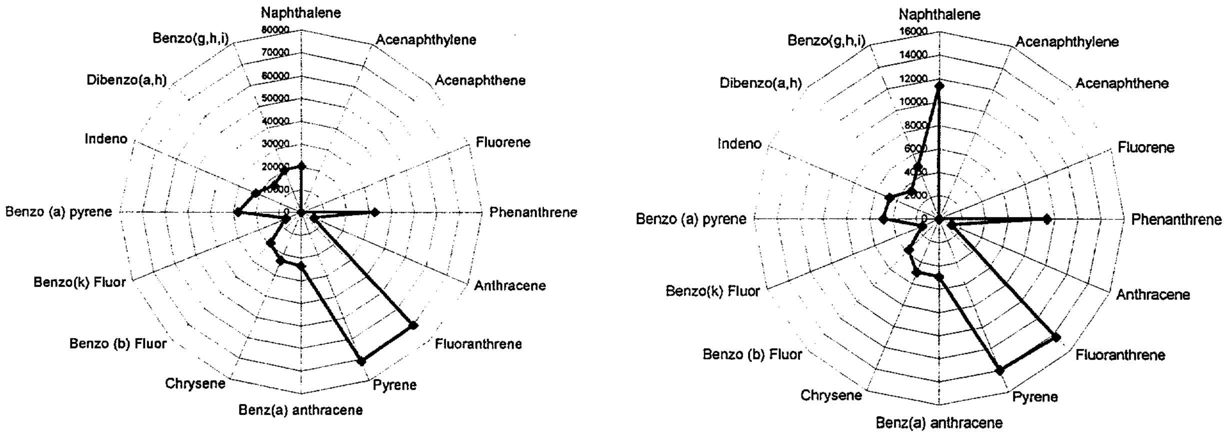
Based on these findings, no cleanup of the TPH initially identified as waste oil was required, and the previous owner, who abandoned the USTs that contained leaded fuel, was required to share in the cleanup costs.

## Polycyclic Aromatic Hydrocarbons

Polycyclic aromatic hydrocarbons (PAH), consisting of two or more fused benzene rings, comprise another major class of hydrocarbons in petroleum of environmental interest. Naphthalene ($C_{10}H_8$), consisting of two fused benzene rings, is the lowest molecular weight PAH. Coronene (MW 300.4) composed of six fused rings in a highly condensed configuration is the highest molecular weight PAH with sufficient mobility to be considered potentially toxic (Neff, 1979). The two- and three-ring PAHs are nearly always much more abundant than higher molecular weight PAHs in crude oils, while the higher weight PAHs are much more characteristic of pyrogenic sources (soot, coal tars, engine exhaust) than petrogenic or biogenic sources. Knowledge that different sources may give rise to different types and distributions of PAHs is important when investigating a PAH impacted site. The following example serves to illustrate this point.

*Case 2 - PAHs*

The site in question this time is an abandoned town gas site. Coal tar and fuel oil had been burned for years to generate gas. The fuels used in the generation plant were transported to the site via rail cars. The site was bounded on one side by the rail line with a short, dead end spur extending onto the site to permit offloading of the fuel. Investigation of the site identified the presence of a full range of PAHs from naphthalene to benzo(g,h,i)perylene. Review of data indicated spatial grouping of lighter PAHs along RR tracks heavier PAHs mid-facility. Graphical component analysis of detected PAHs identified a unique signature suite of PAHs associated with the railroad tracks. The PAHs detected along the railroad tracks were predominately fluoranthene and pyrene (Figure 1a,b).

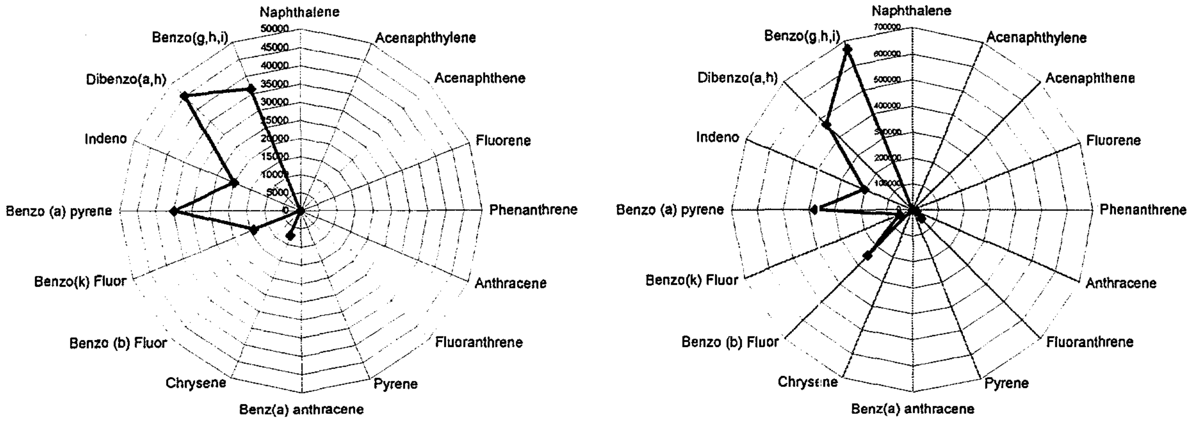


(a) (b)

**Figure 1(a,b)** Plots of PAH composition of samples taken from near the railroad.

Review of technical literature indicated that fluoranthene and pyrene represent between 46 and 88 percent of the total PAH in diesel exhaust (API, 1994). This range corresponded with the signature of the PAHs detected along the railroad tracks.

A suite comprised of benzo(a)pyrene, dibenzo(a,h) anthracene and benzo(g,h,i)perylene dominated within the interior areas. These heavier PAHs with little or no occurance of the railroad suite (naphthalene, pyrene) dominated the signature suite of PAHs, detected within the middle of the site. Distribution plots of their composition are shown in Figure 2 (a,b). Based on the recognition of different suites of PAHs being discernable and related to different sources, the impact resulting from the town gas site operations was able to be separated from the impact associated with use of diesel fueled railroad engines. Remediation undertaken by the utility company was limited to the town gas site specific impacts.



(a) (b)

**Figure 2(a,b)** PAH composition of samples taken from within the middle of the site.

## Halogenated Hydrocarbons –Chlorinated

Halogenated hydrocarbons, particularly chlorinated solvents, are some of the most common contaminants other than volatile aromatic hydrocarbons found at sites across the USA. One important characteristic of halogenated hydrocarbon chemistry is the susceptibility of these compounds to breakdown through reductive dehalogenation involving the exchange of hydrogen for an attached halogen. This degradation process produces a sequentially associated suite of compounds as the breakdown progresses, along a pathway, from the original "parent" product through the associated "daughter" products. Careful analysis and characterization of this "family tree" association can be used to identify unique signatures or fingerprints of plumes.

Breakdown pathways observed are shown below in figures 3 through 5.

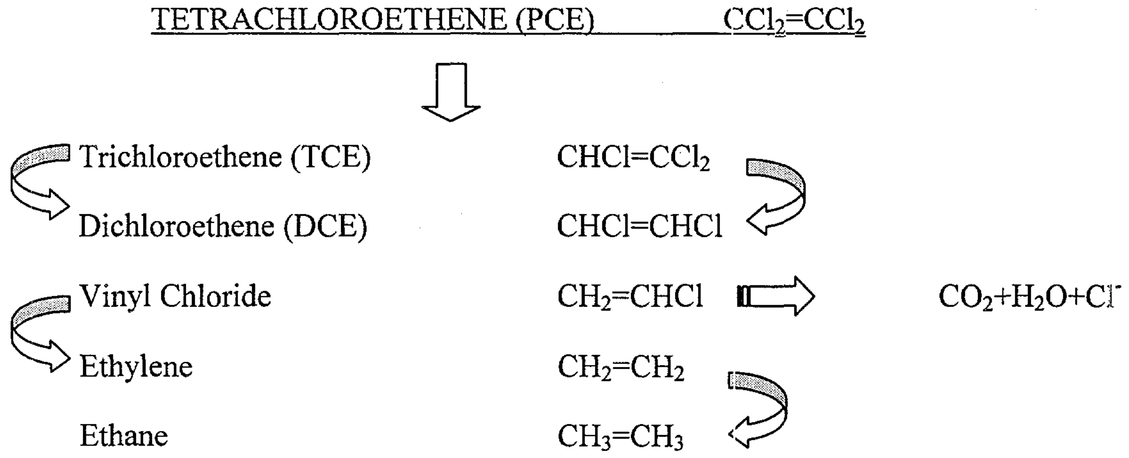


**Figure 3** Breakdown pathway for tetrachloroethene (PCE).

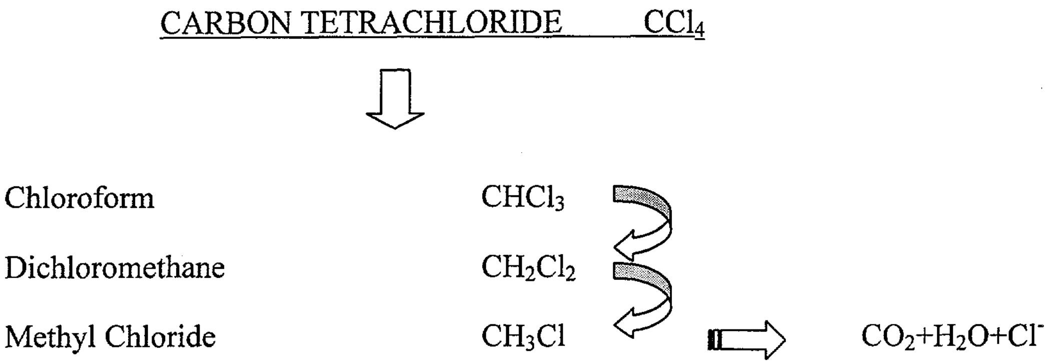


**Figure 4** Breakdown pathway of Carbon Tetrachloride.

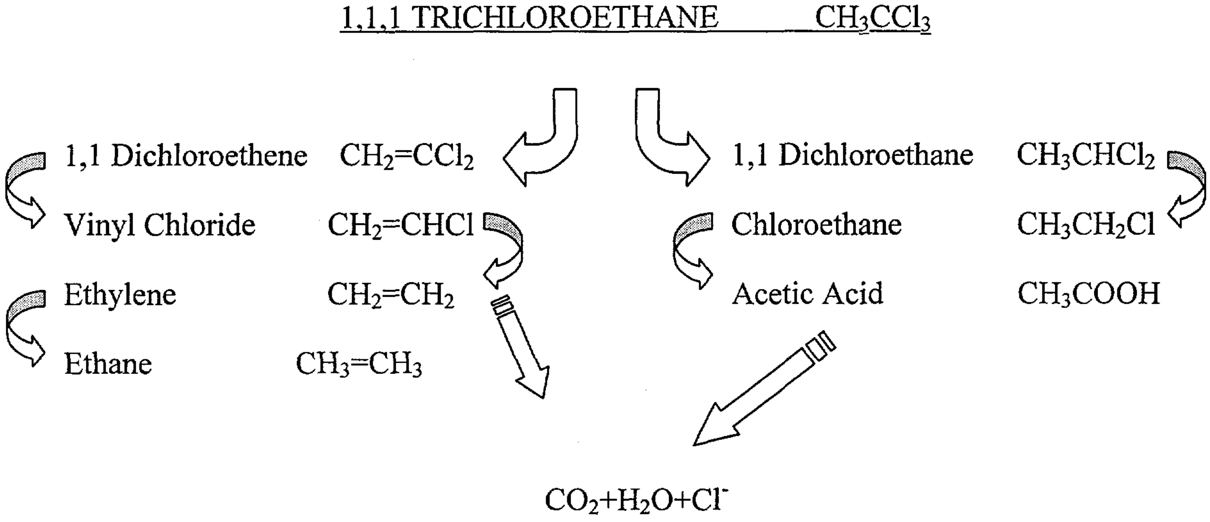


**Figure 5** Primary breakdown pathways of 1,1,1 Trichloroethane.

The relationships observed between parent and daughter products can yield important information about the history of a release. Because the generation of daughter products is dependant upon specific processes, the relationship between parent and daughter products, often presented as ratios, can be expected to vary in a predictable manner based on the position from a source. This is true in both soil and groundwater plumes; though degradation is more readily observable in groundwater plumes. The presence of products not related to the "family tree" can be indicative of unrelated releases. This observation aids in the identification and possible segregation of impacts associated with different releases or in attempting to segregate co-mingled plumes.

Shown below is a plot of selected ratios of compounds observed in six different monitoring wells at a single site (Figure 6). Three distinct groupings are readily identifiable. Group 1 (MW-21, MW-29) exhibits a high DCE/TCE ratio; Group 2 (MW-33, MW-31) exhibits a high DCA/TCA ratio; Group 3 (MW-14, MW-34) exhibits generally low overall ratios. Based on this data, it was identified that there were two, co-mingled plumes present that resulted from two separate releases.

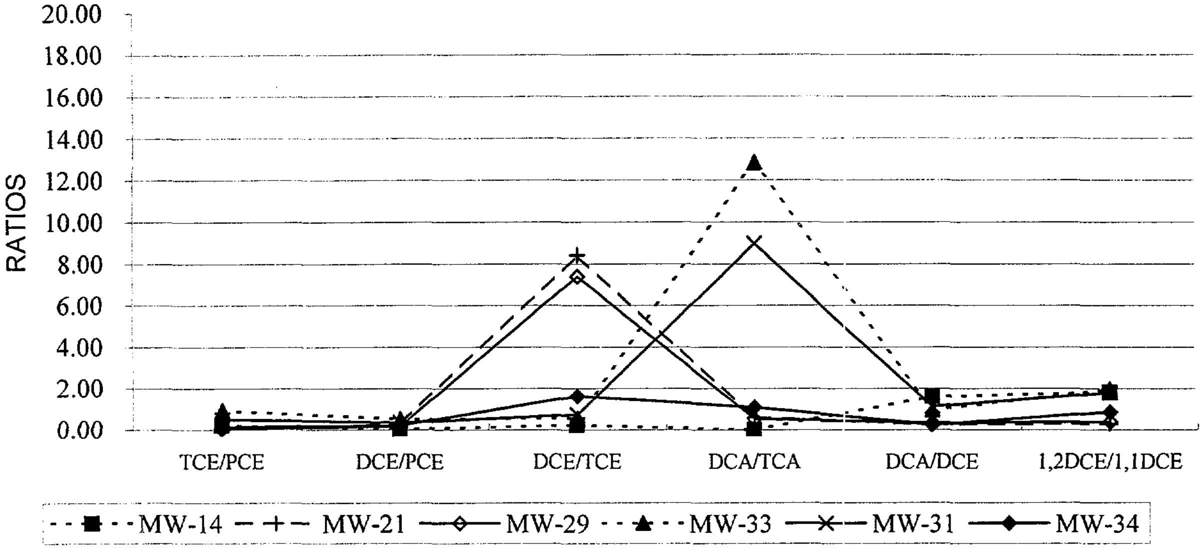


**Figure 6** Parent/daughter product ratios for selected groundwater well samples.

This type of analysis can be quite helpful in establishing identifying a signature suite or fingerprint of chlorinated plumes and has been successfully used to track offsite migration of plumes that become co-mingled with plumes emanating from offsite sources.

## *Case 3 – Chlorinated Hydrocarbons*

PCE and its associated daughter products were found in the groundwater during the investigation of a manufacturing facility that produced fasteners. The facility is located in an industrial park with other similar manufacturing facilities including several large aerospace facilities. Characterization of the fastener site indicated chlorinated solvents dissolved in the groundwater under the site, downgradient of the site, and upgradient to the site. Although there were several sumps and clarifiers on the fastener site, none could be specifically identified as a source for PCE found in the groundwater. Further, no PCE was found in the soil and the facility management claimed that they did not use PCE.

Forensic geochemistry was used with transport and fate groundwater modeling to show to the regulatory agency how the currently observed pattern of chemicals indicates: (1) the most probable sources of contamination to the groundwater, (2) the magnitude of the contamination from various sources, (3) the responsible parties, and (4) the relative risk associated with the various contaminant contributions. Further, from this information, the relative liability of the various responsible parties could be equitably determined, which led to a negotiated settlement rather than a lengthy and expensive lawsuit.

## AGE DATING

Determining when a release took place based on the chemistry of the contaminants is a much more difficult exercise than establishing a fingerprint or unique signature. Most all methods available do not have the resolution necessary to specify a specific year. What can be determined in some circumstances is the general time period when the release took place.

### Petroleum Hydrocarbon - Fuels

The presence or absence of specific additives and fate and transport behavior of petroleum constituents have all been used in attempts to date fuel releases. The success of the use of additives is limited by the extensive time period that usually exists between reformulation of the major fuel products. One of the most significant mileposts in fuel formulation was the elimination of lead and introduction of oxygenating ether compounds

Gasoline prior to 1980 often contained tetramethyl lead, trimethylethyl lead, dimethyldiethyl lead or methyltriethyl lead. After 1980 tetraethyl was used. Lead scavengers were used in leaded gasoline along with the lead alkyl compound. The most common scavengers used were EDB and EDC. Analysis for these compounds can therefore help determine if the product was released before or after 1980. Oxygenates began to be added after 1980. Common compounds used include MTBE, di-isopropal ether (DIPE), ethyl tertiary butyl ether (ETBE), methanol and ethanol. Again, the presence or absence of these constituents can be used to indicate an "older" release from a "newer" release.

Another approach taken to date petroleum releases involves the development of appropriate fate and transport arguments. The fate aspect of the arguments typically incorporates documentation of changes in composition of petroleum hydrocarbon products due to natural processes including volatilization, water washing (leaching) and degradation. The goal is to characterize the release and then compare and contrast it to the characteristics of "fresh" product. The degree of alteration is used as a general gauge of how long the product has been in the environment. For sites with multiple releases, this approach is used to date one release relative to another. For single releases the degree of degradation is compared with observed and published degradation rates to determine the amount of time since the release.

The transport aspect of dating examines the distance that the contaminants have moved in the environment in light of expected transport rates in the affected media to determine the amount of time since the release. This approach is most commonly applied to contaminated groundwater problems where the movement of the contaminant is assumed to be dominated by advective groundwater flow. Factors that need to be considered in this approach primarily includes the permeability, hydraulic gradient, and retardation factor that is typically based on organic carbon content. If these factors are known, the argument is quite simple. For example, if the contaminant is observed to have traveled 50 feet downgradient from the release point and the calculated effective groundwater transport velocity is 10 feet per year, then with no retardation the release is determined to be approximately 5 years old.

Though attractive in their simplicity, both fate and transport arguments are based on a number of assumptions regarding the natural processes taking place. Without the determination of site specific degradation and transport rates, application of these types of arguments can only be considered as providing major league ballpark approximations. And, even with the determination of site specific values, one is still left with having to make and use assumptions for the condition of the site and associated fate and transport characteristics for the unknown period of time from the release to the beginning of collection of site data. Given these complexities, age-dating based on fate and transport arguments should only be used to provide general guidance to the age of a release, and the age determined solely by these types of arguments should only cautiously be used.

### Halogenated Hydrocarbons –Chlorinated

As with petroleum hydrocarbons, age-dating of chlorinated releases is typically based on either the determination of the degree to which degradation has taken place and estimation of a degradation rate or, when groundwater has been impacted, the transport distance from a known. And, as with petroleum, these approaches can usually only provide a general idea, or probability, of when a given release took place.

## DOCUMENTATION OF NATURAL ATTENUATION

Recognition that compounds can naturally degrade in the environment, coupled with the high cost and questionable success of many engineered remediation approaches, has lead the regulatory and legal communities to view natural attenuation and biodegradation as increasingly viable approaches to the management of risk associated with contaminated sites. Central to the acceptance of this approach is the ability to document and substantiate the past and present roles that natural degradation processes have played and are playing in limiting or even reducing risk. Once determined, this information can be used to indicate the degree to which the identified processes can be expected to continue into the future and the ultimate end state of the contaminant

The sophistication of the approaches used to document remediation by natural attenuation (RNA) has increased over time. Early approaches used to document RNA involved resampling sites over time to demonstrate that levels were declining. It was then assumed that natural processes were the cause. As more knowledge has been gained regarding the actual dynamics of reductive and biodegradation processes, documentation of RNA has expanded to include the use of the analytical assessment of changes in the makeup of the contaminants. For petroleum fuel sites, the reduction of the more degradable components of a release (e.g. benzene) relative to the less degradable components (e.g. xylenes) is one observation that has been used to support RNA. For chlorinated compounds, identification of parent and daughter products related by accepted breakdown pathways and the observed variations of the mass ratios of daughter/parent compounds over space and time has been used to support RNA.

Documentation of RNA is now advancing into the use of computerized, fate and transport models combined with the increasing body of knowledge of reactions, reaction rates, controlling parameters and by-products. In support of this type of analysis, the nature of information collected as part of site investigations has grown to include the collection of data necessary to understand the active role that natural processes are playing in the environment. Examples of models now used to characterize and document RNA include BIOSCREEN (Newell et al., 1996) which is used primarily for refined petroleum fuel releases, and the relatively new RT3D reactive transport modeling code (Clement, 1997).

Use of forensic techniques in documenting that RNA has been occurring, and the impact of that knowledge is described in our Case 4.

### *Case 4 – Chlorinated Hydrocarbons*

PCE, TCE, and associated daughter products were found in low concentrations in several groundwater monitoring wells around a closed municipal landfill. The landfill received municipal waste in the 1960's. The state regulatory agency issued a "Clean-up and Abatement" order against the current owner of the property containing the closed landfill. Further actions against the current landowner were filed by neighboring landowners concerned about contamination coming onto their properties and diminishing the value. The current owner bought the property after the landfill was closed and believed that he was not responsible for "clean-up" of the groundwater or for contaminating his neighbor's properties. Numerous negotiations ended with no results; litigation ensued.

Forensic geochemistry was used with integration of other site characterization parameters, to reinterpret the complicated groundwater flow and contaminant transport in and out of the landfill. The occurrence of chlorinated chemicals and their associated daughter products showed a typical (first order) chemical decay pattern, indicative of a source in the landfill and not from more recent activities of the current owner on the surface. Further, projecting the decay pattern into the future showed attenuation below the drinking water Maximum Contaminant Levels within ten years, arguing for a containment strategy rather then a more costly remediation.

## CONCLUSIONS

As has been demonstrated by these examples, application of knowledge of chemical speciation, reactions, relationships, and fate and transport characteristics of compounds found in the environment is of great benefit and many times critical to gain understanding, resolve disputes, and develop meaningful and responsible risk management approaches to contaminated sites. To benefit from the application of forensic geochemical analysis, site investigative techniques and approaches need to go beyond merely assessing the extent of contamination, to assessing the true nature of the compounds, the impacted media, and the nature of the interactive fate and transport processes at play.

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# CHARACTERIZATION OF SOIL BENEATH A SURFACE IMPOUNDMENT USING GEOCHEMICAL MODELING

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## ABSTRACT

The 100-D Ponds served as a surface impoundment between 1977 and 1994, receiving effluent from a water treatment facility and wastes from nearby laboratories. The ponds are located at the Hanford Site in Washington State, which is operated by the U. S. Department of Energy (DOE), and were constructed in an ash disposal basin. Physical and chemical characterization of sediment in the pond indicated that contamination was limited to the upper 1 meter of the pond floor.

In order to approve closure of this unit, the regulating authority required evidence that the ponds did not contaminate the underlying soil or groundwater. Because there are no data for vadose zone samples beneath this unit, the regulators required the collection and analysis of deep soil samples from beneath the surface impoundment in order to approve its closure. An alternative proposed by DOE was to combine the available near-surface data with geochemical modeling of subsurface reactions to formulate a conceptual model for the fate of contaminants associated with the ponds.

The computer code PHREEQC was used to evaluate the possibility that dangerous wastes or dangerous waste constituents had migrated into the vadose zone and groundwater. The model simulated reactions between infiltrating water and the various sediment types that occur beneath 100-D Ponds. The model and available chemical analyses show that contamination was restricted to the sediments in the pond, and that this unit did not contaminate the subsurface soil or groundwater. Based on the results from the modeling and the available soil and groundwater data, the regulators have agreed that the ponds can be clean closed without collecting additional, costly subsurface soil samples.

## INTRODUCTION

The 100-D Ponds is a *Resource Conservation and Recovery Act* (RCRA) Treatment, Storage, and/or Disposal (TSD) unit located in the northern portion of the Hanford Site in Washington State (Figure 1), which is operated by the (DOE). Prior to the construction and operation of the ponds this location served as disposal basin for bottom ash from a coal-fired powerhouse. This ash basin was retired in 1966, and the ponds were constructed and began operating in 1977.

The ponds served as a surface impoundment for liquid effluent until discharges ceased in 1994. The majority of the effluent received by the ponds was from a water treatment plant which filtered and purified Columbia River water for use in Hanford operations. Routine maintenance

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of the treatment plant included backflushing mixed-media filter beds and semiannual discharge and cleaning of two large settling basins. These activities released approximately 12 million liters of effluent per year into the ponds.

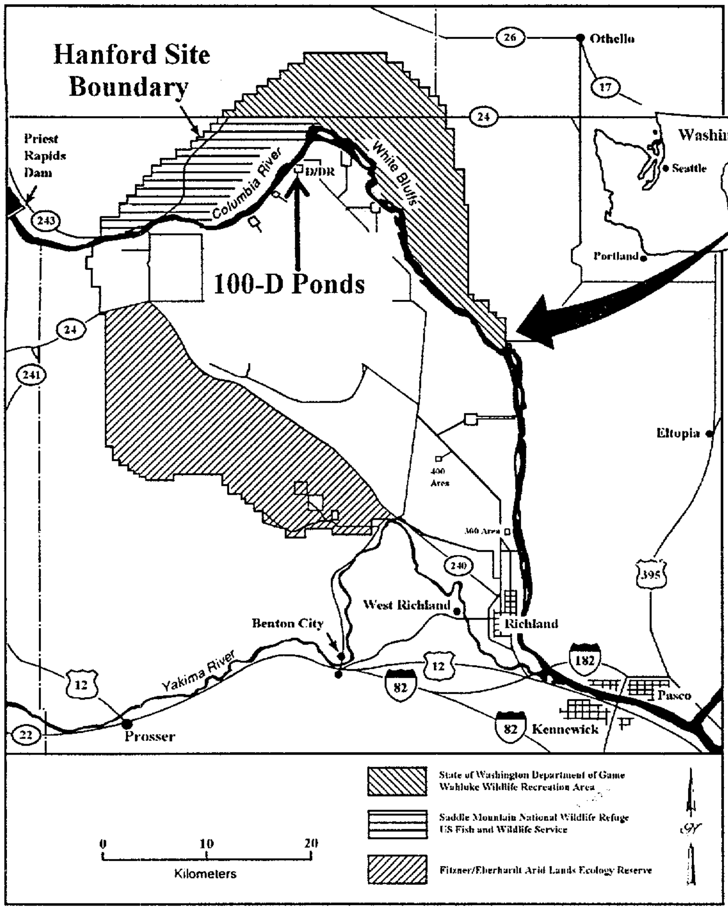


Figure 1. Hanford Site and Regional Map.

The 100-D ponds also received liquid waste streams from miscellaneous laboratories and test facilities in the area. Figure 2 shows the location of the ponds and the process sewer system which collected effluent from various buildings and discharged into the ponds.

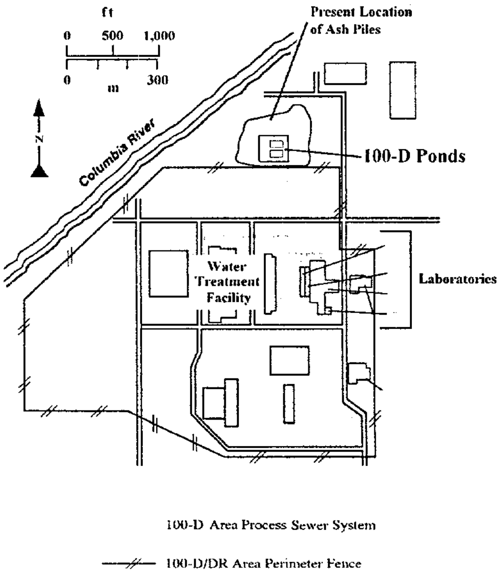


Figure 2. The 100-D Area.

Preparations to close this facility began in 1992 with the release of a closure plan and collection of characterization data. Additional samples collected in 1995 indicated that contamination was limited to a thin (approximately 60 cm) layer of sediment in one of the ponds. Preparations for the excavation and disposal of this sediment, with the objective of clean closing this TSD, included discussions between the DOE and the Washington State Department of Ecology (Ecology), which serves as the regulating agency for RCRA. Although both parties agreed that the bulk of contamination associated with 100-D Ponds was located in this sediment, Ecology required evidence that the soil and groundwater beneath the ponds had not been adversely affected by operations at this TSD. To demonstrate this Ecology directed that soil samples be collected at regular intervals from the surface to the groundwater table beneath the ponds (approximately 14.5 m below the ponds) in at least two locations.

To avoid the expense and delay of drilling and sampling the soil beneath the ponds, the DOE and its contractors, Bechtel Hanford, Inc., and CH2M HILL Hanford, Inc., used available groundwater and soil data combined with geochemical modeling to demonstrate that this TSD has not impacted the soil or groundwater. The following is a physical and chemical description of the ponds and associated environment, and details of the modeling effort which ultimately succeeded in regulator agreement that this unit could be clean closed without the additional collection of subsurface samples.

## PHYSICAL AND CHEMICAL CHARACTERIZATION OF THE PONDS

This TSD consists of two ponds separated by a dike. The settling pond is the southermost of the two and received nearly all of the effluent discharged into the system. This is connected to the northern percolation pond by overflow pipes through the dike. Operational records suggest that the level of the settling pond rarely if ever rose high enough to spill into the percolation pond; samples from the settling pond do not show any evidence of contamination. Each pond is approximately 30 meters wide, 50 meters long, and 4 to 5 meters deep.

Figure 3 shows the outline of the ash pile, the RCRA monitoring wells associated with the ponds, and the position of the ponds in the ash pile. Figure 4 is a cross section through 100-D Ponds showing the topographic profile along a northwest-southeast transect and subsurface features, including approximate boundaries of the coal ash and position of the water table. Sediments below the ash are composed of loosely cemented sands and gravels of the Ringold Formation.

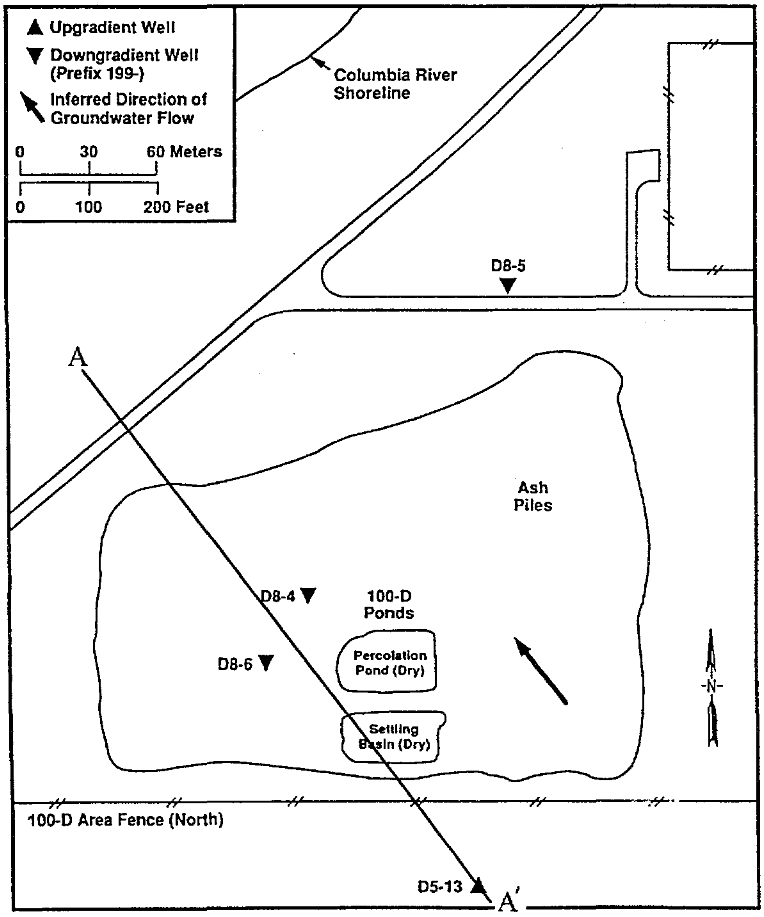


**Figure 3. 100-D Ponds and Monitoring Wells; A-A' is transect for cross section in Figure 4.**

### Contaminant Sources

Several different facilities discharged to 100-D Ponds during its 17 years of operation. The following is a description of contaminants that may have been discharged to ponds and the likely origin of these contaminants:

- Corrosive chemicals. Three demineralizers occasionally discharged potentially corrosive regeneration fluids into the ponds. These effluents may have exhibited pH levels below 2.0 or above 12.5 upon arrival at the ponds, although

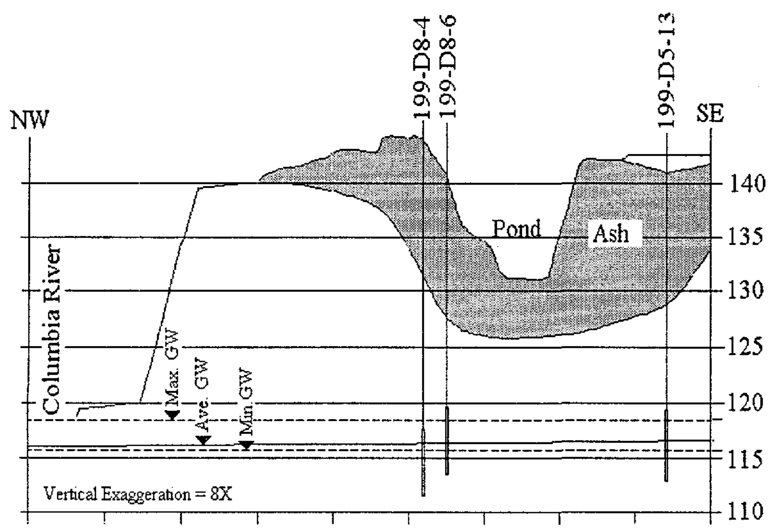


**Figure 4. Cross Section Through 100-D Ponds. See Figure 3 for transect location. Patterned area is inferred extent of coal ash. Vertical axis is in meters above sea level.**

their actual corrosivity level was never established. It is the potential for this site to have received these corrosive chemicals that led to the classification of the 100-D Ponds as a TSD unit.

- Mercury. No records exist that identify disposal of mercury into 100-D Ponds; however, the presence of liquid metallic mercury was visibly confirmed in the floor drain of a laboratory which discharged to the ponds. Mercury traps were installed three years before the ponds began receiving effluent in 1977, but some mercury could have persisted in the sewer system and been deposited in the ponds

- Dangerous shop chemicals. Until 1988, when most of the laboratories were permanently closed, standard volatile organic shop chemicals such as thinners and solvents could have been released to the 100-D Ponds from open floor and sink drains. However, such chemicals were not normally stored in bulk quantities nor were they procedurally discharged to the drain system when spent.

- Radioactive constituents. Unirradiated uranium fuel elements used at a test facility may have contributed radiological contamination to 100-D Ponds.

- Naturally occurring metals from Columbia River water and sediment. The filters used at the water treatment facility removed suspended and colloidal minerals from the river water, which would have been discharged into the 100-D Ponds during periodic backflushing of the filters. Semi-annual washdowns of the 183-D water storage basins also discharged river sediment and flocculent into the 100-D Ponds along with Columbia River water.

## Characterization of Contamination

Because this is a RCRA TSD, there has been a groundwater monitoring program around the ponds since 1992. Two different sampling and analysis efforts have been conducted to characterize soils and sediments in the ponds, one in August 1992 and the other in January 1995 (BHI 1995). Samples were analyzed for metals and organic analytes using both total (SW-846) and toxic characteristic leaching procedure (TCLP) analytical preparation and analysis techniques. Samples of the coal ash surrounding the ponds were also collected in September 1992.

Characterization data indicated that some contaminants were present in the sediment on the bottom of the settling pond. These constituents likely originated from the laboratory facilities and arrived by way of the process sewer system. Constituents that were present above cleanup levels established by Ecology include polychlorinated biphenyls (PCBs), arsenic, barium, total chromium, lead, nickel, and zinc. The coal ash underlying the sediment was also chemically evaluated and found to have contaminant levels below cleanup limits.

The contaminated sediments, which consisted of naturally occurring fine-grained material and flocculent, were removed and disposed of in August 1996. The floors of the ponds were sampled shortly after this remediation. Data from all of these samples are discussed below.

## Evaluation Of Groundwater Data

Groundwater monitoring at 100-D Ponds began in 1992. As required by 40 CFR 265.92, groundwater has been analyzed for groundwater quality parameters, drinking water parameters, and contamination indicator parameters. Statistical comparisons of contamination indicator parameters upgradient and downgradient of the site are made on a quarterly basis. This phase of groundwater monitoring is commonly called "indicator evaluation" or "detection" monitoring.

The groundwater monitoring network for the 100-D Ponds is composed of one upgradient and three downgradient wells (Figure 3). The wells are completed at the top of the unconfined aquifer. Four quarters of data were collected in 1992 and 1993 and analyzed for a complete suite of organic and inorganic constituents and radionuclides. Semiannual samples collected since 1993 have been analyzed for a suite of metals, anions, field measurements, and radiological components.

A statistical summary for contaminants of potential concern from the three downgradient wells shows that groundwater concentrations are below Ecology's *Model Toxics Control Act* (MTCA) Method B groundwater cleanup standards. Of special concern are the chemicals that were found to be above MTCA Method B soil cleanup standards for groundwater protection in the sediments of the settling pond, namely PCBs, arsenic, barium, cadmium, chromium, copper, lead, mercury, nickel, vanadium, and zinc. None of these constituents were found in the downgradient wells at levels that would indicate contribution from 100-D Ponds. These results indicate that effluent disposal activities at the ponds did not have any adverse effects on groundwater.

Although discharges to 100-D Ponds did not create a groundwater mound detectable by water levels in the monitoring wells, the effect of the discharges can be seen in the water chemistry data. The greatest volume of effluent routed to the Ponds was raw or treated river water released from the water treatment facility, which diluted the groundwater beneath the Ponds. The groundwater upgradient of 100-D Ponds is contaminated with chromium, tritium, and nitrate. The discharges into 100-D Ponds effectively diluted this groundwater to values typical of or below background concentrations for the Hanford Site, as shown by analyses from downgradient monitoring well samples (DOE-RL 1996a).

Figure 5 shows chromium concentrations and conductivity measurements over time for the upgradient and downgradient monitoring wells. These plots show that water quality in the upgradient well has degraded since the decrease of discharges to 100-D Ponds and final cessation in June 1994, while concentrations in the downgradient wells have changed little since that time. This is interpreted to be the result of the lack of "clean" water from past discharges to dilute the contaminated water entering the area from upgradient sources. The RCRA groundwater monitoring program for interim status units requires a comparison of concentrations of various indicator parameters from downgradient wells with critical mean values calculated from an upgradient well. Over the course of groundwater monitoring at 100-D Ponds, pH is the only parameter that has exceeded the critical value (which is 9.14). This exceedence occurred in February 1996 in the two downgradient wells, 199-D8-4 and 199-D8-6. It has been concluded that the coal ash underlying the Ponds is the source of the elevated pH in the groundwater.

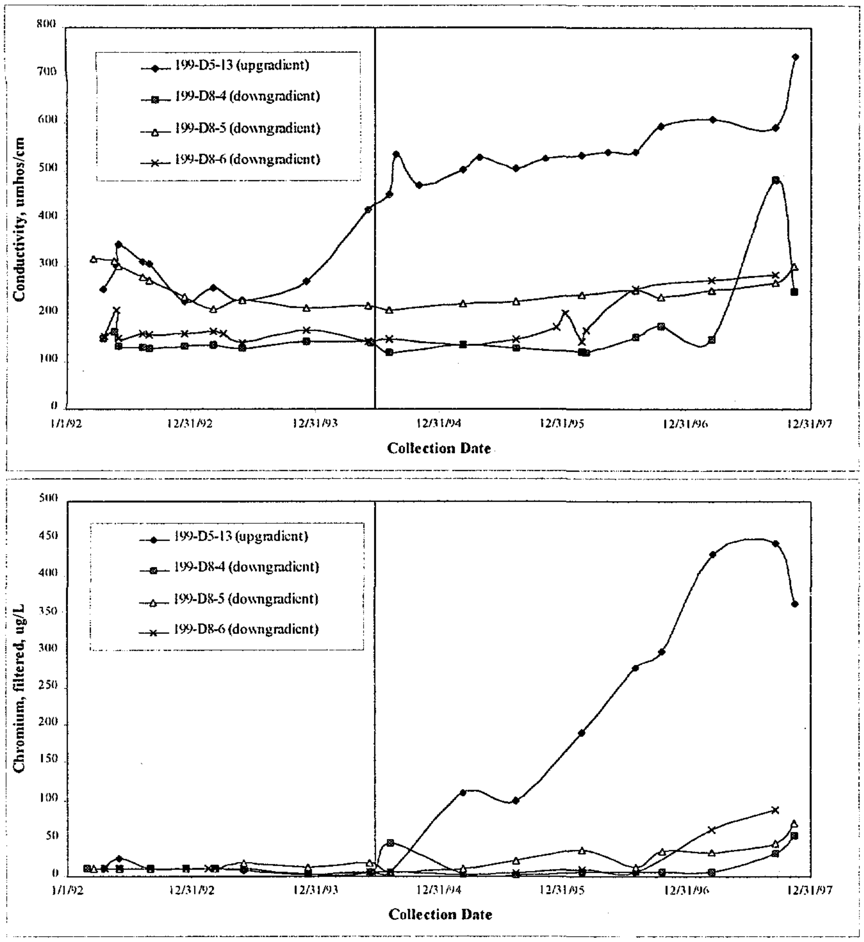


**Figure 5. Conductivity and Chromium Values from 100-D Ponds Monitoring Wells from March 1992 to November 1997. Vertical line represents end of discharges to the ponds.**

## Evaluation Of Subsurface Soils

Data collected in the 1995 characterization effort were from surface samples and various depths sampled from four different test pits with a maximum depth of 2.4 meters. These data and analyses of the 1992 samples were used in the decision to remediate this TSD unit by removing the sediment from the settling pond. The 1995 data show that the ash beneath the fine grained settling pond sediment is not contaminated. The contaminants are restricted to the fine-grained sediment in the settling pond. These contaminants include PCBs, arsenic, total chromium, and lead (DOE-RL, 1996b). The data also show that the concentrations of these contaminants drop sharply in the ash underlying the sediment. Figure 6 shows this relationship for several contaminants.

Several samples intended to characterize the background composition of the coal ash surrounding and underlying 100-D Ponds were also collected in 1992. These have compositions very similar to the materials underlying the settling pond sediment, collected and analyzed in 1995.

Additional samples were collected from the bottom of the ponds after removal of the contaminated sediments in August 1996. Data from these samples are below Ecology MTCA

Method B cleanup standards, indicating that contamination was fixed in the fine-grained sediments and did not migrate into the vadose zone.

## PHYSICAL AND CHEMICAL FACTORS AFFECTING CONTAMINANT MIGRATION

The effluent discharged to 100-D Ponds was predominantly water from the water treatment facility. Some corrosive liquids and miscellaneous chemicals were also discharged through the process sewer system into the ponds, along with river sediment and flocculent used in the water treatment process. These latter solids are important to consider when evaluating the mobility of metals and PCBs, as fine-grained sediment and flocculent have the ability to adsorb many chemicals and effectively immobilize them in an aqueous environment. It is thus possible that chemicals discharged into the ponds were fixed in the upper layer of sediment composed of flocculent and solids filtered from Columbia River water. A discussion of the use of flocculents for binding contaminants in water follows.

Coagulants and flocculents are used in liquid/solids separation applications to neutralize the ionic charges that surround solid particles dispersed in water, and cluster them together to promote settling. Most naturally occurring particles have a negatively charged surface in water due to the release of cations such as $Na^+$ and $Ca^{2+}$ from the surface of the particle into the surrounding water. When microscopic particles of like charge approach one another, they repel and cannot coalesce to form larger particles. This leads to very stable systems of particles in water that will not settle. Cationic coagulants adsorb onto the negatively charged particle surfaces and neutralize the negative charges that are causing repulsion. Optimum coagulation occurs when the particle surface charge is reduced to near zero.

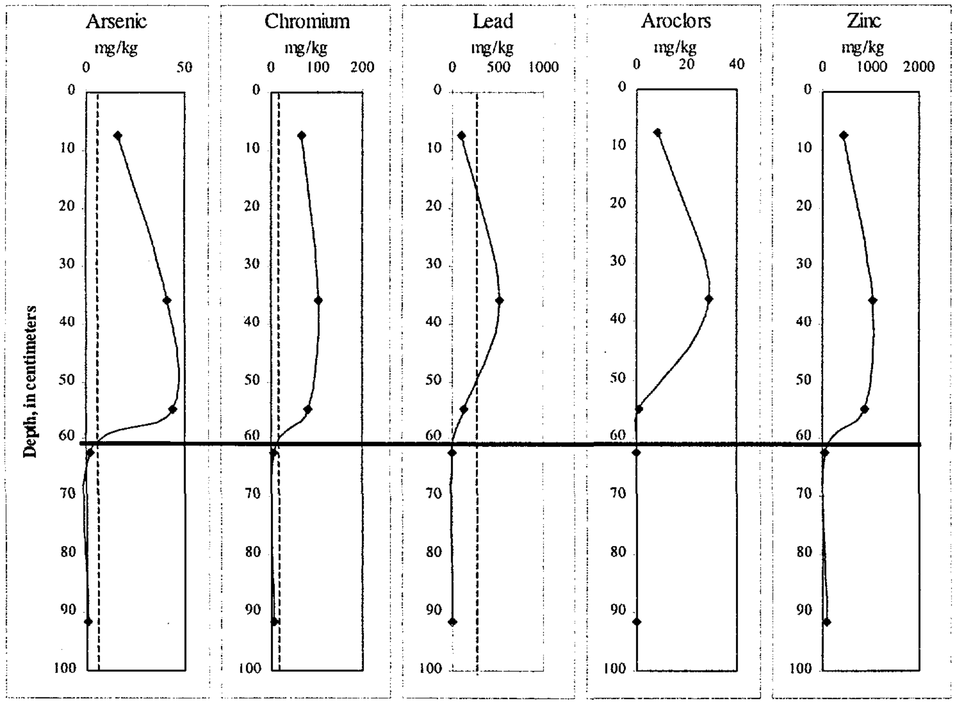


**Figure 6. Concentration Profile of Several Constituents in 100-D Ponds Sediment and Underlying Ash (below horizontal line). Dashed lines are cleanup limits (near zero for aroclors and off scale for zinc).**

The agent used at the water treatment facility as a coagulant and flocculent was aluminum sulfate (alum). This compound, and others like it (e.g., ferric chloride), have trivalent metal ions ($Al^{+3}$ and $Fe^{+3}$) that are strongly attracted to any negatively charged surface. Trivalent cations are desirable coagulants when compared to divalent and monovalent cations, which have very weak coagulating abilities. The use of alum usually produces a fairly clean supernatant water since the metal hydroxides produced assist in the capture of very fine particles. Use of alum also tends to lower the pH of the system as anions are adsorbed.

The flocculent released into the ponds would carry with it the contaminants (natural or anthropogenic) adsorbed at the water treatment facility, but would also probably have excess adsorption capacity when it was deposited on the surface of the settling pond. It is, therefore, likely that this alum would bind much of the contamination entering with the liquid effluent and prevent contaminants from migrating through the vadose zone.

## MODELING OF SUBSURFACE SOIL

In order to evaluate the possibility that dangerous wastes or dangerous waste constituents have migrated and been deposited into the vadose zone, geochemical modeling was performed to simulate reactions between infiltrating water and the various sediment types that occur beneath 100-D Ponds. The computer code PHREEQC was used for this simulation to identify the composition of solutions reacting with subsurface mineral assemblages and identify any phases that may precipitate. PHREEQC is distributed and maintained by the U.S. Geological Survey.

### The Computer Program PHREEQC

The computer code PHREEQC is based on an ion-association aqueous model with capabilities for speciation and saturation-index calculations, and other calculations involving mixing of solutions, mineral and gas equilibria, and ion-exchange reactions. The model uses thermodynamic data to simulate equilibrium conditions between different phases. A manual detailing the theory and operation of this program is available (Parkhurst 1995). This program and its precursor, PHREEQE, have been used for over 15 years for modeling surface and subsurface aqueous geochemical reactions.

### Application of PHREEQC to 100-D Ponds

The computer model PHREEQC calculates geochemical conditions at *equilibrium*, which necessitates the assumption that water-rock contact time is adequate to achieve equilibrium conditions. This was probably not the case during much of the time the ponds were active as an effluent disposal facility, because large amounts of water were discharged in a short time period and quickly reached the groundwater table. Evidence of this can be seen from a January 1993 incident where 1,136,000 liters of water from the settling basins were inadvertently emptied into 100-D Ponds (Alexander 1993). A rise of several centimeters was measured in most of the monitoring wells within several days of this discharge, indicating fast infiltration rates and thus little time for equilibration to occur.

After discharges to the ponds ceased in June 1994, recharge to the vadose zone beneath the ponds effectively ceased and travel time for residual vadose zone waters increased. This residual water had longer to react with the ash and Ringold Formation and was more likely to be at equilibrium with the solid phases. The assumption of equilibrium should yield the most dissolution and precipitation and thus represents a "worst case" situation.

PHREEQC invokes a separate database file for the requisite thermodynamic data on the components, species, and phases necessary to perform the calculations. The database used for this modeling effort was adopted from the program MINTEQ, which has a comprehensive list over 1,100 species and more than 500 phases.

**Methodology**. The modeling parameters were formulated to mimic the reactions that would be expected to occur beneath 100-D Ponds. PHREEQC allows several steps to be performed in one run; the output gives the results of each step and the final result of the run. For 100-D Ponds, the various steps were as follows:

1. React infiltrating water with coal ash underlying the ponds,
2. React the solution derived in step 1 with minerals typical of the Ringold Formation,
3. Mix this solution with groundwater, maintaining equilibrium with the Ringold Formation.

The initial solution composition and coal ash composition were selected without precise knowledge of their chemical properties. Ideally, the infiltrating water would be defined by some average or upper statistical bound of the effluent composition released into 100-D Ponds. This information is not available, so the actual composition used was a combination of average Columbia River water for the major elements (PNL 1994) and the average of TCLP analyses performed on the sediments at the bottom of the settling pond for the metals (BHI 1995). The Columbia River is a likely primary water source, as approximately 200 million liters of Columbia River water were received from the water treatment facility during operation of the ponds. The rationale for using TCLP analyses for metals is that the maximum concentration of metals in infiltrating water would be the leachate from the contaminated sediments; TCLP analyses represent the "worst case" leachate likely to be produced from a sample.

Reaction of a solution with a solid requires the mineral phases of the solid to be known. Lacking mineral analyses of the coal ash, appropriate phases were chosen from published tables of mineral constituents in ash from various coals (Falcone and Schobert 1986). The minerals anhydrite ($CaSO_4$), quartz ($SiO_2$), and hematite ($Fe_2O_3$) were used to represent the coal ash in the PHREEQC program. In addition, calcium hydroxide in the form of portlandite ($Ca(OH)_2$) was included as a mineral phase in the ash because high calcium contents are typical of subbituminous coal (Huffman and Huggins 1986), which was the type used at Hanford.

The solution resulting from reaction of the infiltrating water with coal ash was then reacted with minerals typical of the Ringold Formation. These include quartz, plagioclase feldspar, calcite, and montmorillonite.

The third step was performed to determine if precipitation of any mineral phases was likely to occur when the reacted water was mixed with groundwater. The groundwater chosen was an average of pre-1994 analyses from the upgradient monitoring well, 199-D5-13. The restriction on the date was necessary because this well started to become contaminated with chromium and other constituents (Figure 5) from upgradient sources in 1995, due to dissipation of the groundwater mound beneath the ponds as discharges diminished and finally ceased in June 1994.

**Results of Modeling**. The model PHREEQC was run with the above inputs. The output produced by the program contains the composition of the modeled solution after each step, the distribution of the various aqueous species, and the saturation index of all minerals in the thermodynamic database that contain the components considered in the aqueous and solid phases. Phases that are in equilibrium with the solution have a saturation index equal to 0. Phases with a saturation index greater than 0 indicate that they are thermodynamically oversaturated and may precipitate from solution. After each reaction step, those phases with a saturation index greater than 0 were evaluated and allowed to precipitate if they were geologically feasible.

The first step in the modeling procedure was speciating the initial solution, which is Columbia River water with metals from TCLP analysis of the sediments added to it. This solution was then reacted with the vadose zone in two steps. Reaction with ash materials resulted in precipitation of a small amount of barium arsenate, Ca-nontronite (a member of the smectite group of clay minerals), hematite, and sepiolite (a member of the palygorskite group of clay minerals). The minerals anhydrite, portlandite, and quartz reacted with the solution to form the precipitates. The composition of the solution and mass of precipitates and reactants are listed in Table 1.

The calculated pH of the vadose zone solution in equilibrium with coal ash phases is 12.3. The portlandite, a hydrous lime mineral, is responsible for the high pH. The model inputs were varied to determine the influence of small amounts of portlandite in the system, simulating a situation where preferred pathways through the coal ash were used for transport from the surface to the water table and reactive surfaces of portlandite are neutralized. The qualitative result is that only a small amount of portlandite in the system is necessary to increase pH above 12.

The water-ash solution was then equilibrated with minerals typical of the Ringold Formation. This resulted in albite, calcite, and montmorillonite reacting to precipitate anorthite and quartz, with no change in pH of the solution.

The solution produced by reaction with vadose zone minerals was then mixed with groundwater at a ratio of 10% meteoric water to 90% groundwater. This mixing and precipitation of plagioclase, calcite, and montmorillonite reduced the pH to 9.7. Barium arsenate and lead hydroxide are also identified as supersaturated phases in PHREEQC, although the amounts of precipitate are very small (Table 1). Small amounts of hematite, quartz, and boehmite were consumed in this reaction.

## CONCEPTUAL MODEL

The soil, groundwater, and geochemical modeling data presented above can be combined into a conceptual model to describe the interaction of the percolating fluid with subsurface materials and groundwater. This conceptual model considers the entire aqueous system associated with 100-D Ponds, including interaction with sediments, vadose and saturated zone materials, and groundwater. The model is presented in Figure 7 and described in the following steps:

**Table 1. Results from Geochemical Modeling of 100-D Ponds, Using PHREEQC. Solution compositions in mg/L.**

| Analyte | Beginning Solution, Col. R. water + TCLP* | Solution after Reaction w/ ash | Solution after Reaction w/ Ringold | Ave. Upgradient, Well D5-13 | Mix 10% Ringold 90 % Upgradient | Solution, Mixed water w/ Ringold | Average Comp. of Downgradient Wells |
|---|---|---|---|---|---|---|---|
| Al | 1.28E-03 | 0.0000 | 9.90E-02 | 8.10E-02 | 8.28E-02 | 2.51E-01 | 2.60E-01 |
| As | 1.00E-01 | 8.92E-02 | 8.92E-02 | 4.30E-03 | 1.28E-02 | 1.29E-08 | 2.61E-03 |
| Ba | 3.00E-02 | 6.46E-07 | 6.46E-07 | 8.00E-02 | 7.20E-02 | 3.69E-02 | 2.96E-02 |
| Ca | 21.25 | 5599.2 | 5567.1 | 43.73 | 596.0 | 218.04 | 25.46 |
| Cl | 1 | 1.000399 | 1.000399 | 11.801305 | 10.72 | 10.720080 | 3.31 |
| Cr | 1.50E-02 | 1.50E-02 | 1.50E-02 | 7.50E-02 | 6.91E-02 | 6.90E-02 | 6.43E-02 |
| F | 1.00E-01 | 1.00E-01 | 1.00E-01 | 2.93E-01 | 2.74E-01 | 2.74E-01 | 1.92E-01 |
| Fe | 3.50E-02 | 7.84E-07 | 1.19E-03 | 2.52E-01 | 2.27E-01 | 1.49E-09 | 6.01E-01 |
| Hg | 2.00E-04 | 2.00E-04 | 2.00E-04 | 2.00E-04 | 2.00E-04 | 2.00E-04 | 8.60E-05 |
| K | 1.1 | 1.10 | 1.10 | 3.56 | 3.32 | 3.31 | 3.00 |
| Mg | 5.1 | 7.20E-06 | 1.14E-03 | 111.024 | 99.94 | 5.64E-09 | 3.50 |
| N | 2.00E-01 | 2.00E-01 | 2.00E-01 | 23.41 | 21.10 | 21.09 | 2.03 |
| Na | 2.15 | 2.15 | 38.37 | 5.66 | 8.932 | 8.856 | 4.29 |
| Pb | 1.00E-01 | 1.00E-01 | 1.00E-01 | 5.00E-03 | 1.45E-02 | 7.83E-04 | 2.61E-03 |
| S | 11 | 281.2 | 281.2 | 17.59 | 43.94 | 43.935900 | 22.86 |
| Si | 17.8 | 3455.1 | 3457.9 | 5.21 | 350.3 | 2.876416 | |
| V | 2.00E-03 | 2.00E-03 | 2.00E-03 | 0.00E+00 | 2.00E-04 | 2.00E-03 | 1.07E-02 |
| pH | 8.6 | 12.328 | 12.328 | 7.98 | 11.861 | 9.659 | 8.46 |
| | **Phase** | **mg/kg** | | | **Phase** | **mg/kg** | |
| Precipitate: | Ca-nontronite | 0.061 | | | Ba3(AsO4)2 | 0.059 | |
| | Ba3(AsO4)2 | 0.05 | | | Anorthite | 2316 | |
| | Hematite | 0.027 | | | Albite | 0.53 | |
| | Sepiolite | 32.2 | | | Calcite | 110.2 | |
| | Anorthite | | 218.6 | | Montmorillonite | 3147 | |
| | Quartz | | 187.0 | | Pb(OH)2 | 0.016 | |
| Reactant: | Anhydrite | 624.5 | Albite 413.1 | | Hematite | 148.6 | |
| | Portlandite | 9670 | Calcite 0.448 | | Quartz | 2198 | |
| | Quartz | 7398 | Mont. | | Boehmite | 1869 | |

* Average TCLP analyses of sediments for Ba, Cd, Cr. Hg, Pb, Sb, V, and Zn.

*1. Effluent discharged to the ponds consisted predominately of releases from the 183-D water storage basins.*

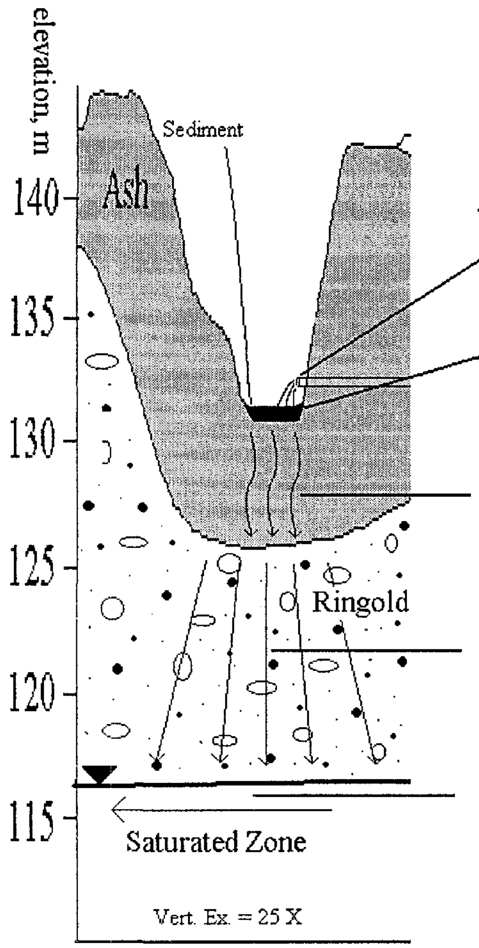
These releases consisted of backwash from the multimedia water filters and effluent released from semi-annual washdowns of the water storage basins. This latter effluent consisted of treated water, Columbia River sediment, and flocculent.

*2. The effluent deposited and reacted with flocculent in the upper portion of the settling pond.*

The flocculent served to trap ions, small particles, and colloids in the water treatment facility and after deposition in the pond. This effectively immobilized the contaminants which were discharged from the laboratories.

*3. The effluent percolated through the coal ash underlying the ponds.*

The percolating solution reacted with the coal ash phases, increasing the pH of the solution to 12.3 and its calcium and sulfur contents.



| Physical Process | Conceptual Model |
|---|---|
| 1. Effluent Discharge | Bulk of influent is Columbia River water |
| 2. Flocculent + Sediment Deposited | Flocculent traps and immobilizes contamination discharged from laboratories |
| 3. Percolation through ash | Reaction with coal ash increases pH of solution, along with calcium and sulfur content |
| 4. Solution moves through unsaturated Ringold Fm. | Solution reacts with Ringold Fm. to dissolve and precipitate several rock-forming minerals |
| 5. Solution enters groundwater | Solution decreases in pH as it reacts with groundwater; minor dissolution and precipitation |

**Figure 7. Schematic Representation of Conceptual Model for 100-D Ponds Vadose Zone.**

4. *The solution continued through the coal ash and into the Ringold Formation.* Geochemical modeling shows some dissolution and precipitation of several rock-forming minerals, but no significant precipitation of heavy metal compounds.

5. *The solution entered the groundwater.* Modeling shows that pH decreases to 9.7, similar to measured values. The predominant solid reactions are quartz and hematite dissolving to form montmorillonite and plagioclase feldspar. Very small amounts of barium, arsenic, and lead phases precipitate as solids.

The conclusion from this conceptual model is that virtually all of the contamination contributed to 100-D Ponds was trapped in the sediments deposited in the settling pond (Figure 6). None of the data examined indicate that this TSD has contributed significant amounts of heavy metals to the vadose zone or groundwater beneath the ponds.

# CONCLUSIONS

The 100-D Ponds received effluent from several different sources in the 100-D Area. The water treatment facility was the source of the greatest volume of effluent, which contained flocculent and sediment entrained in Columbia River water. The laboratories that discharged to the process sewer system contributed a much smaller volume of contaminants but were the likely sources of contaminants such as PCBs.

Data from over 6 years of groundwater monitoring demonstrate that operation of 100-D Ponds has not had an adverse effect on groundwater. None of the contaminants associated with sediment in the ponds are elevated in groundwater, and most analyses of contaminants from the downgradient wells are below detection limit. Levels for all contaminants are below MTCA Method B groundwater standards.

Elevated pH values have been recently recorded in two of the three downgradient wells (Hartman 1996). These two wells have historically had higher pH values than the upgradient wells, which is ascribed to the alkaline characteristics of the coal ash underlying and surrounding the ponds. The recent increase in pH in the downgradient wells is probably related to cessation of discharge to the ponds, allowing more time for infiltrating water to be in contact with the ash and more completely approach equilibrium.

Data collected from different depths show that soil contamination in 100-D Ponds was restricted to the upper layer of sediment (Figure 6), and the constituents of interest are not elevated in the ash immediately underlying the sediment. A geochemical model was employed to evaluate the possibility that contaminants were transported through the upper portions of the vadose zone and deposited in sedimentary deposits beneath 100-D Ponds. This process was postulated by Alexander (1993) in a hydrochemical conceptual model that suggested that the abrupt changes in mineralogy between the coal ash-Ringold interface would create a "geochemical trap" for cationic heavy metals. This argument was purely qualitative and based on some assumptions which are not supported by recently collected data. For instance, coal ash was invoked as the source for the heavy metals, but analyses of the ash have shown very low values for leachable heavy metals (DOE-RL 1992). Leachate compositions of samples from surface sediment in the settling pond also show very low levels of leachable heavy metals (e.g., <0.1 ppm lead, <0.02 ppm total chromium; BHI 1995).

The geochemical model PHREEQC was employed to simulate subsurface reactions between water infiltrating from 100-D Ponds and minerals in the vadose zone and saturated zone. The input parameters were chosen to represent an upper bound of values for heavy metals (using results of TCLP analyses from contaminated surface sediments) and caustic conditions (using portlandite as the calcium oxide phase) in the ash beneath the ponds. Results from this quantitative geochemical analysis show only a trace amount of precipitation of heavy metal-containing minerals at the water table. Most minerals containing the constituents of interest are strongly undersaturated, and would not be expected to precipitate.

Results from the PHREEQC model do not perfectly match conditions measured beneath the ponds. For example, the modeled solution has a final pH of 9.7 after mixing with groundwater and precipitation of minerals in the saturated zone. Recent measurements from monitoring wells downgradient of 100-D Ponds had pH values as high as 9.3 (Hartman 1996). Calcium is markedly higher in the modeled solution than in prevailing groundwater conditions, and iron and magnesium concentrations are lower. With the exception of these deviations, results from the modeled solution correspond closely to those in the groundwater and indicate that large amounts of minerals containing heavy metals are not present in the subsurface beneath the ponds.

The chemical and modeling data support the argument that most or all of the contaminants discharged to 100-D Ponds were immobilized in the flocculent and sediment deposited on the surface of the settling pond. This sediment was removed in August 1996, and samples collected from the bottom of the ponds after this removal show no evidence of contamination in the coal ash. The cleanup action, empirical data, and modeling results indicate that the contamination at 100-D Ponds has been successfully remediated and requires no further action.

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# COMPUTERIZED INTEGRATION AND VISUALIZATION OF DATA FOR SITE CHARACTERIZATION

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## ABSTRACT

Expedited site characterization (ESC) emphasizes the use of existing data of sufficient quality, multiple complementary characterization methods, and on-site decision making to optimize environmental site investigations. This requires rapid integration and analysis of large volumes of disparate data. Argonne's ESC process is flexible and adaptable to the unique characteristics of each site. Therefore, integration and visualization of ESC data require a wide range of techniques. This paper illustrates three of these methods: (1) spatial data integration in a geographic information system (GIS), (2) two-dimensional visualization through the use of automated cross section generation, and (3) three-dimensional modeling where data are sufficiently dense.

The Applied Geosciences and Environmental Management Section (AGEM) of the Environmental Research Division at Argonne National Laboratory uses software components that include a GIS, spreadsheets, database management systems, computer-aided design (CAD), graphing programs, geotechnical programs, contouring and modeling software, and custom routines to provide dynamic support for ESC. The best features of each program provide computer visualization that supports geoscientists in making correct, timely, and cost-effective decisions.

## INTRODUCTION

Expedited site characterization is an interactive, integrated process emphasizing the use of existing data of sufficient quality, multiple complementary characterization methods, and on-site decision making to optimize environmental site investigations (Burton and Walker 1997). Argonne's ESC is a flexible process that can be tailored to the unique characteristics of each site, rather than a prescriptive regimen. An important component of ESC is computerized visualization of large volumes of data. Just as not every geoscientific technique works for every site characterization, not every computer program in the ESC suite of visualization applications is suitable for every site. A varying subset of computer programs handles dynamic data requirements to allow rapid integration and visualization of relevant site data.

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# TECHNIQUES

This paper illustrates three techniques of data visualization as applied to ESC: (1) spatial data integration in a GIS; (2) two-dimensional visualization via cross section automation; and (3) three-dimensional visualization where data are sufficiently dense.

One of the hallmarks of successful ESC is the efficient use of existing site data. The goal of the first phase of an ESC investigation is to understand the geologic and hydrogeologic controls on a site. This understanding guides formation of scientific hypotheses to be tested, refined and revised throughout the site work. In preparation for the Phase I work, existing regional and local geographic and geoscientific data are extensively researched. Results of any previous investigations are studied. Preparation of the Phase I work plan usually reveals a large amount of data from various sources that requires organization and analysis. As the on-site investigation begins, the site database grows to even more challenging proportions and diversity. The AGEM suite of computer applications helps the scientists assimilate the growing body of information about the site.

## Spatial Data Integration in a GIS

A GIS provides order for disparate data by allowing spatial access to relevant information as it is georeferenced to the base map. Two current AGEM ESC projects will illustrate ESC GIS and other visualization techniques. The first is a rural site in Kansas where the Commodity Credit Corporation/U.S. Department of Agriculture (CCC/USDA) formerly operated a grain storage facility. As at many similar sites, the grain storage bins were fumigated in the 1950s and 1960s with carbon tetrachloride, a then commonly used pesticide that is now known to be a carcinogen. AGEM is investigating potential groundwater contamination at this site and many other CCC/USDA sites. The second project for illustrative purposes is a study of geology and hydrogeology at Argonne National Laboratory.

Figure 1 shows the integration of an orthorectified aerial photo from the U.S. Geological Survey, a street map, and the various locations of Kansas Department of Health and Environment monitoring wells, domestic wells, public wells, and the former CCC/USDA site. Site data are georeferenced; the system can allow spatial access to related analytics, lithology, and groundwater hydrology. When the user selects a well, a table of recorded parameters is displayed.

Zooming out presents a more regional view. Figure 2 shows the area centered on the town in Figure 1, but covering nearly 400 square miles as compared to less than one square mile in Figure 1. At the regional scale, the GIS incorporates logs from Kansas Geologic Survey test holes and from public and domestic wells, as gathered from publications and agency offices. Through this graphic interface, a geologist can select a line of section at a regional scale. Figure 2 shows the A-A′ section marked for cross section generation.

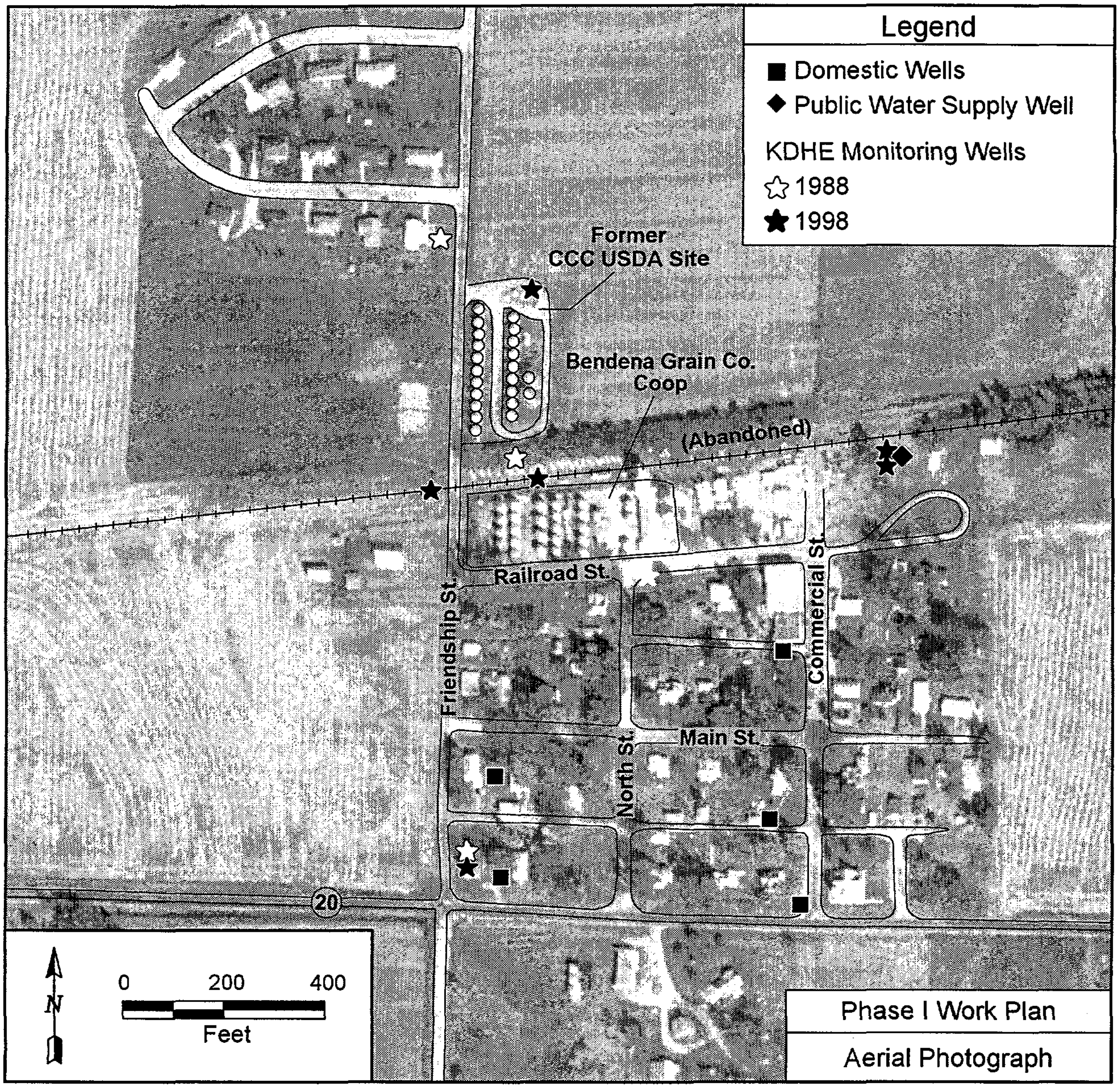

**FIGURE 1** Spatial Database for a Rural Kansas Site, Prepared for the Phase I Work Plan

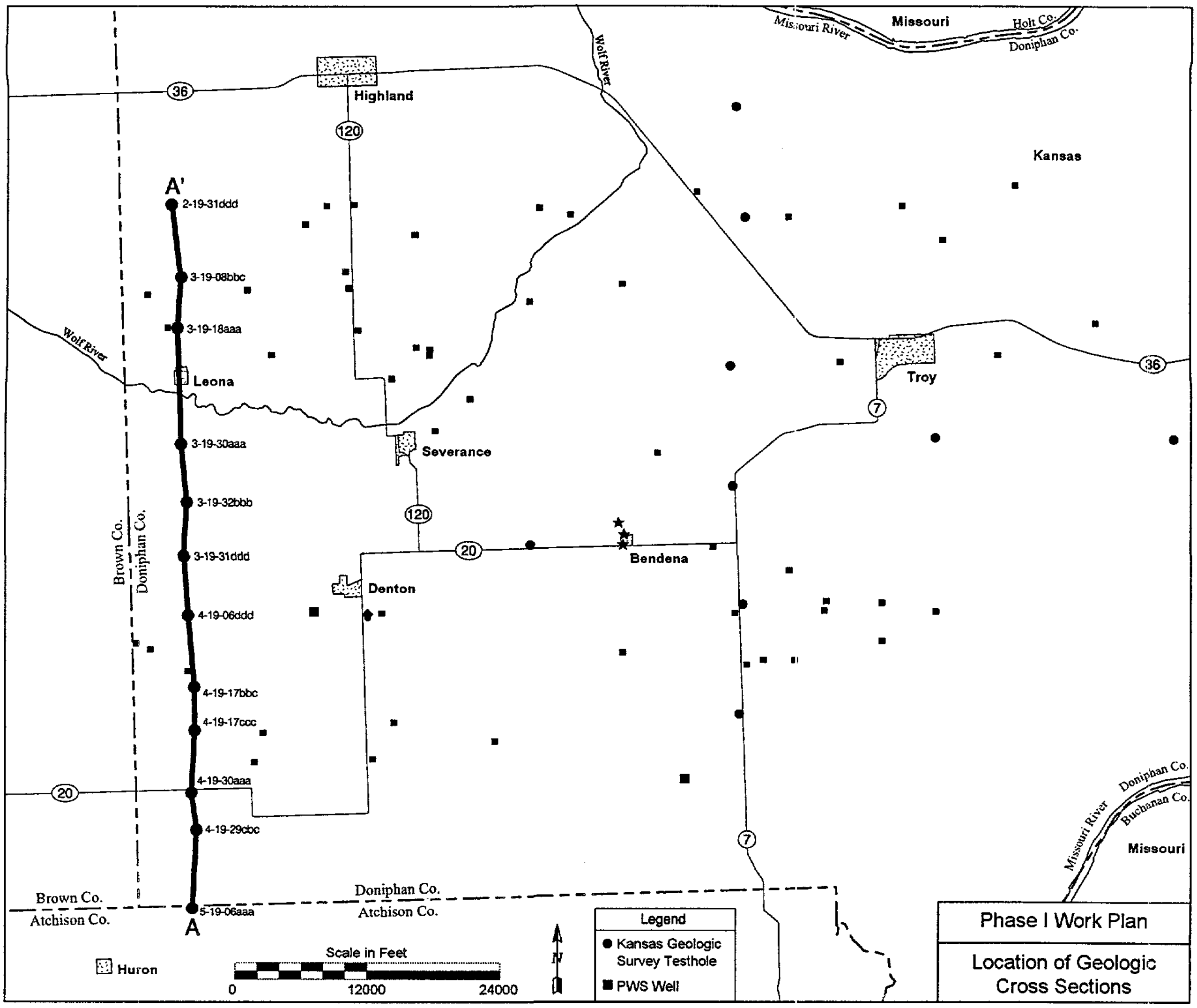

**FIGURE 2** Cross Section Location Selected from Regional View

## Two-Dimensional Visualization: Regional Scale

Lithologic data from the boring locations shown in the GIS become the basis for a cross section that can be automatically generated from the database. A selection like that shown in Figure 2 is automatically entered into a program that generates cross sections in AutoCAD Data Exchange Format (DXF). Figure 3 shows the output generated by this custom routine. The initial cross section output in the work plan phase prints to a large plotter. The section format is designed to include all the descriptive text detail, rather than symbols or patterns. Other section formats include cone penetrometer data curves, downhole geophysics, analytics, or other parameters, in addition to lithologic descriptions. The purpose of this section is to display as much detail as possible to aid the geologist in creating an interpretation. The example in Figure 3 includes extreme vertical exaggeration over the section length of approximately 15 miles

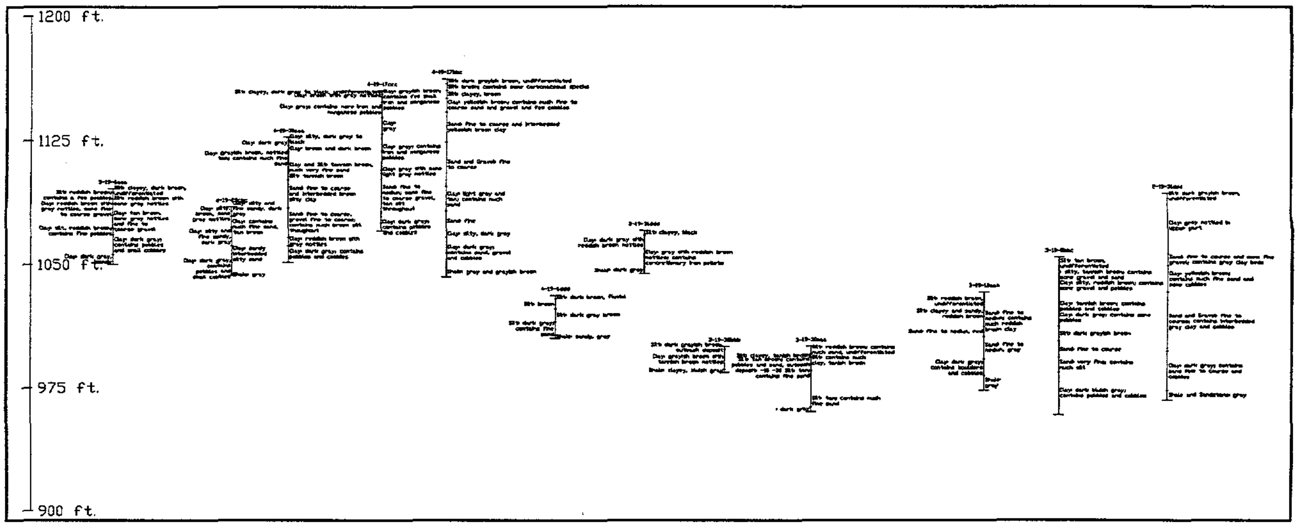

**FIGURE 3** Automated Cross Section, Which Must Be Printed on a Large Plotter to See Detailed Lithologic Descriptions

in order to see the unit descriptions. The DXF file generated by the cross section program is read into AutoCAD for printing, display, and (later) addition of the interpretation.

The skeletal cross section shown in Figure 3 is the basis for the interpretation, shown in Figure 4. The latter figure shows the geologists' interpretation of connections in lithologic units. The simplification from the very detailed descriptions shown previously requires the input and skills of the human experts, not automated computer processing. The computer assists by displaying the complexity, but the scientists do the interpretation.

## Two-Dimensional Visualization: Local Scale

The second example of visualizing the subsurface comes from Argonne National Laboratory, a site very different from the rural CCC/USDA site. Here, in an area of less than two square miles, data exist from nearly 900 wells and borings. In the process of studying the geologic and hydrogeologic controls on the site, the geologists evaluated data from all of these locations and selected 359 logs for their "pick file" database. These logs became the basis for creating a series of 11 detailed cross sections to study very localized subsurface structures. Figure 5 illustrates the clustering of data in several operational areas, along with the lines of section chosen for study. The GIS interface allows selection of these sections to create a table that is input to cross section generating programs.

For each of the 11 selections, the custom program accessed the lithologic database to create a skeletal cross section similar to that of Figure 3. The program also calculated the topography for each line of section by automatically accessing the topographic database at each intersection of the line of section and a contour line. The program then added the line of topography to the section drawing as another DXF layer. One of the final interpreted sections is shown in Figure 6. This example shows a striking contrast in current surface topography compared to the original boring elevations, reflecting the construction of a berm.

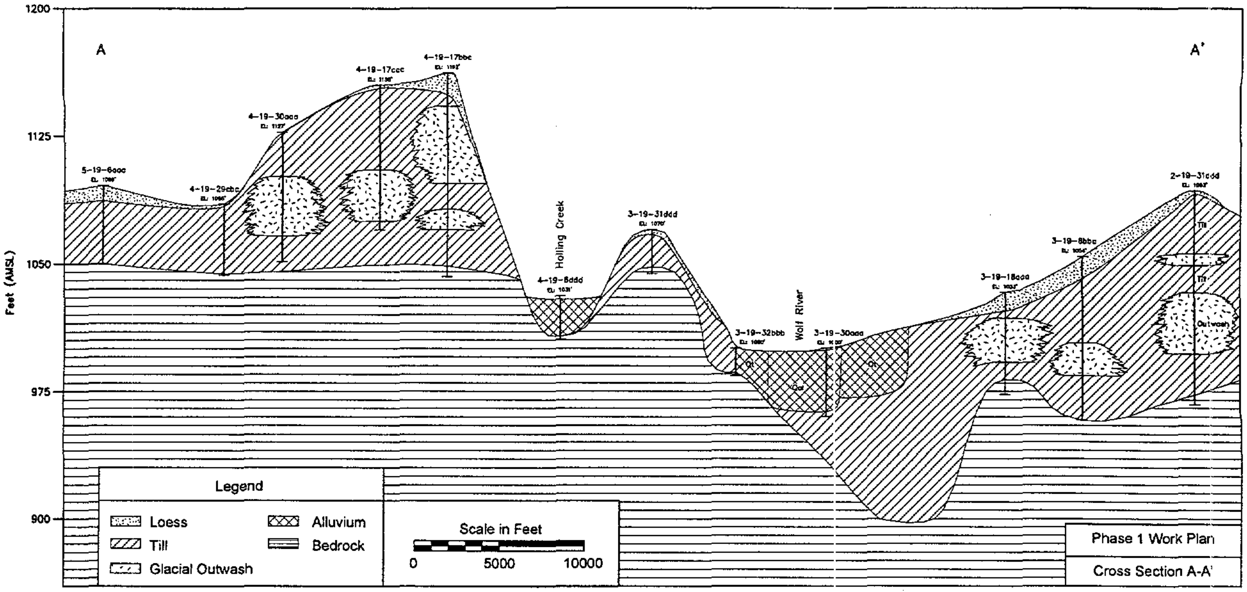

**FIGURE 4** Final Cross Section, Showing Geologists' Interpretation

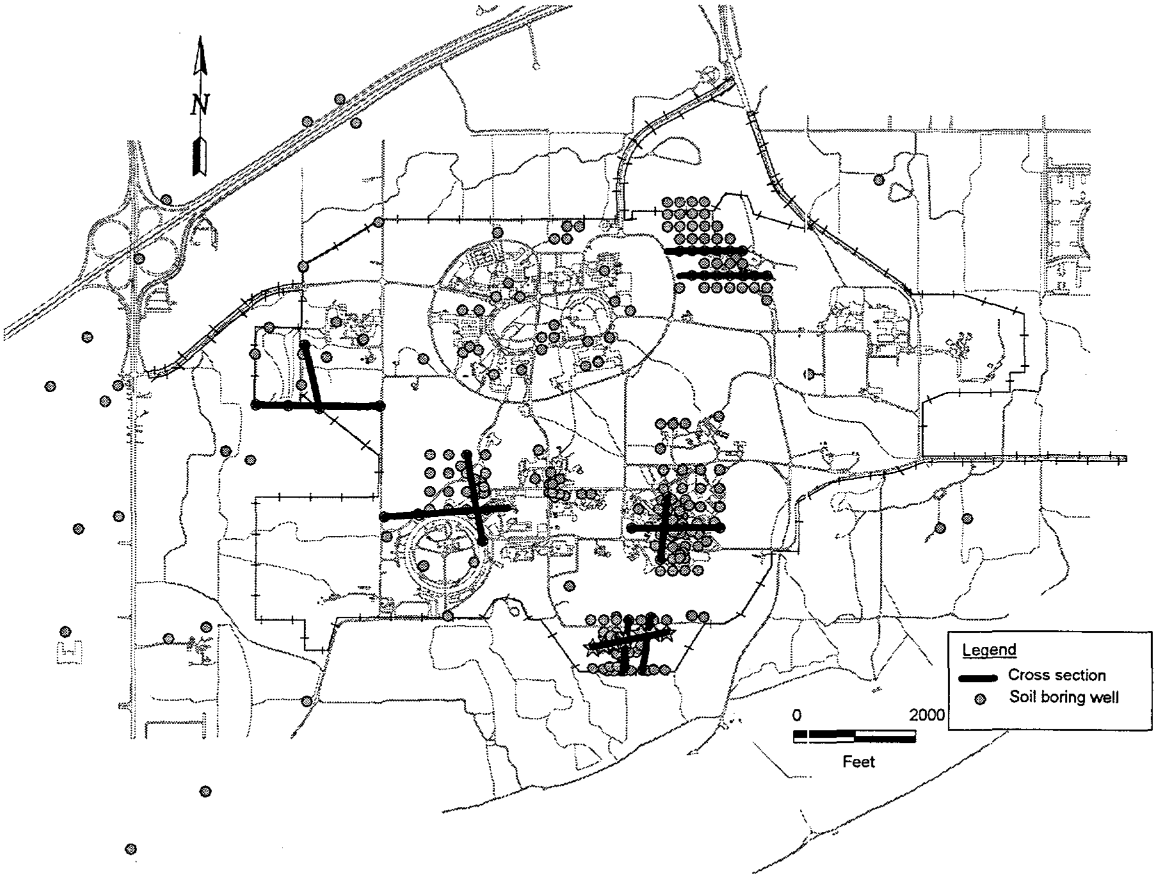

**FIGURE 5** Eleven Cross Sections Selected from a Database of 359 Logs of Sufficient Quality for Detailed Local Study

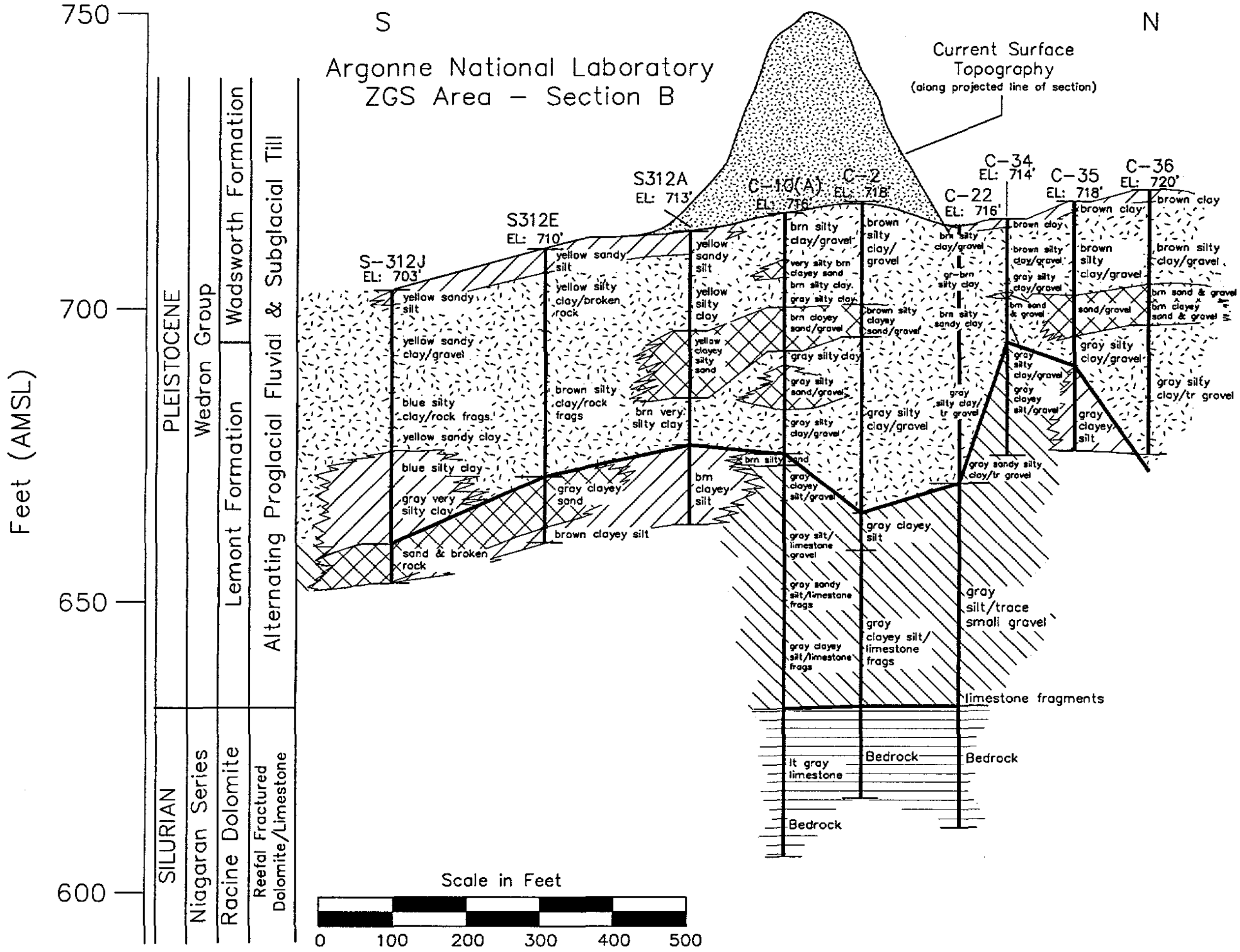

**FIGURE 6** Line of Topography on Interpreted Section, Automatically Generated from Topographic Database

Figure 6 includes the final interpretation that was added manually after analysis by geologists. The ease of automatically generating multiple sections from the database of logs allows greater visual access to the data than would be possible otherwise.

## Three-Dimensional Visualization Where Data Are Sufficiently Dense

As shown by the number of borings in Figure 5, several operational areas at Argonne have been studied extensively over the years. The 317 Area, an early waste disposal site, offered good lithologic information from 110 logs in an area of less than 30 acres. This density provided the data for a three-dimensional model that shows the potential for groundwater movement. The model is not, however, a true representation of geologic units, but shows the generalized distribution of sand and gravel within the local area. The model was developed by dividing the lithologic descriptions into fine-grained and coarse-grained (sand) areas and calculating the percent sand in each five-foot horizontal slice. This description was extrapolated into horizontal cells 50 feet on a side. The resulting matrix is displayed with a color table representing a continuum of percent sand. The black-and-white depiction in Figure 7 represents the model results. However, the color model shows the percent sand differences more clearly. When it is animated by making increasing percentages of sand transparent, the model reveals the sandiest units. At around 25-30% sand, the areas with most potential to allow water movement become apparent, as shown in Figure 8.

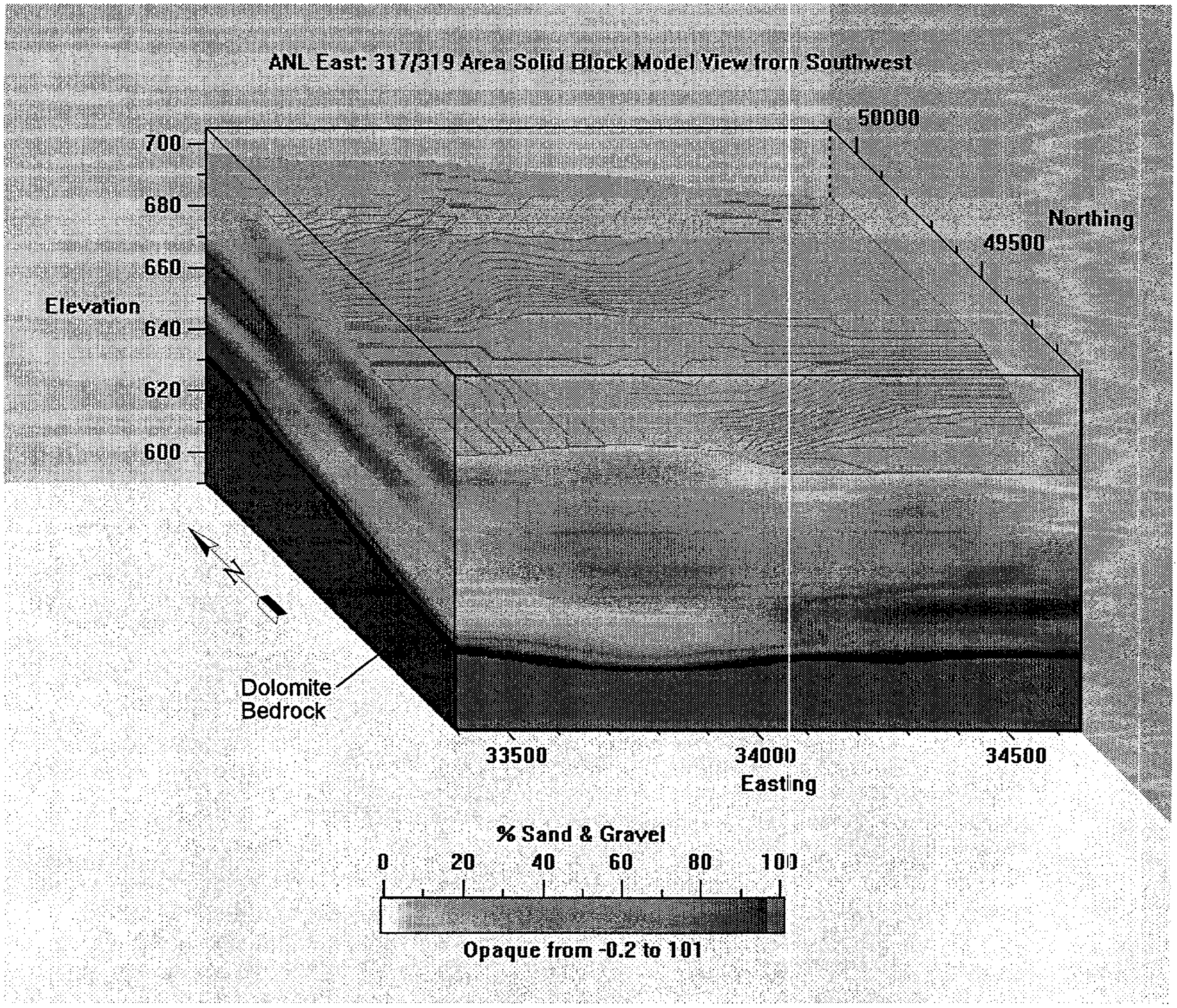

**FIGURE 7** Solid Block Model, Showing Generalized Distribution of Sand and Gravel above the Bedrock Surface

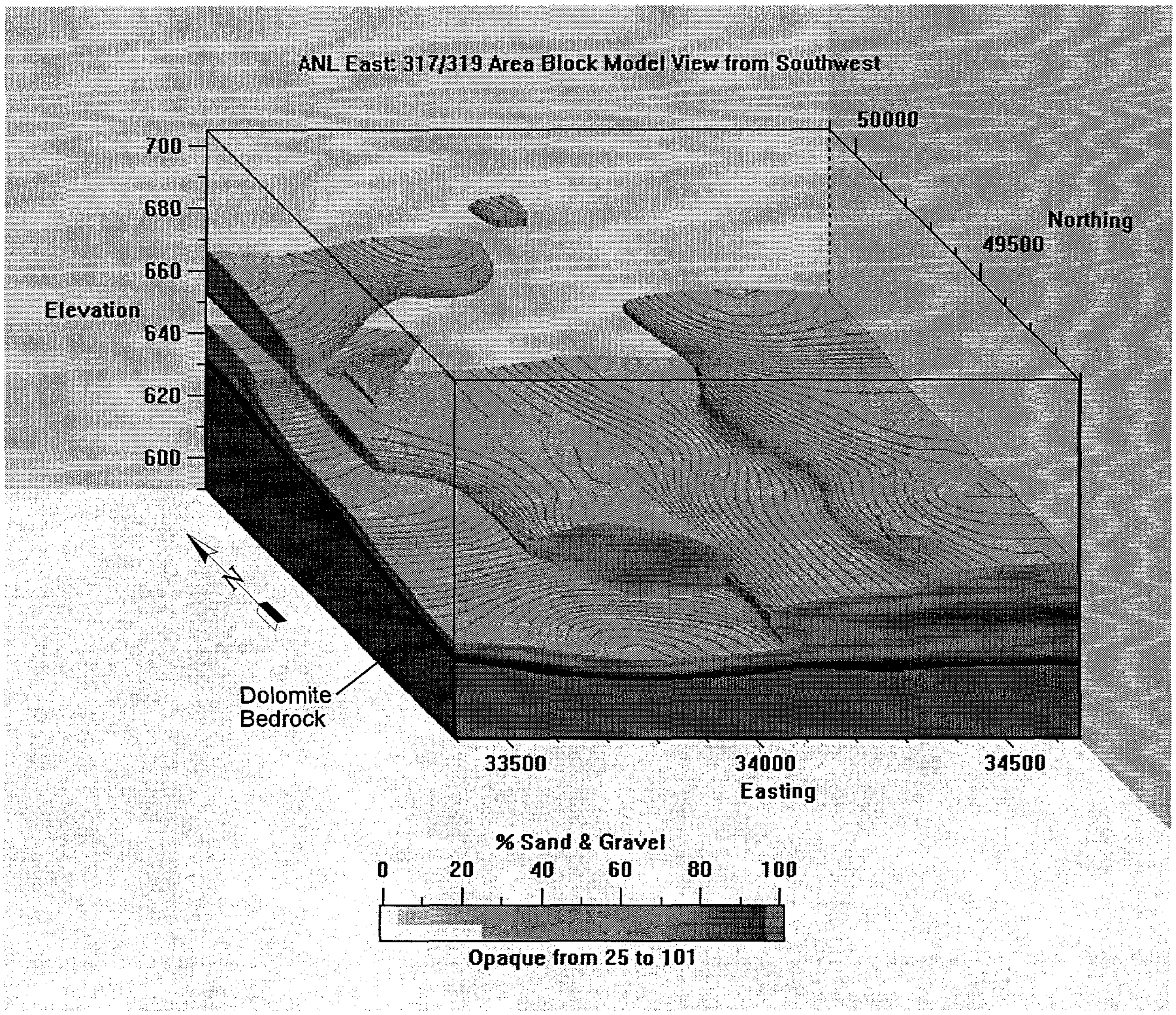

**FIGURE 8** Solid Block Model at about 25-30% Sand, with Areas of Most Potential to Allow Water Movement Becoming Apparent

## CONCLUSIONS

In the AGEM experience, no single computer system has been able to fulfill all data integration and visualization needs. The ESC is a dynamic process, and our computer systems have developed dynamically as well. We are continually establishing the suite of applications that contribute to the ESC process. The key requirement of data integrity is carefully maintained. Our data are accessed via the network and our servers. Few users have write access to the data in our Oracle, FoxPro, and MapInfo databases.

MapInfo provides users with spatial access to our data. One of the strengths of that software is its ability to access data in many formats. We use it to access files directly from Oracle, FoxPro, Excel, Access, and AutoCAD, as well as bitmapped and ASCII text files.

We use geotechnical applications from RockWare, Spyglass, Visual Logic, Golden Software, and AutoDesk. In addition, we have written our own program to automate cross section generation and allow access to data in any of our formats.

Our computer systems have been described as a "software democracy," where every scientist has a favorite, and the challenge is to combine the best features from a wealth of tools. This dynamic mix and our custom routines allow us to integrate input from many data sources and output from many programs. The goal in employing all these systems is data visualization that will guide the geoscientists in making correct decisions.

## ACKNOWLEDGMENTS

R.H. Becker of AGEM did much of the computer programming for the automated cross section generation. W.T. Meyer of AGEM developed the solid block model. The work described was supported by Argonne National Laboratory and by the U.S. Department of Agriculture, Commodity Credit Corporation, under interagency agreement with the U.S. Department of Energy through contract W-31-109-Eng-38.

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# THE ROLE OF THE CONCEPTUAL HYDROGEOLOGIC MODEL IN SITE CHARACTERIZATION AND DYNAMIC RISK ASSESSMENT

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## ABSTRACT

A fundamental aspect of the Expedited Site Characterization (ESC) methodology developed by Argonne National Laboratory is the use of a dynamic conceptual hydrogeologic model to guide site investigations. A preliminary conceptual model is progressively tested and refined as additional data are integrated to yield a more detailed understanding of the physiographic, geologic, hydrologic, and geochemical processes that together control groundwater flow and contaminant migration within the aquifer system. As the conceptual model evolves, the characterization program is tailored to address the specific data needs identified at each stage of the site investigation. Through this approach, technically defensible, process-oriented hydrogeologic and, if necessary, mathematical site models are developed to facilitate the dynamic analysis of risks arising from the distribution, fate, and transport of contaminants at the investigation site.

An overview of site characterization studies conducted for the hazardous waste contamination site in Bruno, Nebraska, is presented to illustrate Argonne's use of this approach in the investigation of a relatively complex groundwater flow and contaminant transport system and in the evaluation of risk. An extended monitoring program was implemented during the characterization of this site, in order to address critical uncertainties in the hydrogeologic factors controlling long-term groundwater flow and contaminant migration. The final conceptual and mathematical site models provided justification for the definition a hypothetical, downgradient residential location as the primary observation point for a risk-based evaluation of remedial alternatives, using Argonne's dynamic risk assessment approach.

## INTRODUCTION

The site characterization methodology developed by Argonne National Laboratory serves as the technical basis for the Standard Provisional Guide for Expedited Site Characterization of Hazardous Waste Contaminated Sites (ASTM 1997). A central theme of the ESC approach is the use of a conceptual hydrogeologic model throughout the site investigation process, as a framework for the selection of appropriate characterization techniques and for the integration and interpretation of site data. Information obtained from the site is used to test and refine the conceptual hydrogeologic model in an iterative process, so that subsequent investigations can be effectively targeted to address critical data needs. Through this approach, technically defensible, process-oriented conceptual and, if necessary, mathematical site models are developed to support the evaluation of risks associated with contaminant fate and transport at the investigation site. To demonstrate Argonne's approach to the use of conceptual hydrogeologic models in site

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characterization and dynamic risk assessment, an overview of studies conducted by Argonne for the hazardous waste site in Bruno, Nebraska, is presented.

## BACKGROUND

Bruno is a small (population 150) agricultural community located approximately 50 mi west of Omaha in Butler County, Nebraska, that was the site of a grain storage facility operated by the Commodity Credit Corporation of the U.S. Department of Agriculture (CCC/USDA) in the 1950s and 1960s. During this period, fumigants containing carbon tetrachloride and carbon disulfide were commonly used within the commercial grain storage industry and by the CCC/USDA for treating grain in storage. Since the mid 1960s, grain storage facilities have been operated at the Bruno site by a number of private and commercial organizations.

All Bruno residents receive their domestic water supply from a municipal groundwater distribution system. Prior to 1990, the municipal system was served by two wells (36-1 and 65-1) located within the limits of the village, as shown in Figure 1. In 1984, routine screening for volatile organic compounds (VOCs) by the Nebraska Department of Health (NDH) identified carbon tetrachloride and chloroform in water from the Bruno municipal system. Follow-up analyses by the NDH and the Region VII U.S. Environmental Protection Agency (EPA) confirmed the presence of carbon tetrachloride and chloroform in the public supply wells at concentrations at or above the maximum contaminant levels for these compounds. The CCC/USDA was identified as one of several potentially responsible parties at the Bruno site. In 1990, the contaminated municipal wells were abandoned and replaced by two new wells, located approximately 1 mi west of the town, that are free of VOCs.

In 1993 the CCC/USDA, working under an interagency agreement with the U.S. Department of Energy, requested Argonne to perform an investigation of the groundwater system at Bruno by using Argonne's QuickSite$^{SM}$ ESC methodology. Bruno was subsequently listed on the CERCLA National Priorities List (NPL) by the Region VII EPA.

## PRELIMINARY HYDROGEOLOGIC MODEL

For use in the formulation of a preliminary conceptual hydrogeologic model for the Bruno area, geologic, hydrogeologic, groundwater geochemical, and basic climatic data of good quality (but of fairly regional scope) were obtained primarily from studies conducted in Butler County by the Nebraska Water Survey (NWS) (Ginsberg 1983). These data were supplemented by geologic logs available for a very limited number of water wells and test borings in the more immediate vicinity of the village. The topographic and physical characteristics of the site were determined from U.S. Geological Survey mapping (USGS 1968) of the Bruno area, from several aerial photos taken during the period of CCC/USDA operations at the site, and from Argonne staff visits to the site and discussions with residents of the community.

The preliminary conceptual model assembled for the Bruno hydrogeologic system is illustrated in Figures 2 and 3. Bruno lies within an area of rolling hills, bluffs, ridges, and narrow, deeply incised creek valleys developed in the thick Pleistocene loess that blankets the southeastern third of Butler County. The village is sited on the relatively steep southeastern flank

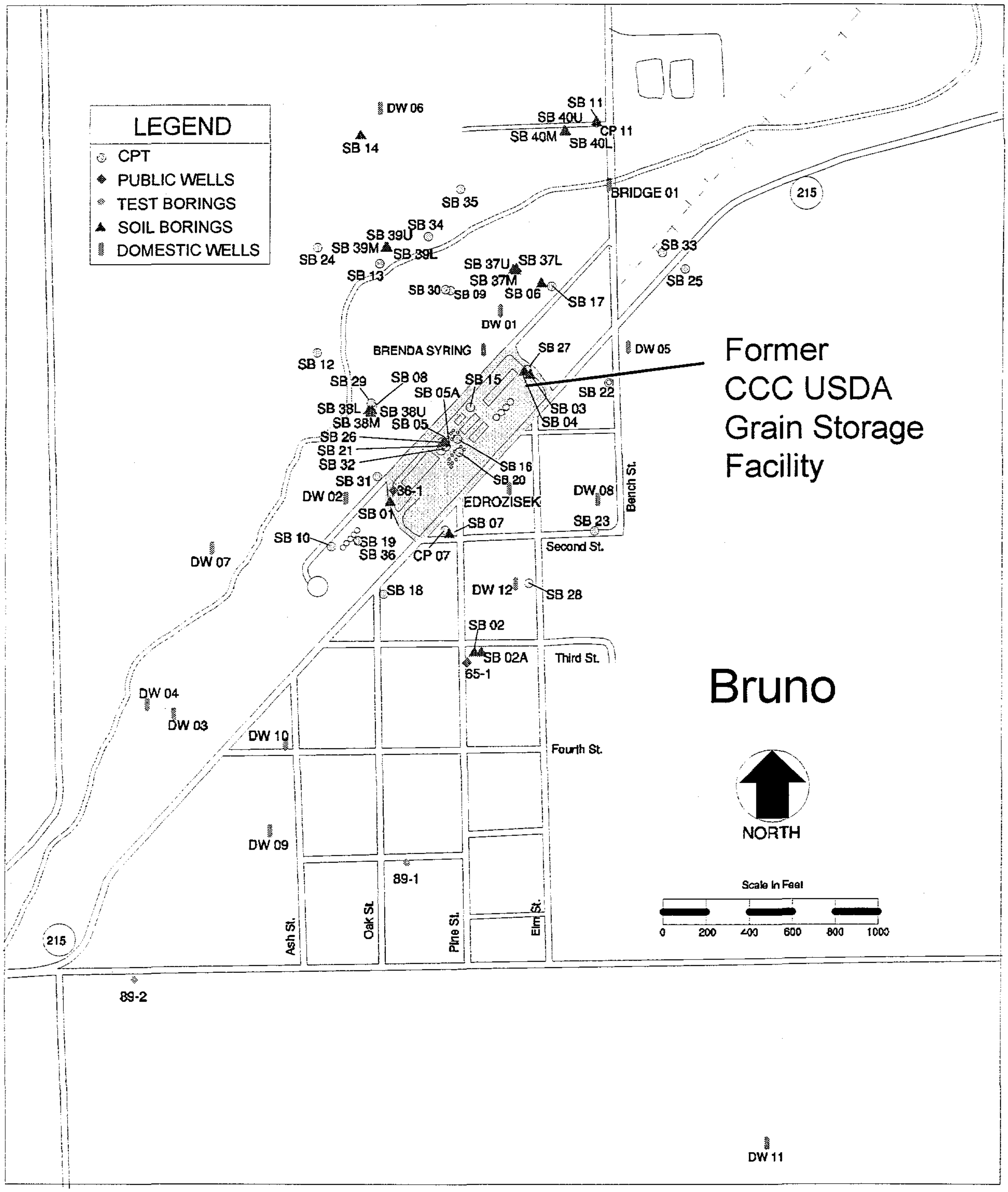

**FIGURE 1** Map Showing Locations of All QuickSite$^{SM}$ Phase I, Phase II, and Extended Monitoring Activities

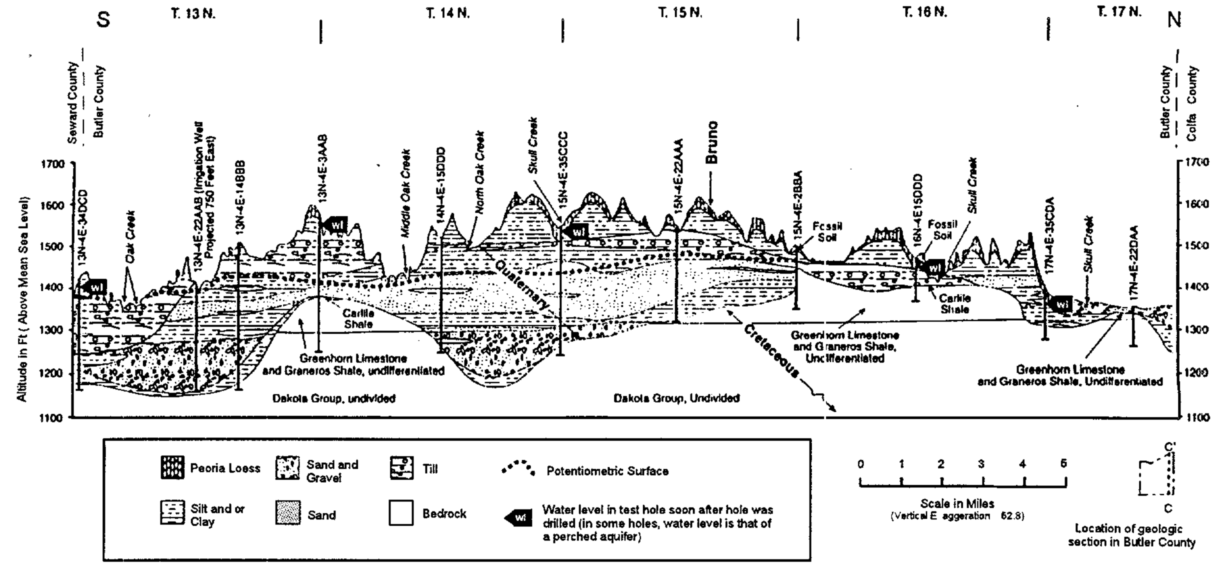

**FIGURE 2** South-North Geologic Section through the Eastern Part of Butler County, Nebraska (Source: Ginsberg 1983)

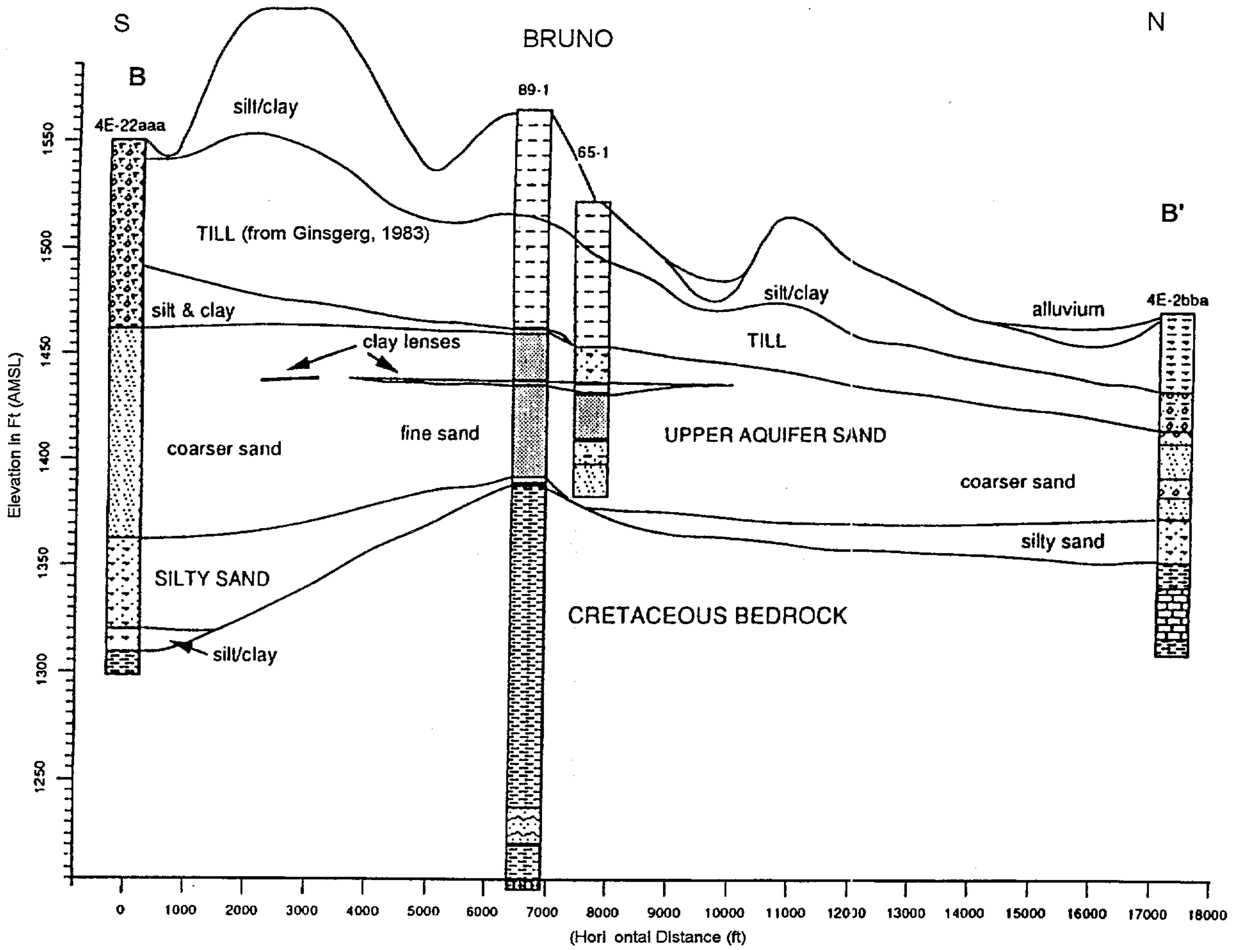

**FIGURE 3** South-North Geologic Cross Section through Bruno, Nebraska

of one such northeastward-draining ephemeral creek, in which water levels rise 10 ft or more in response to heavy rains.

The general geologic and hydrogeologic setting of the Bruno area is represented in a south-north cross section (Figure 2) lying approximately 1 mi east of the village. The surficial loess overlies a variable sequence of glacial till and proglacial to glaciofluvial silts, sands, or sands and gravels deposited over an irregular Cretaceous bedrock surface. These Pleistocene deposits form the only groundwater reservoir of significance in eastern Butler County. The regional cross section suggests that the Pleistocene deposits thin northward and are absent 2-3 mi north and northwest of the village. Bedrock units in the vicinity of Bruno consist of relatively impermeable limestones and shales. Regional mapping of an average potentiometric surface for the Pleistocene aquifer sequence, based on sparse well control, suggested a general northwestward direction of groundwater flow across the Bruno area.

Drillers' logs were available for only three borings located within roughly 0.5 mi of Bruno, precluding the development of a detailed local geologic or hydrogeologic picture for the site. A north-south cross section tying two of these wells to two wells in the regional section (Figure 2) is shown in Figure 3. The logs for these wells suggest the local presence of a bedrock high beneath the town, as well as a possible clay aquitard within the relatively flat-lying sandy aquifer unit, overlain by till and surficial loess. No groundwater levels or flow data for wells in the town were available. Information on the distribution of VOC contaminants within the aquifer system was limited to the results obtained for the public water supply wells by the NDH and the EPA, described above.

## PHASE I AND PHASE II STUDIES

A phased program of field investigations was conducted at the Bruno site, in order to develop the conceptual model of groundwater flow and contaminant transport within the aquifer system. Phase I of the Bruno ESC study focused primarily on defining the local stratigraphy, hydrostratigraphy, and patterns of groundwater movement at the site. Information obtained from the Phase I studies was used to guide detailed groundwater sampling and supplemental hydrogeologic studies during Phase II of the investigations.

Six conventional borings were drilled to provide a detailed record of lithologic variations within the Pleistocene sequence (see Figure 1). Boring SB01D and portions of borings SB02 and SB03 were continuously cored, and all borings were logged geologically and geophysically. All additional activities at the site were performed by using an electronic cone penetrometer (ECPT) variably equipped with soil sampling, groundwater sampling, or physical and geophysical logging probes. Experimental calibration of the ECPT log responses was first performed adjacent to the continuously cored borings, to verify that the mechanical and geophysical profiles obtained with the ECPT probe could be used as a tool for correlation of the main lithologic intervals identified from the geologic logs and for the selection of sampling intervals at uncored locations. Groundwater sampling was performed at selected depths by using the HydroPunch II during the drilling of the conventional boreholes, as well as with the ECPT, to develop vertical profiles of the variations in groundwater geochemistry and contaminant distribution within the aquifer system. The six conventional borings were completed as temporary well pairs screened in the upper and lower portions of the aquifer system (see below), to permit the periodic determination of groundwater levels and flow directions during the investigations. A single piezometer (SB25) was also installed in the upper portion of the aquifer to extend the water level observation network in this aquifer interval. Aquifer tests were conducted by pumping of the former public water supply wells 36-1 and 65-1, two temporary wells in the lower portion of the aquifer, and one temporary well in the upper portion, to estimate the hydraulic properties of the aquifer materials.

## REVISION OF THE PRELIMINARY CONCEPTUAL MODEL

The ESC hydrogeologic investigations confirmed the surficial silt/loess; Cretaceous bedrock; and generally flat-lying, predominantly sandy units predicted from the preliminary hydrogeologic model; however, no distinct glacial tills (as suggested from previous drillers' logs) were identified within the study area. A persistent intermediate layer of clay was also not identified; a finer-grained zone of variable thickness and lithology, consisting of silts, silty sands, and clayey silts, was penetrated in most borings, separating the sandy unit into upper and lower zones.

The ECPT logs and boring data were used to map the distribution and thicknesses of the upper and lower sandy zones and the intermediate silty unit, as shown in Figure 4. The subsurface topography on the upper surfaces of the upper sandy zone and the silty unit, in particular, roughly mirrored the modern land surface, suggesting that paleodrainage patterns during the deposition of these sediments may have been similar to those of the present drainage system. Examination of the results in the context of the available regional geologic control supported the interpretation that deposition of the intermediate silty unit was restricted to the paleodrainage valleys and that this unit is not areally extensive.

Groundwater geochemical (major cations, anions, trace metals) and isotopic (carbon, oxygen, deuterium, and tritium) analyses demonstrated a common origin for groundwater throughout the Bruno aquifer system, as the probable result of fairly local, geologically recent infiltration of precipitation. Subtle variations in the distribution of these parameters suggested, however, that vertical hydraulic communication between the upper and lower sandy zones of the aquifer system might be partially or locally impeded by the intermediate silty unit within the study area. This interpretation was independently corroborated by manual water level measurements made in the network of monitoring wells in the upper and lower sandy zones.

Groundwater levels throughout the aquifer system rose during the monitoring period, as shown for the upper sandy zone in Figure 5. The observed water level trends within each aquifer zone and for the upper and lower wells in each well cluster differed significantly, however, indicating a complex, time-varying pattern of both horizontal and vertical hydraulic gradients across the Bruno site. A transient reversal of the apparent groundwater flow direction in the upper sandy unit and a northwestward shift in the lower sandy zone were observed to correspond with a period of very heavy rainfall, high surface runoff, and rapid groundwater rise near the creek during summer 1994.

Estimates of horizontal hydraulic conductivity ($K_h$) for the upper and lower sandy units were obtained from the aquifer pumping tests. These results also suggested low vertical hydraulic conductivity ($K_v$) within the silty unit south and west of the former CCC/USDA facility, with slightly greater $K_v$ toward the north and east.

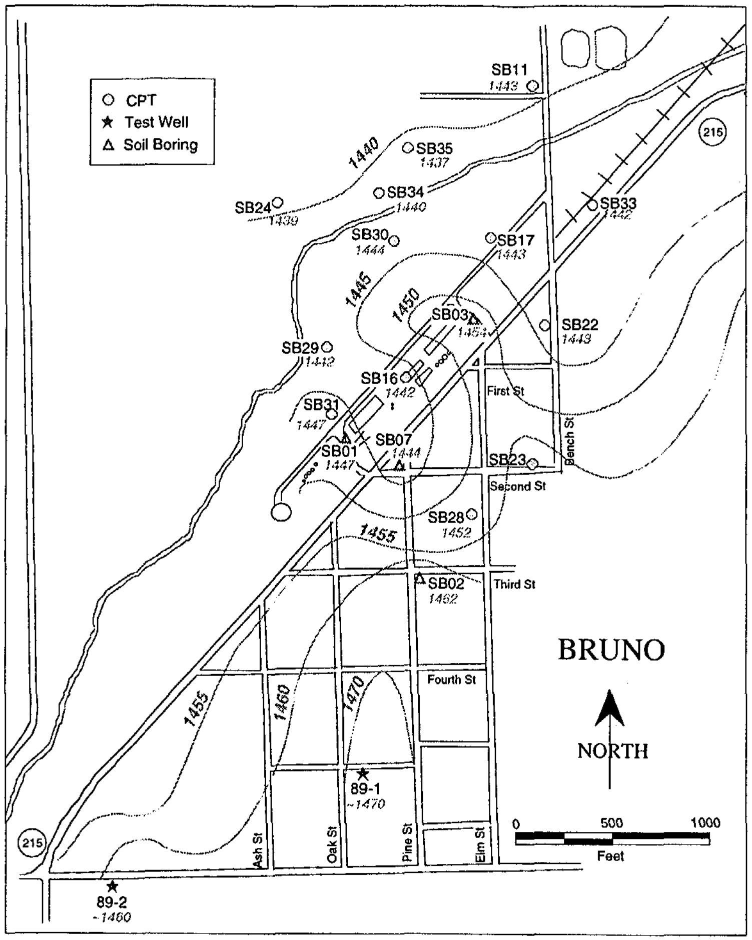

FIGURE 4A Elevation Map (ft AMSL [above mean sea level]) Constructed for the Top Surface of the Upper Sand Zone, Based on Soil Boring and Electronic Cone Penetrometer Data

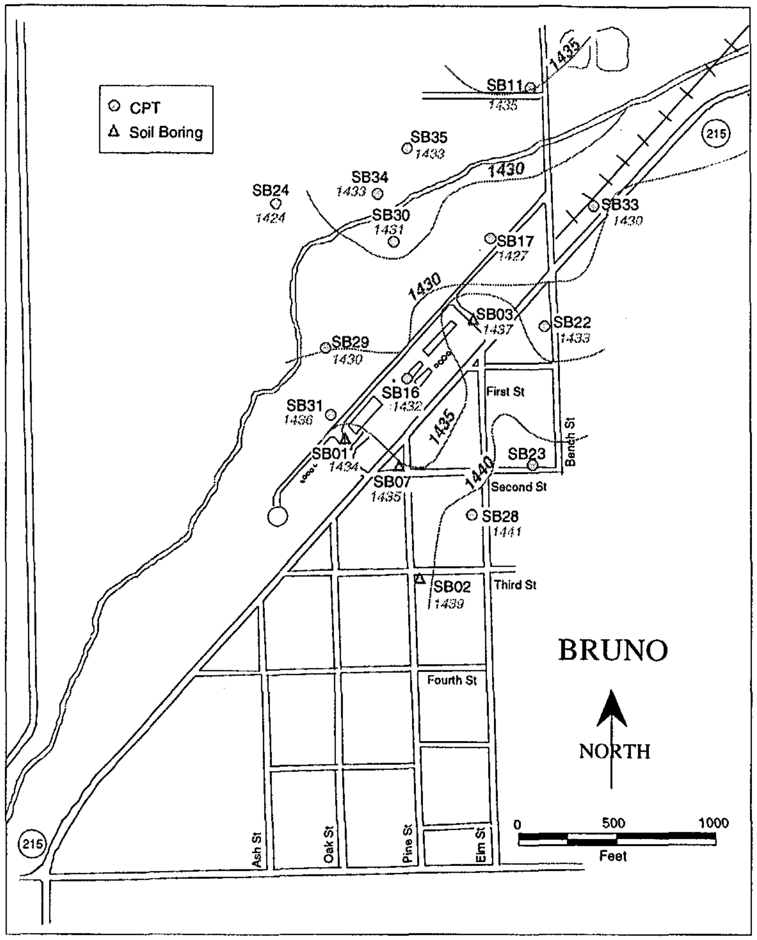

FIGURE 4B Elevation Map (ft AMSL) Constructed for the Top Surface of the Middle Silty Zone, Based on Soil Boring and Electronic Cone Penetrometer Data

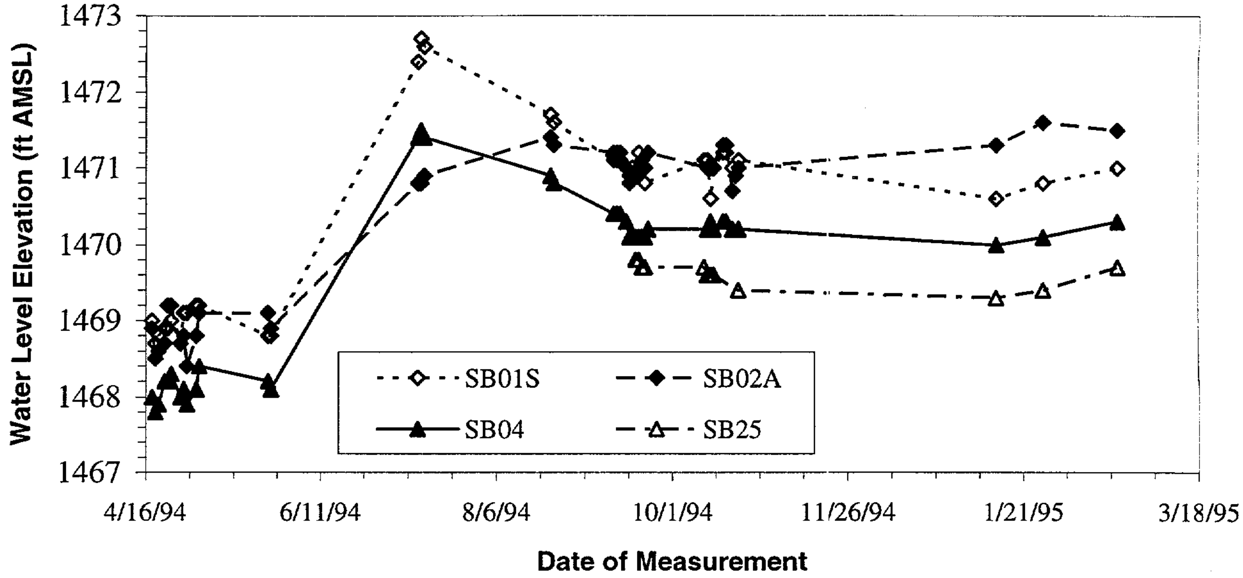

**FIGURE 5** Hand-Measured Water Levels for the Upper Sandy Zone, Spanning the Period of Phase I and Phase II Investigations

Groundwater analyses for VOCs revealed a general pattern of carbon tetrachloride distribution within all three zones of the aquifer system (see Figure 6) that was consistent with an apparent net northward to northwestward movement of groundwater; however, this pattern suggested that the vertical and areal distribution of the contamination within the aquifer system was relatively complex.

## PRELIMINARY MATHEMATICAL AQUIFER MODELING

The ESC investigations defined a conceptual hydrogeologic model for the Bruno groundwater flow system that built on the preliminary model but added significantly greater complexity. The results suggest that the combined effects of regional recharge to the aquifer system; localized, nonuniform recharge to the upper and lower sandy zones in the low-lying area adjacent to the creek; and inferred variations in the vertical and horizontal hydraulic conductivities of the intermediate silty unit could in large measure account for both the variable groundwater flow patterns and the irregular distribution of carbon tetrachloride contamination observed in the Bruno aquifer system.

To examine this conceptual model, preliminary numerical models of groundwater flow and contaminant transport were constructed and calibrated by using the geologic, hydrologic, and groundwater geochemical constraints obtained from the field investigations. Sensitivity testing of these numerical models indicated that uncertainties in (1) the detailed lithologic and hydraulic characteristics of the intermediate silty unit, (2) the potential for locally preferred groundwater flow and contaminant migration pathways within the aquifer system, and (3) the relative frequency and potential longer-term significance of the seasonal shifts in groundwater flow directions observed at the site limited Argonne's ability to reliably predict the future

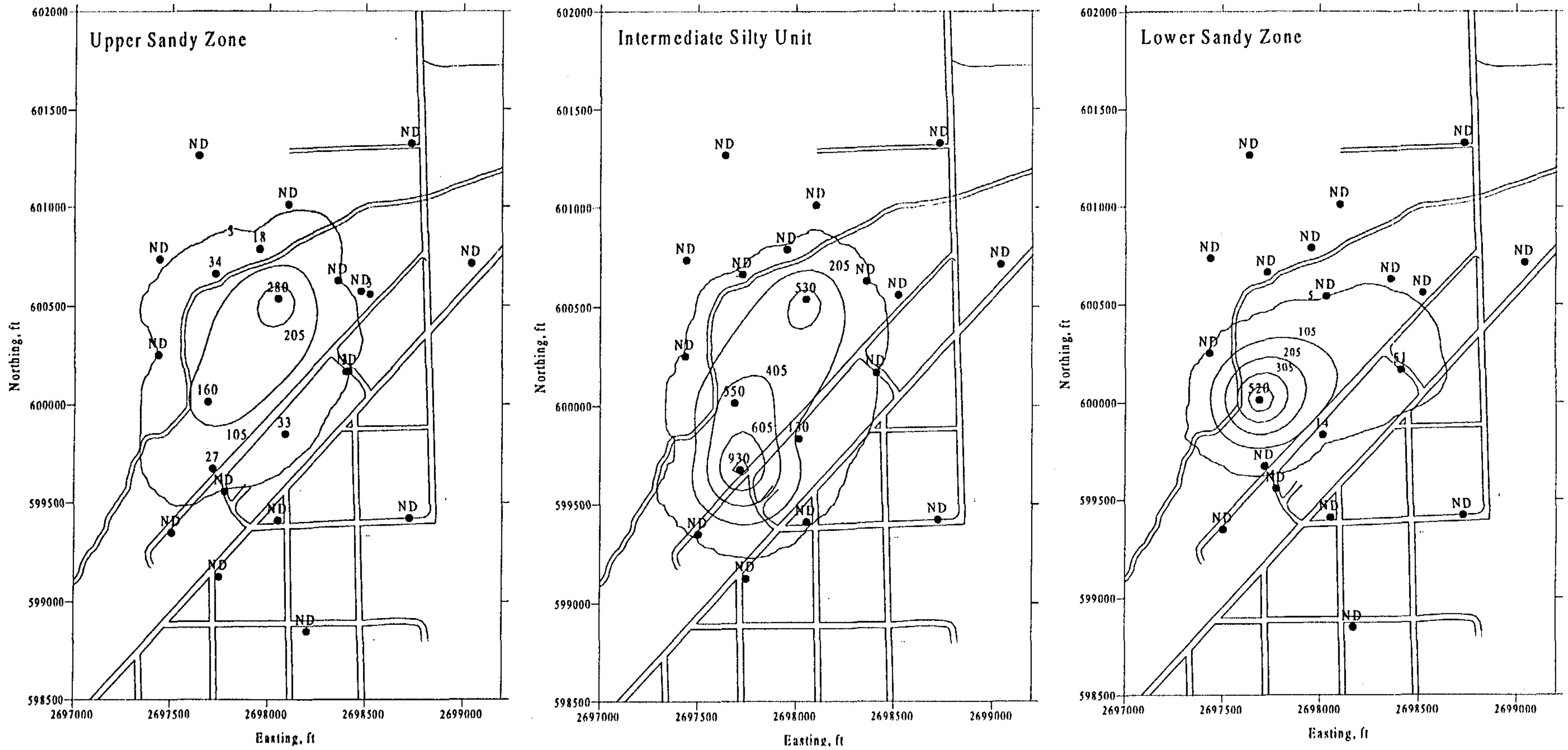

FIGURE 6 Measured Carbon Tetrachloride Concentrations in the Upper Sandy Zone, Intermediate Silty Unit, and Lower Sandy Zone (µg/L)

migration of the carbon tetrachloride contamination within the Bruno aquifer system and hence potential aquifer restoration needs.

## EXTENDED MONITORING PROGRAM

On the basis of these conceptual and numerical models, Argonne received regulatory approval to implement an extended program of targeted hydrogeologic monitoring at the site to provide critical data for calibration of the long-term groundwater flow and contaminant transport models necessary for risk analyses. The activities performed under this program included the following:

- Installation of additional temporary monitoring well and piezometer clusters within the upper and lower sandy zones and the intermediate silty unit of the aquifer system at four key locations, to augment the vertical and areal extent of the observation well network established during Phase I and Phase II.

- Continuous recording of water levels within the observation well and piezometer network to determine the responses of the aquifer system to short-term and/or longer-term fluctuations in rainfall and recharge and to possible local pumping activities.

- Quarterly sampling and analysis of groundwater, collected at two temporary monitoring well locations and in adjacent vertical profiles by using the ECPT, to identify the detailed distribution and possible migration pathways of carbon tetrachloride within the aquifer system during the extended monitoring period.

- Targeted soil sampling, analysis of sediment physical properties, and *in situ* hydraulic testing at selected locations to determine the vertical and lateral heterogeneity of the intermediate silty unit.

Argonne proposed that monitoring of groundwater levels and the contaminant distribution within the aquifer system be continued over a period of three to five years, in order to develop a site-specific database reflecting the range of potential annual climatic, rainfall, and water level conditions that might be expected at Bruno. The actual monitoring was conducted over a period of 22 months. In agreement with the regulatory agencies, Argonne considered the hydrogeologic data collected during the Phase I, Phase II, and extended monitoring periods to be acceptable for development of the long-term groundwater flow and transport models to be used in the risk evaluation.

## ADDITIONAL CONSTRAINTS ON THE CONCEPTUAL HYDROGEOLOGIC MODEL

The extended groundwater monitoring data confirmed that ambient groundwater flow within both the upper and lower sand units is predominantly to the north or northwest in the vicinity of the former CCC/USDA site, as shown in Figure 7. The ambient hydraulic gradients in these zones are similar in magnitude and appear to remain relatively constant despite observed fluctuations in absolute groundwater levels within the aquifer system associated with seasonal to annual variations in rainfall patterns.

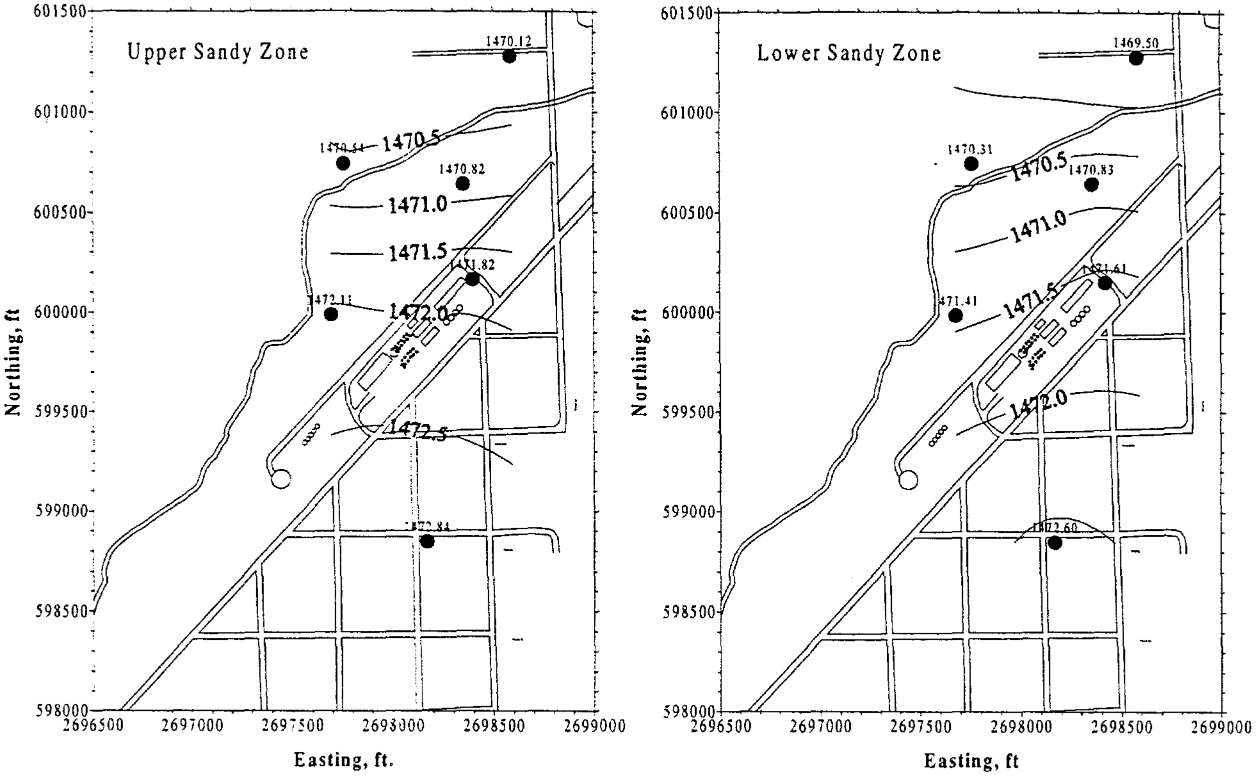

**FIGURE 7** Representative Potentiometric Surfaces for the Upper and Lower Sandy Zones under Ambient Hydraulic Gradient Conditions

Locally enhanced recharge to the aquifer system in the immediate vicinity of the former CCC/USDA site resulted in transient groundwater mounding and altered groundwater flow patterns within the upper and lower sandy zones (see Figure 8), as observed in the Phase I and Phase II manual water level measurements, during extended periods (several consecutive months) of consistently heavy, frequent rainfall. The continuous monitoring data demonstrated, however, that these mounding effects occurred in response to individual rainfall/recharge events during such wet periods and were relatively short lived (see Figure 9). An analysis of historic rainfall data available for the Bruno area indicated that the rainfall conditions required to produce transient mounding effects at the site have probably occurred in approximately 75% of the last 40 years.

A fairly sharply defined, thin, silt-clay layer identified at or near the base of the intermediate silty unit in the western and central portion of the Bruno study area pinches out toward the east and northeast across the site. Where it is present, this layer forms the most significant barrier to vertical groundwater and contaminant migration across the silty unit. Groundwater monitoring data demonstrate that the upper sandy zone and the portion of the intermediate silty unit above the silt-clay layer appear to be in direct hydraulic communication with each other; however, the vertical and horizontal hydraulic conductivities of the silty unit are relatively low. The $K_h$, $K_v$, and sand content of the silty unit increase in the area northeast of the former CCC/USDA facility. These observations account for the lateral offset in transient mounding effects observed in the upper versus lower sandy zones.

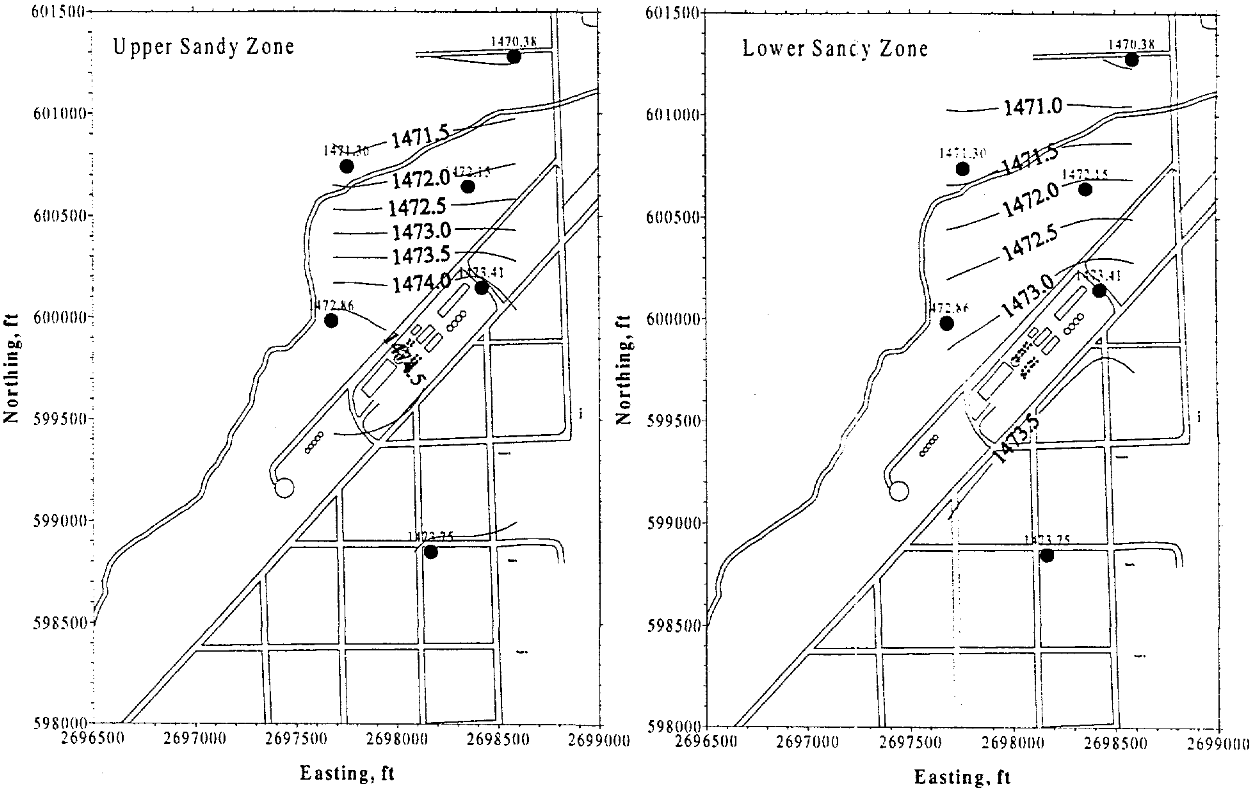

**FIGURE 8** Example Potentiometric Surfaces for the Upper and Lower Sandy Zones under High Rainfall/Recharge Conditions

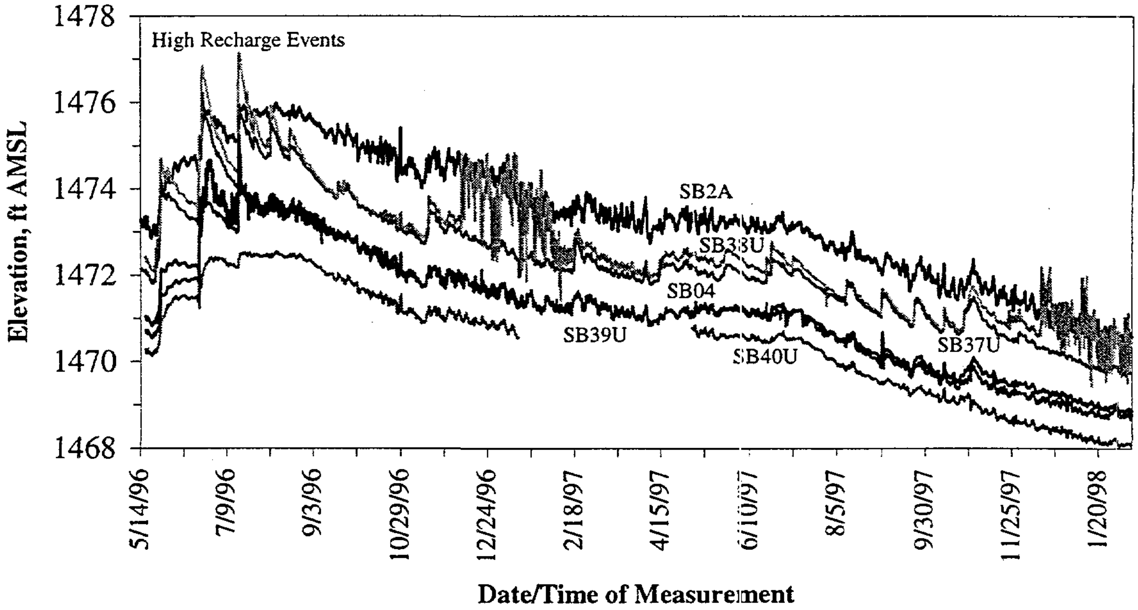

**FIGURE 9** Hydrographs for the Upper Sandy Unit, Recorded during the Extended Monitoring Program

Groundwater sampling data during the period of extended monitoring showed no evidence for significant natural contaminant migration within the aquifer system. The periodic sampling demonstrated, however, that groundwater flow to the monitoring wells during sampling (induced by low-rate pumping) preferentially occurred from portions of the aquifer units with higher (relative) carbon tetrachloride concentrations and, by implication, greater (relative) groundwater and contaminant mobility. On the basis of these observations, the maximum carbon tetrachloride levels identified for each location and hydrostratigraphic zone within the aquifer system were considered most representative for use in predicting contaminant migration, as outlined below.

## FINAL SITE MODELS AND DYNAMIC RISK ANALYSIS

The construction of final site conceptual and (when necessary) mathematical models requires an understanding of (1) the hydrogeologic processes controlling groundwater flow and contaminant transport and (2) the physiographic and cultural setting of the area under investigation, in order to define a practical and technically defensible basis for the analysis of human health risks. In conducting risk analyses, Argonne employs a dynamic assessment approach under which the health risks posed to actual or hypothetical residents at physically realistic locations within the study area are calculated by using the expected time-versus-concentration profiles associated with migration of the contaminated groundwater at those locations.

The preliminary mathematical models of groundwater flow and contaminant transport were recalibrated by incorporating the additional hydrogeologic constraints on the site conceptual model outlined above. Predictive flow and transport runs were used to simulate the effects on long-term contaminant migration of transient recharge events near the former CCC/USDA site, in keeping with the historic patterns of annual rainfall identified for the area. These simulations ultimately demonstrated that significant downgradient migration of carbon tetrachloride is expected only within the upper and lower sandy zones (see Figure 10); under the identified conditions at the site, the contamination within the intermediate silty unit appeared effectively immobile.

All residents within Bruno receive their domestic water from an uncontaminated municipal supply and are at no risk from the existing groundwater contamination. The area surrounding Bruno, particularly the region downgradient, is very sparsely populated and shows no indications of recent or probable population growth. Agricultural irrigation is uncommon in this area because of the fairly rolling local topography. The regional hydrogeologic studies performed by NWS (Ginsberg 1983) further indicated that the Pleistocene geologic units that host the Bruno aquifer system are absent in the area 2-2.5 mi north and northwest of the village; residents in this area obtain their water from deep Cretaceous aquifers.

On the basis of these observations, Argonne identified fewer than 12 occupied residences north and northwest of Bruno that might rely on private wells within the Pleistocene aquifer system for their sole source of domestic water. Of these, the four residences nearest the anticipated contaminant migration pathway (sites 1-4 in Figure 10) were considered as potential observation points for the calculation of long-term health risks; however, the results of the long-term simulations showed no expected risk at these locations.

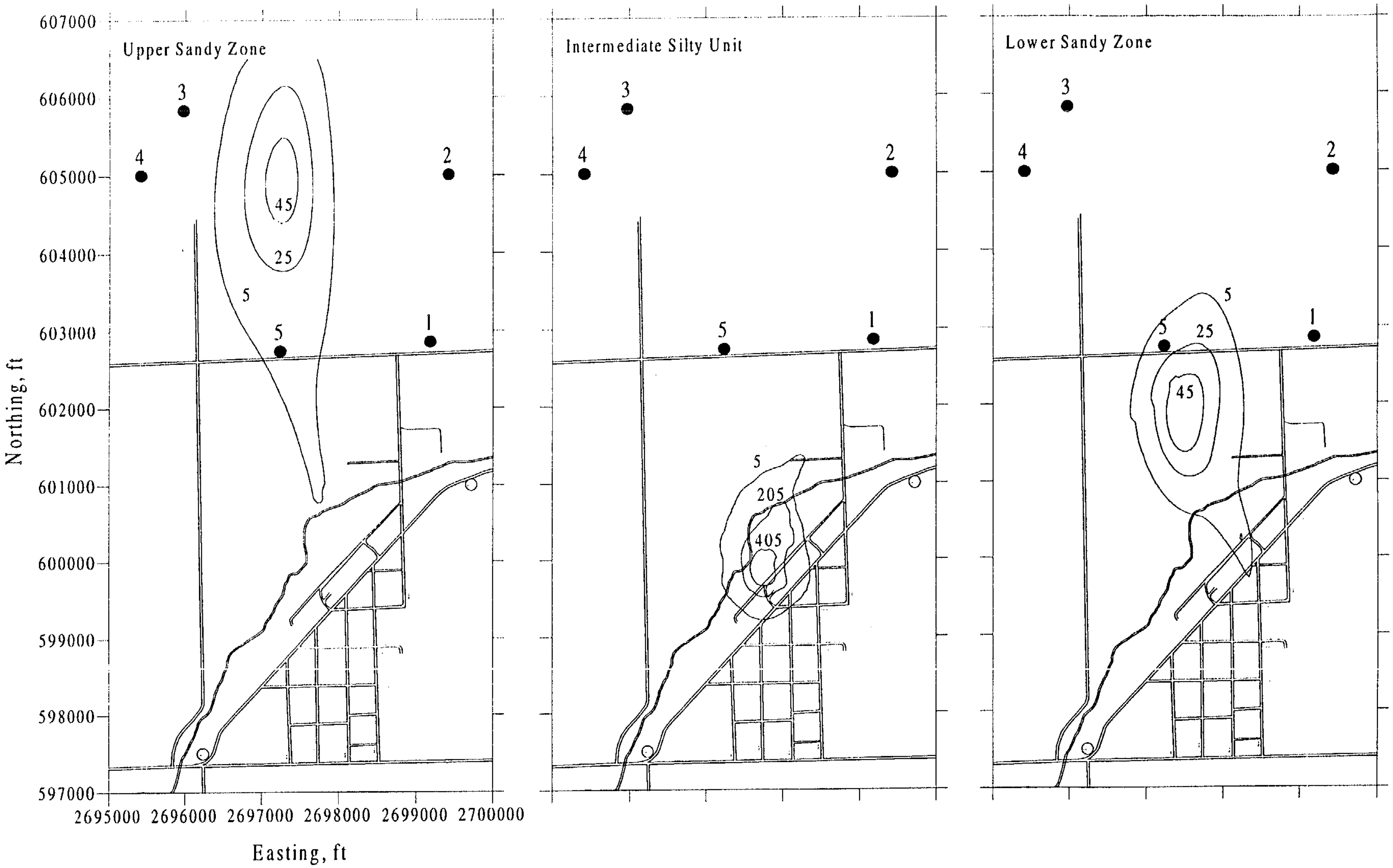

**FIGURE 10** Simulated Plume Configurations in the Upper Sandy Zone, Intermediate Silty Unit, and Lower Sandy Zone after 100 Years of Migration (Concentrations are in µg/L.)

For the final Bruno conceptual and mathematical models, a location (site 5 in Figure 10) along the first existing road north of the village was considered as the *nearest reasonable site* for the potential construction of a new residence that might not be served by a connection to the municipal water supply system and that would lie directly within the expected contaminant migration pathway. The location of this hypothetical residence was used as the primary observation point for the calculation of baseline (no-action) health risks associated with the carbon tetrachloride contamination of the Bruno aquifer system.

The dynamic risk analyses indicated that long-term contaminant migration within the upper and lower sandy units only might pose an unacceptable future health risk at the defined observation point, requiring an evaluation of alternative groundwater remediation scenarios. Subsequent remediation feasibility studies for the site employed the calibrated site models and risk-based evaluation procedures outlined above and focused on the reduction of mobile contaminant levels in these zones only.

## SUMMARY

The systematic development and critical evaluation of an integrated, process-oriented, conceptual hydrogeologic model is an essential element in the expedited characterization of hazardous waste sites. The conceptual model provides a framework for the selection of appropriate characterization techniques, for the integration and interpretation of site data, and for the identification of critical data needs. The Bruno example demonstrates that the effective construction of site conceptual and (when necessary) mathematical models, incorporating an understanding of both the hydrogeologic processes controlling groundwater flow and contaminant transport and the physiographic and cultural characteristics of the area under investigation, also provides the practical and technically defensible basis necessary for the analysis of human health risks with Argonne's dynamic risk assessment approach.

## ACKNOWLEDGMENT

Argonne's work at the Bruno, Nebraska, site is supported by the U.S. Department of Agriculture, Commodity Credit Corporation, under an interagency agreement through U.S. Department of Energy contract W-31-109-Eng-38.

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# INTEGRATING SITE CHARACTERIZATION THROUGH GROUNDWATER FLOW MODELING: THE MURDOCK, NEBRASKA EXAMPLE

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## ABSTRACT

Since the late 1980s, with steady improvement in computer technology and greater regulatory acceptance, groundwater modeling has become an essential component of site characterization and remediation design. The groundwater flow modeling process, as demonstrated on a contaminated site in eastern Nebraska, shows the benefits of modeling as it pertains to site characterization. A fully three dimensional, numerical groundwater flow model of a shallow aquifer system was constructed to (1) better understand the dynamics of groundwater flow in the area of carbon tetrachloride contamination, (2) identify preferred pathways of groundwater flow emanating from the contaminant source area, (3) predict the long-term migration of $CCl_4$ at the site, and (4) support development of an appropriate groundwater monitoring scheme. A steady-state calibrated model was produced that simulates average annual conditions. Pathline analysis was used to estimate the expected trajectory of the contaminant plume as it migrates across the effected area. Finally, a monitoring program was developed based on the expected pathway of the contaminant.

## INTRODUCTION

Throughout the 1970s and early 1980s, groundwater modeling, especially solute transport modeling, was viewed by most hydrogeologists as an academic exercise. It was seen as having little “real world” relevance to site characterization. After many years of steady improvement in modeling techniques, the proliferation of high performance desktop computing, and development of user-friendly groundwater flow and solute transport software packages, groundwater modeling has become an essential component of site characterization and remediation design.

This paper describes the application of groundwater flow modeling to characterization of a site in eastern Nebraska contaminated by carbon tetrachloride. The groundwater modeling *process*

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provided added confidence in the geologic and hydrologic conceptual model of the site by confirming the expected groundwater flow behavior, and consequently, dissolved $CCl_4$ transport.

The proposed ASTM guidelines for expedited site characterization (ESC) include a brief discussion of fate and transport analysis and risk evaluation (ASTM, 1997). The ASTM guidance suggests that the modeling tasks of the ESC are the "final stage of the ESC process." However, in order for the modeling component of any ESC to achieve the maximum success and utility, the ESC Phase I and Phase II must be undertaken with a mind toward the type and level of sophistication of groundwater flow and transport modeling that eventually will be conducted.

## BACKGROUND

The U.S. Environmental Protection Agency identified the former grain storage facility of the Commodity Credit Corporation of the U.S. Department of Agriculture (USDA) at Murdock, Nebraska as the source of carbon tetrachloride contamination in the shallow groundwater. Argonne National Laboratory, under agreement with the USDA, completed an expedited site characterization of the Murdock site in 1992 (Argonne National Laboratory, 1992). As part of the ESC, groundwater flow and dissolved $CCl_4$ transport modeling was undertaken to:

1. Further understand and document the dynamics of groundwater flow in and around the area of $CCl_4$ contamination as they are influenced by recharge from precipitation, discharges to local springs and seeps, and other natural boundaries to groundwater flow

2. Identify preferred pathways of groundwater flow

3. Predict long-term migration of dissolved $CCl_4$ at the Murdock site

4. Support development of an efficient and cost-effective, yet comprehensive, groundwater monitoring scheme.

## MODEL CONFIGURATION

A fully three-dimensional groundwater flow model of the Murdock area was developed for implementation by MODFLOW (McDonald and Harbaugh, 1988). Figure 1 contains the non-uniform horizontal model grid overlain on the 7.5" quadrangle map containing Murdock, NE and the surrounding area. The horizontal cell dimensions are 50 ft by 50 ft in the area of concern, expanding in size out to the model boundaries.

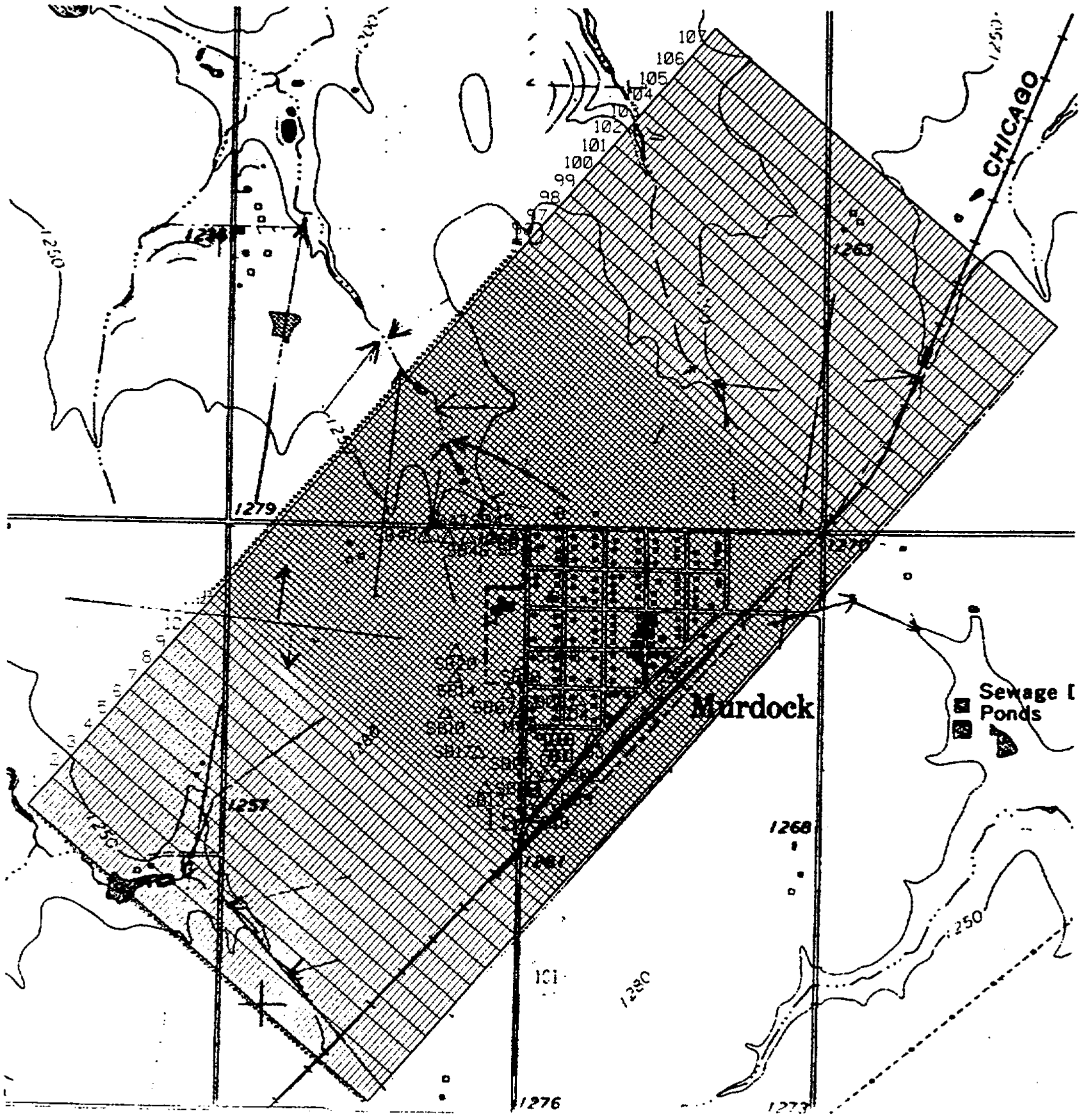

**FIGURE 1** Murdock, Ne Groundwater Model Horizontal Grid Superimposed on the USGS Quadrangle Map of the Site

At Murdock, NE, the shallow aquifer was the focus of the ESC. It is, for the most part, composed of fine to medium grained clean sands continuously overlain by vertically fractured clay and silt. The shallow sand aquifer is bounded on the bottom by a thick unit of low permeability clay. The Murdock groundwater model incorporates the hydrostratigraphy of the shallow groundwater aquifer and overlying silt and clay at the site in 12 model layers. The model layers are non-horizontal to improve the conceptual representation of the physical system (Harte, 1994). Figure 2 shows a typical vertical column section near the center of the model. The grey layers represent the aquifer. Each layer is characterized by a different hydraulic conductivity according to estimates from an aquifer test, grain size, and sand/silt/clay percentages.

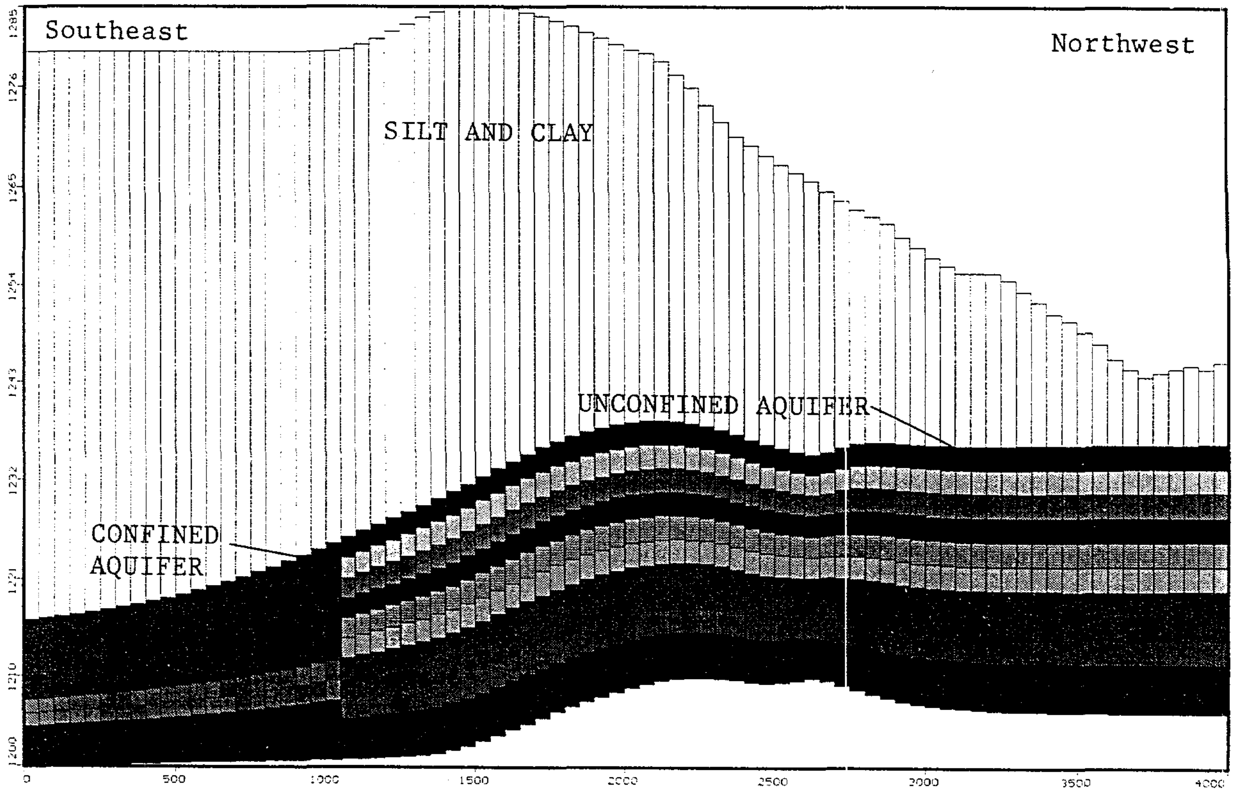

**FIGURE 2** Typical Murdock Groundwater Model Vertical Cross-section Showing Model Layers Representing Confined and Unconfined Sections of Shallow Aquifer and Overlying Silt and Clay (Vertical Exaggeration = 30:1)

## MODEL CALIBRATION

The most important aspect of groundwater modeling for support of site characterization and remedial design is calibration, or history matching. Groundwater model calibration is the activity of adjusting certain model parameters, within predetermined limits, to achieve the best possible fit of model calculated hydraulic heads with those observed in the field. Only through the calibration process is the numerical model validated against the geologic/hydrologic conceptual model. Model calibration integrates the conceptual understanding of the geology and hydrogeology of the site with the dynamics of groundwater flow. The level of vertical discretization in the Murdock model layering was selected so that any vertical flow components at the site could be reproduced by the model and to provide vertical resolution of carbon tetrachloride transport.

A groundwater model representative of long-term average conditions at Murdock, NE was the objective of the calibration process because the model was to be used to address long-term monitoring needs at the site. Bimonthly water level data were available for the wells shown in Figure 3 from April 1997 through February 1998. The Murdock groundwater model was calibrated against the average of the observed water levels in each of these wells (Figure 4) by adjusting hydraulic conductivities of the geologic units, recharge applied to the top layer, and the conductance of the drains that represent the groundwater discharge areas in the model. Calculated steady-state water levels were visually compared with the "target" water levels, and by the root mean squared error (RMS error) and average difference between calculated and target water levels.

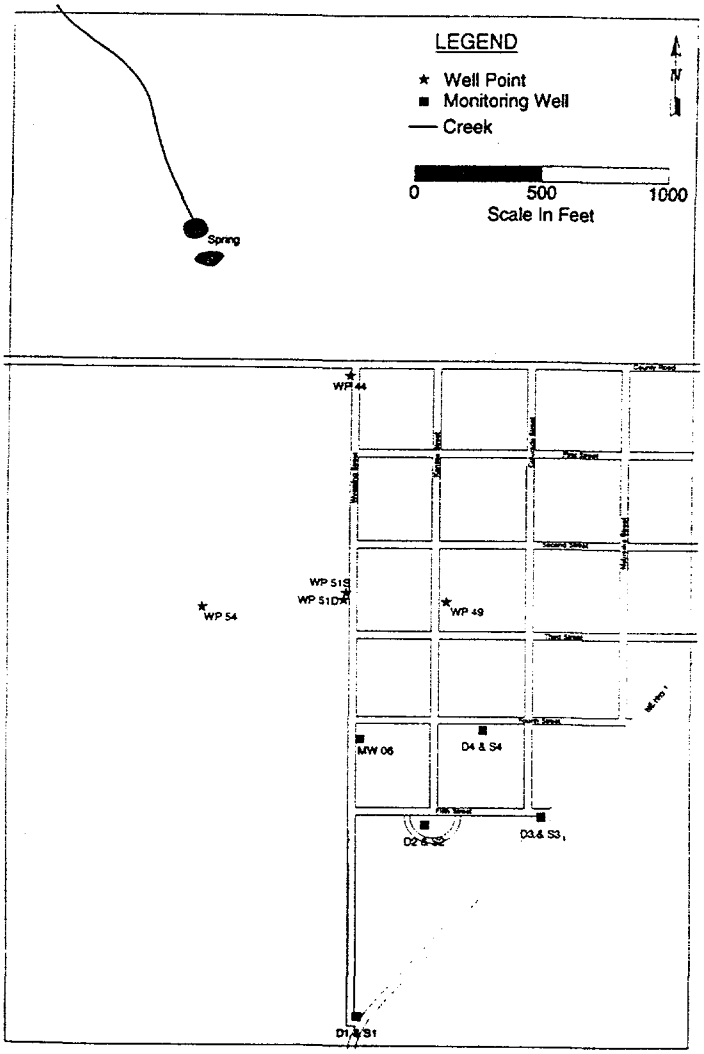

**FIGURE 3** Map Showing Locations of Water Level Data Used for Groundwater Flow Model Calibration

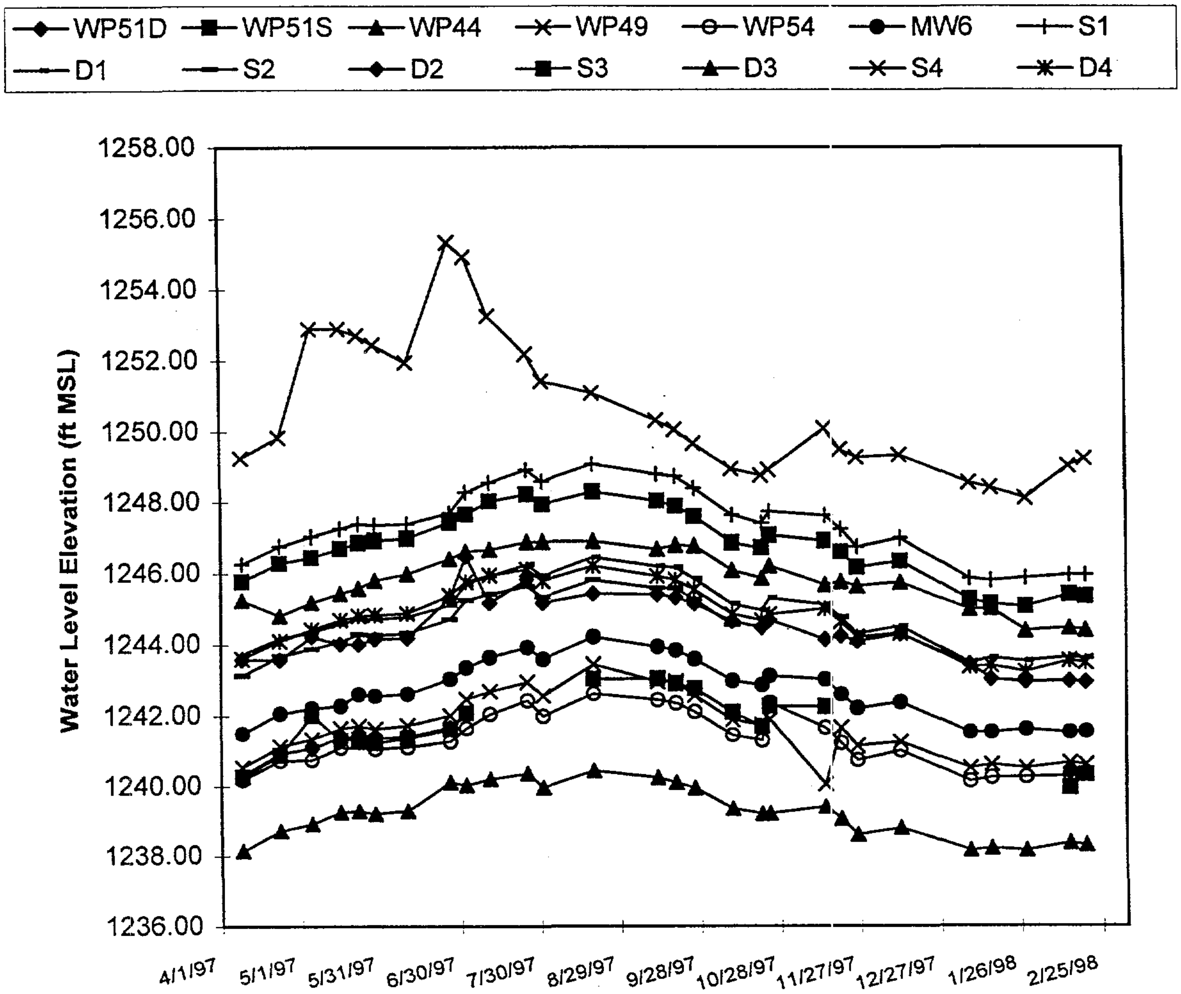

**FIGURE 4** Well Hydrographs Used for Groundwater Flow Model Calibration

Figure 5 shows the results of the calibration exercise. The calculated steady-state water levels closely match the target water levels. Final hydraulic conductivity values are well within the bounds suggested by the site characterization and open literature. To achieve the close match of calculated water levels with average observed water levels, different recharge rates were applied to farmland versus the Murdock community area. No recharge was applied to areas below elevation 1,250 ft AMSL where the topography slopes to the creeks.

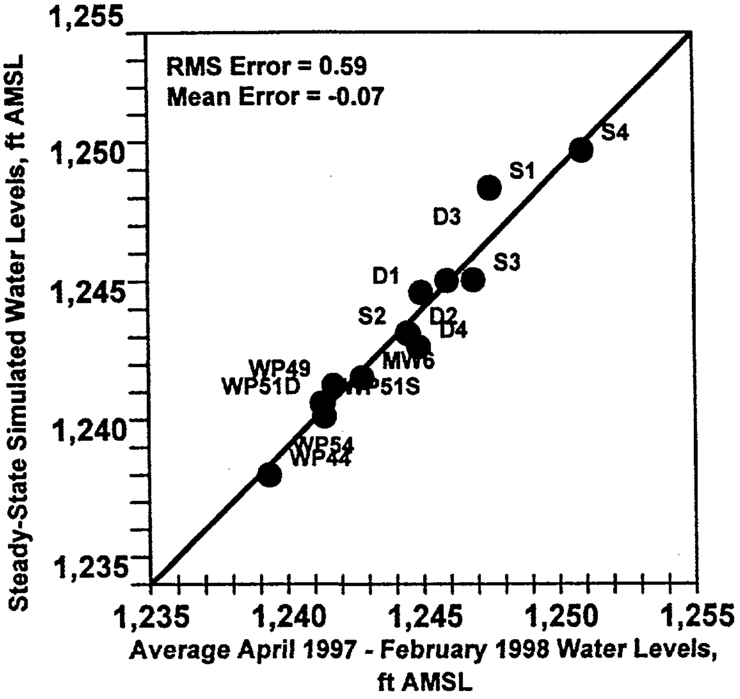

**FIGURE 5** Murdock Groundwater Flow Model Calibration Results

Figure 6 presents an additional evaluation of the success of the Murdock groundwater flow model calibration. The simulated steady-state water level for each calibration well is plotted against the April 1997 through February 1998 range of observed water levels for that well. This presentation shows that while in some cases the simulated water levels deviate somewhat from the average observed water levels (e.g., MW6, S1, S3: Figure 5), in all cases the simulated water levels are within the range of observed water levels used to compute the average "target" calibration water levels.

## RESULTS

The calibrated Murdock groundwater flow model was used to identify the probable pathways for the migration of $CCl_4$ during natural attenuation. Figure 7 is the calculated potentiometric surface for model layer six that is the layer where the bulk of the dissolved $CCl_4$ resides. Figure 8 shows the horizontal groundwater pathlines in model layer six emanating from the area of the former grain storage facility suspected of being the $CCl_4$ contaminant source area. All of the pathlines converge to Pawnee Creek to the northwest of Murdock. The triangles represent locations of soil borings and monitoring wells where sampling for $CCl_4$ has been conducted. The northeastern extent of the pathlines is nearly coincident with the rather sharp demarcation between locations where carbon tetrachloride has been detected and locations where it has not been found.

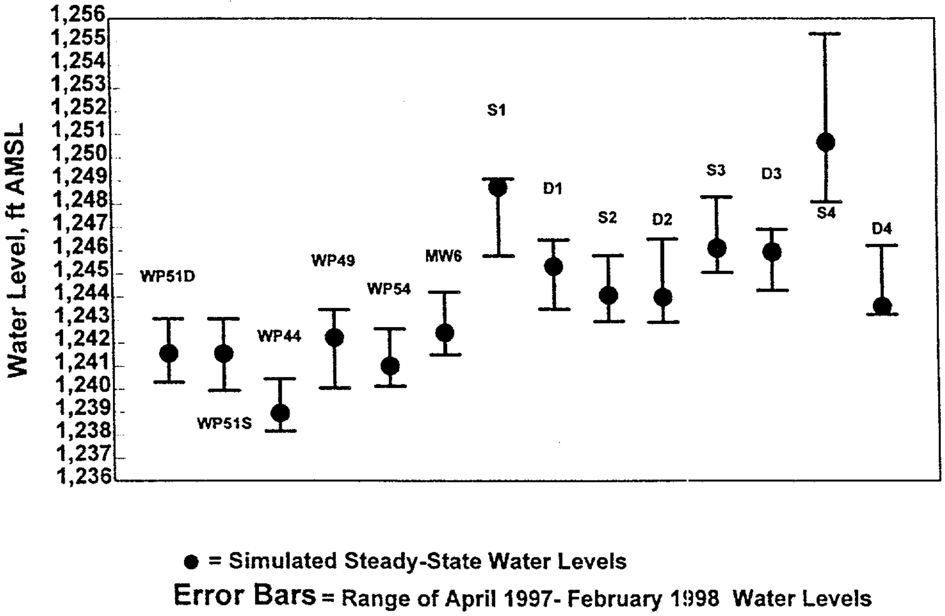

**FIGURE 6** Comparison of Simulated Steady-state Water Levels to Range of April 1997 - February 1998 Observed Water Levels

Flow path analysis, predicated on the calibrated flow model, confirmed that the dissolved $CCl_4$ will traverse a narrow corridor of groundwater flow as it discharges to the creek northwest of Murdock. A long-term groundwater monitoring plan was developed based on the results of the groundwater modeling.

The groundwater modeling program completed for the USDA/CCC site at Murdock, NE demonstrated the application of groundwater modeling within the overall expedited site characterization effort. The groundwater model integrated the geologic and hydrologic information generated from the ESC, consistent with the conceptual model of the system, to form a predictive tool to be used in support of aquifer rehabilitation decisions. In this case, the model confirmed that the $CCl_4$ plume will most likely continue to migrate to Pawnee Creek where it will discharge to surface water.

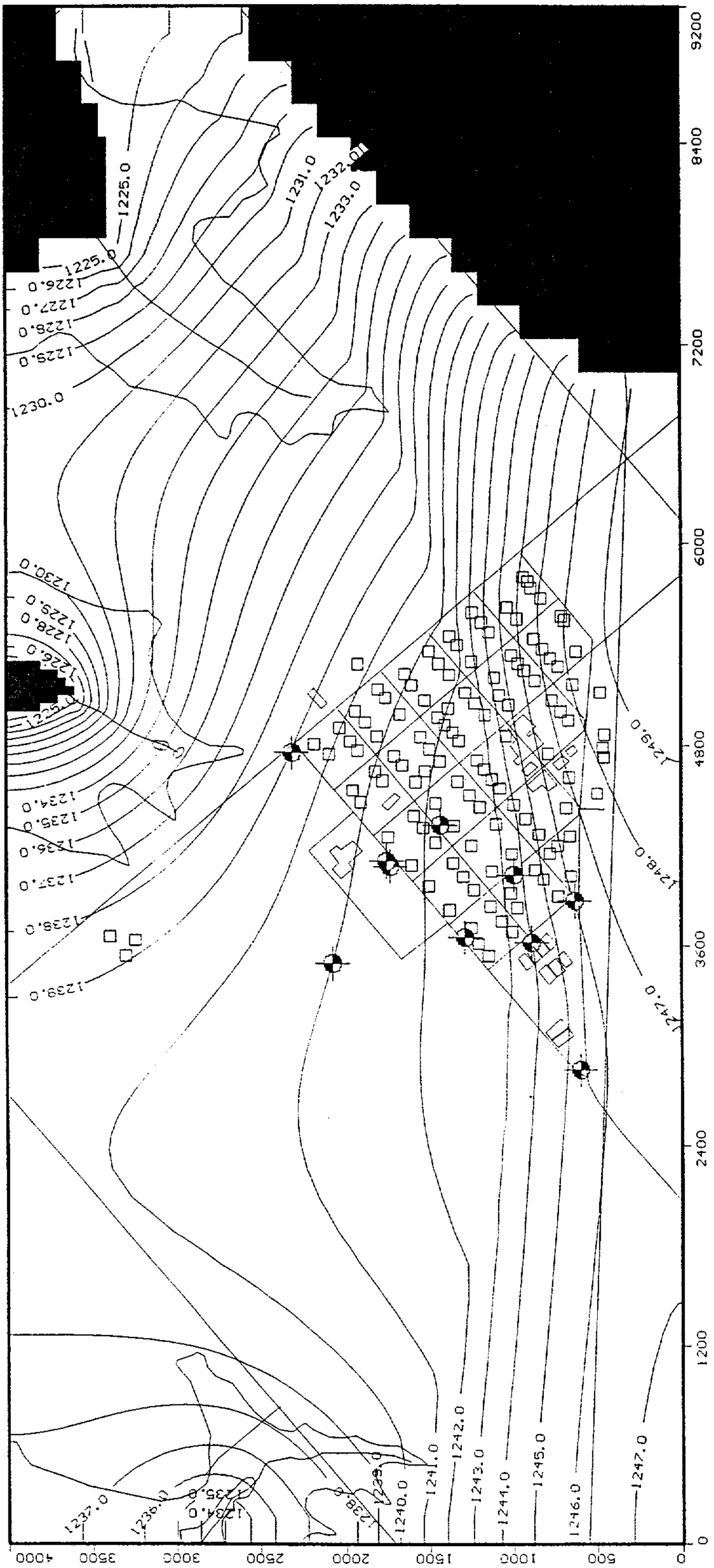

**FIGURE 7** Simulated Potentiometric Surface for Murdock Groundwater Flow Model Layer Six

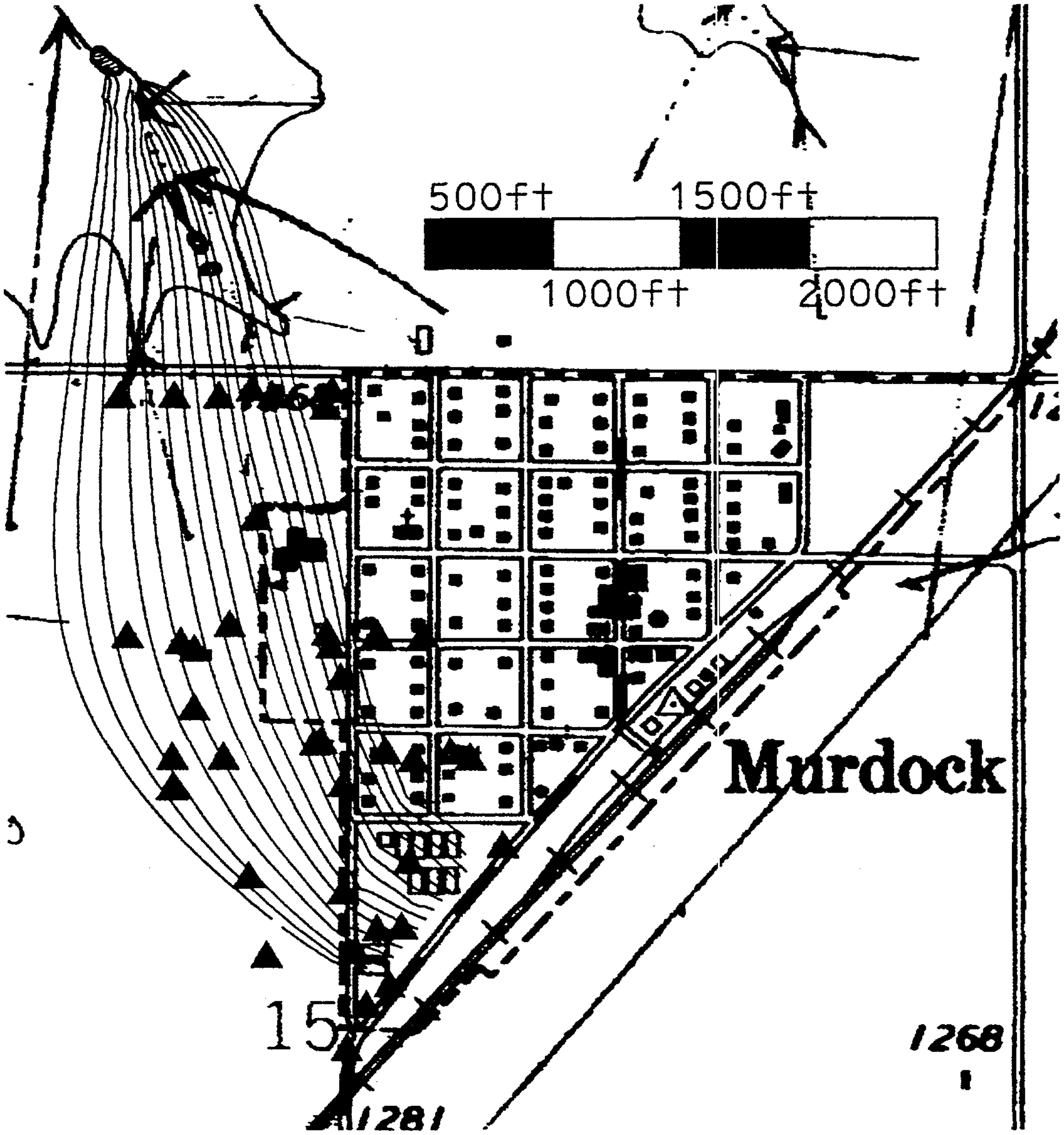

**FIGURE 8** Horizontal Groundwater Pathlines in Flow Model Layer Six

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# USE OF SEISMIC REFLECTION AMPLITUDE VERSUS OFFSET (AVO) TECHNIQUES TO IMAGE DENSE NONAQUEOUS PHASE LIQUIDS (DNAPL) AT THE M-AREA SEEPAGE BASIN, SAVANNAH RIVER SITE, SOUTH CAROLINA

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## ABSTRACT

One of most difficult problems in designing a remediation plan for cleaning up DNAPL contamination is locating the pools of free-phase DNAPL. The seismic modeling of a DNAPL saturated sand versus a water saturated sand suggests that with frequencies of 120 Hz or higher there would be an amplitude versus offset (AVO) anomaly. Seismic survey acquisition parameters for imaging the DNAPL were derived from an AVO model, which was based upon previously acquired seismic and well data. The seismic line was located in such a manner that it started in an area where the unconsolidated sand was water saturated and crossed a known pool of free-phase DNAPL saturated sand and continued back into a water saturated sand. Using a weighted stack processing technique (Smith and Gidlow, 1987) a "fluid factor" stack indicated an anomaly at the depth and location of the known free-phase DNAPL plume. The initial results suggest that under certain conditions free-phase DNAPL can be imaged using high-resolution seismic reflection techniques.

## INTRODUCTION

Imperative to any DNAPL remediation effort is the ability to locate high concentrations of contaminants. Traditional techniques such as borehole sampling run the risk of cross-contamination of aquifers. In addition, high concentrations of DNAPL can be missed because of inadequate spatial sampling. Seismic reflection profiling is a geophysical technique that can provide densely sampled subsurface measurements. A high-resolution two-dimensional survey can be conducted to yield horizontal measurements every foot and vertical measurements every 3-5 feet depending on the survey design. The principal data collected from a seismic reflection survey are the arrival time and amplitude of acoustic waves reflected from subsurface boundaries. These data are processed to create a vertical travel time section of the subsurface. The section can reveal faults, buried channels, and subsurface lows that might influence the migration of DNAPL in the subsurface.

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The amplitude and arrival time of seismic waves is dependent on the elastic parameters of the subsurface including bulk modulus, shear modulus, density, Poisson ratio, and angle of the incidence of the impinging energy. The last two parameters can, in certain instances, be used to infer the fluid content within the pore spaces. In the Petroleum industry seismic amplitude versus offset (AVO) methods are used to directly detect hydrocarbon bearing strata. In this study we adapt some of these techniques to directly detect the presence of DNAPLs at the United States Department of Energy Savannah River Site (Waddell and Domoracki, 1997). If these techniques can be found to be applicable to other sites, remediation of DNAPLs can be facilitated and be achieved at lower cost.

## Savannah River Site

The Savannah River Site (SRS) is located in South Carolina on the South Carolina-Georgia border. During the Cold War SRS was a major production facility of nuclear materials for defense purposes. Since the late 1980's an emphasis on environmental restoration has led to the development of programs and strategies to remediate DNAPL spills at the site. One area of SRS targeted for remediation is the M-Area seepage basin.

The M-Area seepage basin was constructed in 1958 to contain uranium wastes and residual solvents produced from reactor fuel and target degreasing operations (Figure 1). An estimated two million pounds of residual solvents were released into the eight million gallon unlined surface impoundment over a period of nearly thirty years. In 1988 the basin was closed, backfilled, and covered with an impermeable cap. Chlorinated solvents, including free-phase constituents, have been detected in the groundwater near the seepage basin since 1981. The majority of the DNAPL found in the subsurface is composed of Trichorethylene (TCE), Tetrachloroethylene (PCE) and Trichloroethane (TCA) (Looney, 1992). Environmental remediation strategies have included groundwater pump and treat, soil vapor extraction, in situ air stripping, and in situ bioremediation.

The near-surface geology at the M-Area seepage basin comprises Eocene age Upper Coastal Plain sedimentary units. On the surface is the "Upland unit" which consists of cobbles and coarse sand ranging in thickness from zero to fifty feet. Underlying the "Upland unit" are the Tobacco Road and Dry Branch formations which are composed of fine to medium grain sand, clayey sand, and discontinuous layers of clay. The amount of clay in the formations decreases with depth. Directly below the Dry Branch Formation is the Warley Hill Formation, which is composed of sand and glauconitic green clay. In the study area the "green clay" interval of the Warley Hill Formation ranges in thickness from 0 to 10 feet and occurs at a depth of approximately 155 feet below the surface. This clay, when present, is considered the confining unit which separates the overlying surficial aquifer from the semi- to confined aquifer below. The DNAPL in the M-Area pools on top of the "green clay."

# OBJECTIVES

The primary objective of this study was to test the feasibility of using high-resolution seismic techniques and direct hydrocarbon indicator analyses to image free-phase and dissolved phase

DNAPLs at the M-Area seepage basin. Other objectives were to use the seismic data to map the subsurface geology and to determine the geologic controls on the distribution of the DNAPL plume.

## METHODOLGY

The approach taken was three fold consisting of 1) evaluation of existing geological and geophysical data concerning the amount and distribution of DNAPL, 2) seismic modeling to determine whether or not an AVO anomaly would be expected from DNAPL saturated sediments, 3) acquisition and processing of a seismic line designed specially to image the DNAPL.

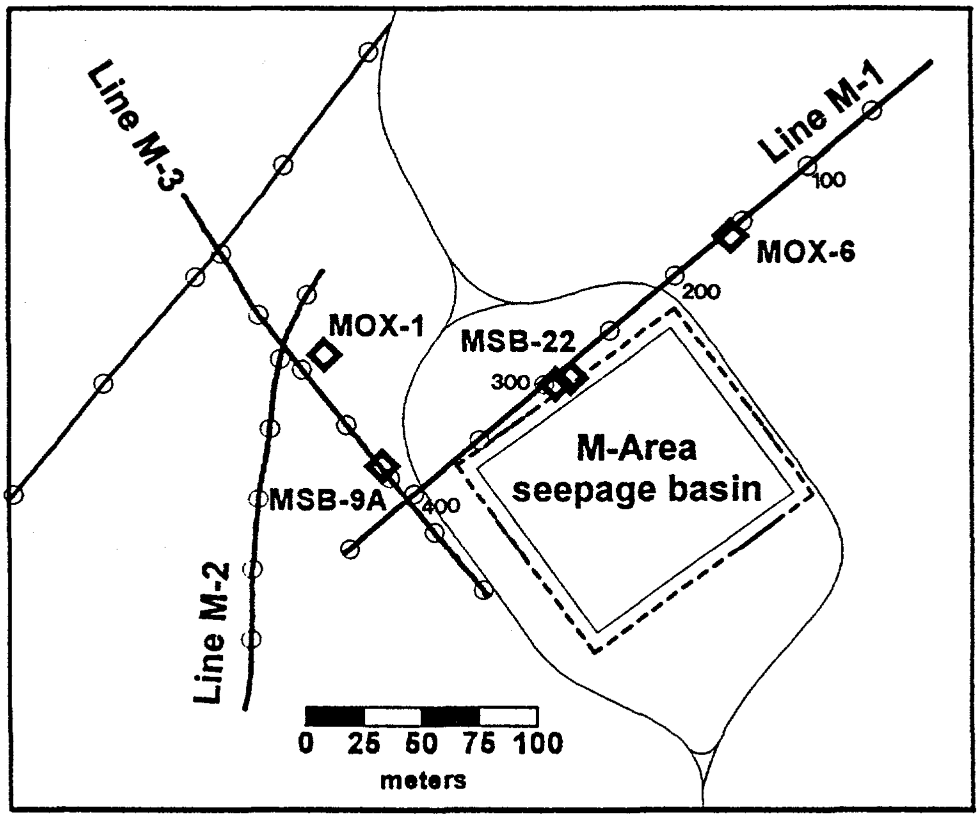

**FIGURE 1** Location map of all the 2-D seismic lines acquired for AVO analysis. Well MSB-3 is adjacent to well MSB-22.

## Seismic Amplitude Techniques

Seismic amplitude can provide an abundance of information that can be used to infer subsurface properties such as lithology and porosity. In the Petroleum industry, one relatively recent use of seismic reflection data is to distinguish between lithologic zones that are filled with hydrocarbons (oil and gas) versus those filled with water. The origin of these methods dates from the 1960's when petroleum companies began to recognize in young clastic sediments (Tertiary age) large seismic amplitudes associated with gas saturated sands (Verm and Hilterman, 1995). The method of correlating lithology to stacked seismic section reflectivity was called the "bright spot" technique. It did not take long before it was realized by that not all large amplitude anomalies were associated with gas reservoirs. This led to intensive research on the previously ignored subject of offset dependent reflectivity. Modern implementation of AVO techniques dates from Ostrander's (1984) work on gas sands. Today, seismic AVO analysis is used routinely to directly detect subsurface hydrocarbons (Castagna and Backus, 1993).

As implemented in the Petroleum industry, AVO analysis involves comparing modeled AVO responses versus field data to find a deviation from an expected background response. The expected background response is usually taken to be a water saturated reservoir; thus, the deviation from the expected response is an indication of hydrocarbons. If these techniques are applicable to aquifers, deviation from the expected response would be an indication of DNAPL.

The CDP stacked seismic section represents the result that would be obtained if the sources and receivers were coincident. This simplistic assumption is essentially correct in terms of the arrival times of the seismic waves; however, in terms of the amplitude of the seismic waves it is not. The amplitude of reflected seismic waves is also dependent on the angle of the impinging energy and the change in Poisson ratio between the reflecting media. Mathematically, the amplitude relationships are described by the Zoeppritz (1919) equations. Implementation of the full Zoeppritz equations, however, is computationally intensive and the formulation is not in a convenient form for geophysical applications.

Most AVO work is developed from an approximate form of the Zoeppritz equations derived by Aki and Richards (1980) by modification of an approximate form by Bortfield (1961). The Aki and Richards formulation was rearranged by Shuey (1985) to express offset dependent reflectivity in terms of P-wave velocity, bulk density and Poisson ratio. The Shuey formulation is important in that reflectivity, R, can be expressed in terms of a normal incidence (NI) reflectivity and an offset or Poisson reflectivity (PR) that arises primarily as a result of changes in the Poisson's ratio between media, i.e.:

$$R(\theta) \cong \mathrm{NI} + [9/4\Delta\sigma - \mathrm{NI}]\sin^2\theta$$

or

$$R(\theta) \cong \mathrm{NI}\cos^2\theta + \mathrm{PR}\sin^2\theta$$

where

| | |
|---|---|
| $\theta$ | is angle of incidence |
| $\sigma$ | Poisson's ratio |
| $\Delta\sigma$ | is $\sigma_2 - \sigma_1$; change in Poisson's ratio across the interface |
| NI | is normal incidence reflectivity, i.e. the reflection coefficient for zero-offset |
| PR | is "Poisson reflectivity" |

(Verm and Hilterman, 1995).

The quantities NI and PR are defined as:

$\mathrm{NI} = (\alpha_2\rho_2 - \alpha_1\rho_1)/(\alpha_2\rho_2 + \alpha_1\rho_1) = (z_2 - z_1)/(z_2 + z_1)$;  z is the acoustic impedance;
$\mathrm{PR} = \Delta\sigma/(1 - \sigma_{avg})^2$

where

| | | | | |
|---|---|---|---|---|
| $\alpha$ | is P-wave velocity, | 1 subscript denotes upper layer, | 2 subscript denotes lower layer | |
| $\beta$ | is S-wave velocity, | " | " | " |
| $\rho$ | is bulk density, | " | " | " |

Thus, seismic AVO analysis is based on the simple idea that changes in the fluid content of a reservoir (or aquifer for this research) can cause a large enough change in the Poisson's ratio so that a significant change in seismic reflectivity as a function of offset occurs. Furthermore, this change in reflection AVO is greater than what would be expected for a change in lithology. To successfully implement these techniques for environmental applications, information is required on the P-wave and S-wave velocities and density of water saturated and DNAPL saturated sediments. Seismic models can then be constructed to determine whether for a given site there is likelihood that a seismic AVO anomaly can be detected from the DNAPL saturated sediments.

## Modeling

The most important aspect of this study is the AVO modeling, which was used to design the field acquisition parameters for seismic profiles M-1, M-2, and M-3. The first type of model was generated using the Aki-Richards (1980) and Smith and Gidlow (1987) approximations to the Zoeppritz equations. The model is a sand wedge saturated with either water or TCE overlying either a clay layer or a water saturated sand (Table 1).

Using the parameters in Table 1, the results of the modeling suggested that there would be an AVO effect caused by the presence of DNAPL (Figures 2, 3, 4). Furthermore, these results indicated that changes in the reflection coefficient would begin to occur at approximately 22° angle of incidence. Using this information the seismic lines were designed such that half the receivers would be under this incident angle and half would be over.

**TABLE 1** Parameters used to generate AVO models.

| Lithology | Vp | Vs | Density |
|---|---|---|---|
| | ft/s | ft/s | g/cc |
| Wedge | | | |
| Water Sand | 5800 | 1450 | 1.9 |
| TCE Sand | 4968 | 1634 | 2.07 |
| Substrate | | | |
| Clay | 5600 | 1300 | 1.85 |
| Water Sand | 5600 | 1460 | 1.89 |

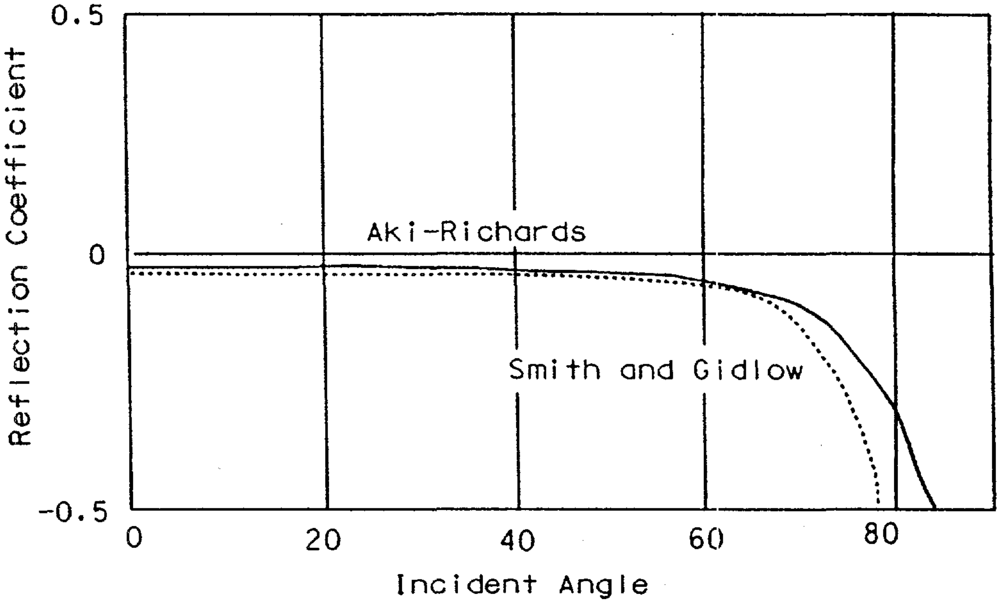

**FIGURE 2** Graph of reflection coefficient versus angle of incidence using the Aki-Richards (solid line) and Smith and Gidlow (dashed line) approximations to the Zoeppritz equations for water saturated sand overlying the "green clay". At the sand/clay interface the reflection coefficient is slightly negative and becomes more negative with increasing angle of incidence. At large angles of incidence (greater than 50°) this effect is pronounced.

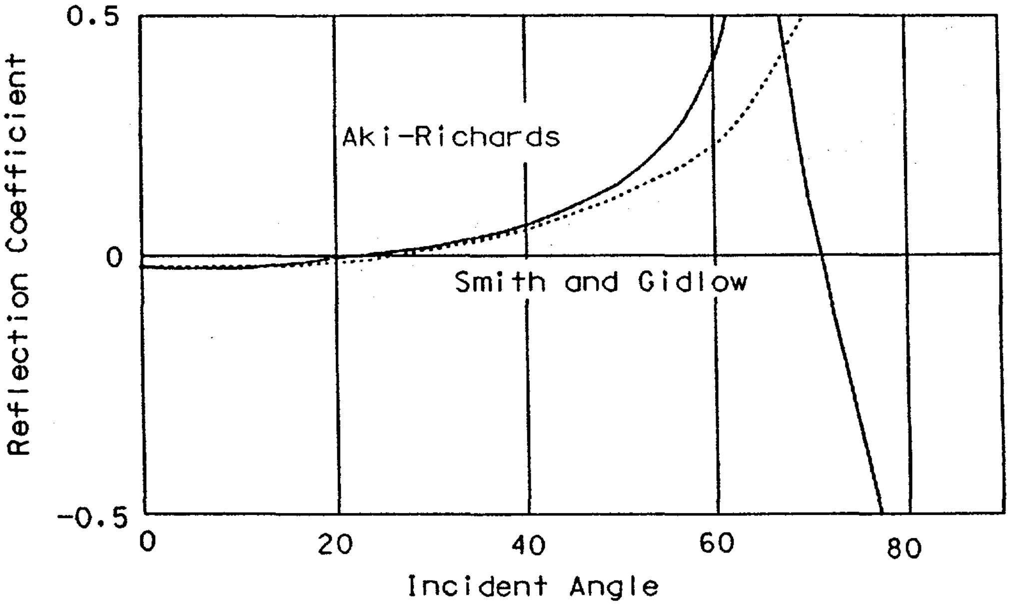

**FIGURE 3** Graph of reflection coefficient versus angle of incidence using the Aki-Richards (solid line) and Smith and Gidlow (dashed line) approximations to the Zoeppritz equations for TCE saturated sand overlying the "green clay". In this scenario, the amplitude is slightly negative, but at 22° the reflection coefficient goes from slightly negative to positive and increases with angle of incidence.

The second type of model was generated using P-wave, S-wave, and density data from an existing well. For this type of modeling a synthetic CDP gather was generated to determine if there would be an AVO effect associated with DNAPL contaminated sediments. Well MHM-21 is near the study area and is not contaminated. The synthetic CDP gather generated using the velocity and density data from the well is shown in Figure 5 (left). To investigate the AVO response caused by the presence of DNAPL a ten foot interval of the logs corresponding to the depth where the DNAPL is accumulating was replaced with the same velocity and density parameters for TCE used to generate the models shown in Figure 2, 3, and 4. Also, the model was convolved with a 120 Hz Ricker wavelet to simulate typical high-resolution seismic data. Figure 5 (right) is the modeled CDP gather for a TCE contaminated sand layer.

Comparison between the synthetic CDP gather models demonstrates that, in this case, an AVO effect can be expected due to the presence of TCE. This AVO effect is manifested as a large increase in amplitude with increasing shot to receiver offset. The increase in amplitude is much larger than if no TCE were present.

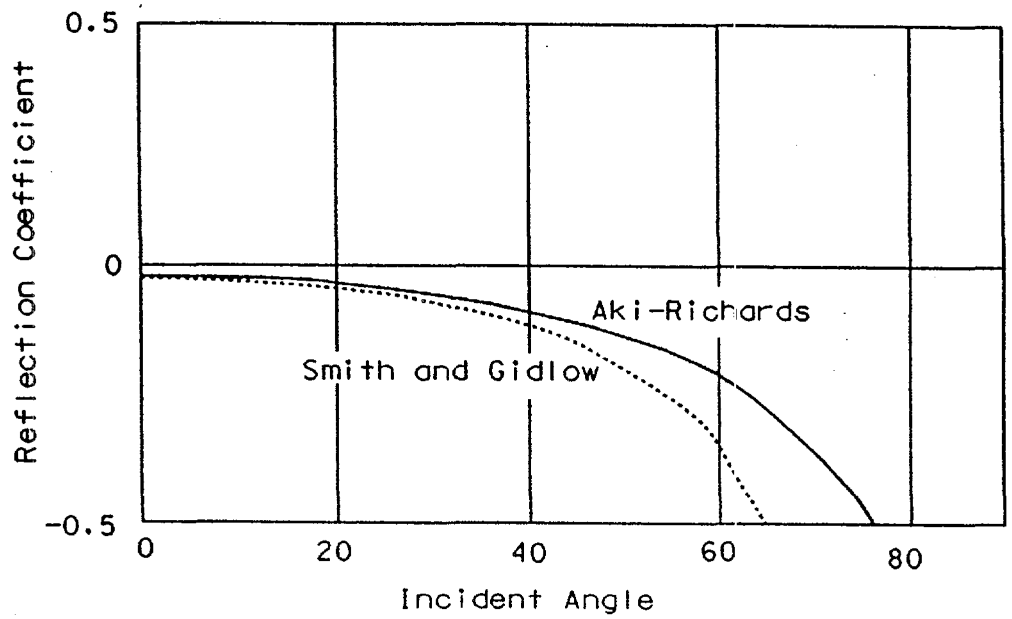

**FIGURE 4** Graph of reflection coefficient versus angle of incidence using the Aki-Richards (solid line) and Smith and Gidlow (dashed line) approximations to the Zoeppritz equations for water saturated sand overlying TCE saturated sand. The reflection coefficient at 0° angle of incidence is near 0, or is slightly negative, and at 22° becomes increasingly negative.

## Seismic Data Acquisition

The original project consisted of recording one seismic profile, line M-1, across a known DNAPL plume that has a free-phase component (Figure 1). However, after processing M-1 and preliminary AVO analysis (fluid factor stack) was preformed, an AVO anomaly was detected at the location and depth of the known DNAPL plume. As a result, it was decided to acquire two additional lines M-2, and M-3 and a vertical seismic profile (VSP) at well MSB-9A (Figure 1).

All of the data were collected with a 24 bit OYO DAS-1 seismograph recording either 48 channels (M-1) or 96 channels (M-2 and M-3). The M-Area is a notorious low signal-to-noise seismic data area. Two test lines were shot prior to the acquisition of the M-series lines using mini-vibrator, downhole Seisgun™, and EWG-1 weight drop sources. None of these sources were able to combine the requirements of adequate signal penetration, high frequency content, and minimal source generated noise. Lastly, a 10 lb. sledgehammer was tested. The sledgehammer was found to be a repeatable high frequency source that generated a relatively small surface wave.

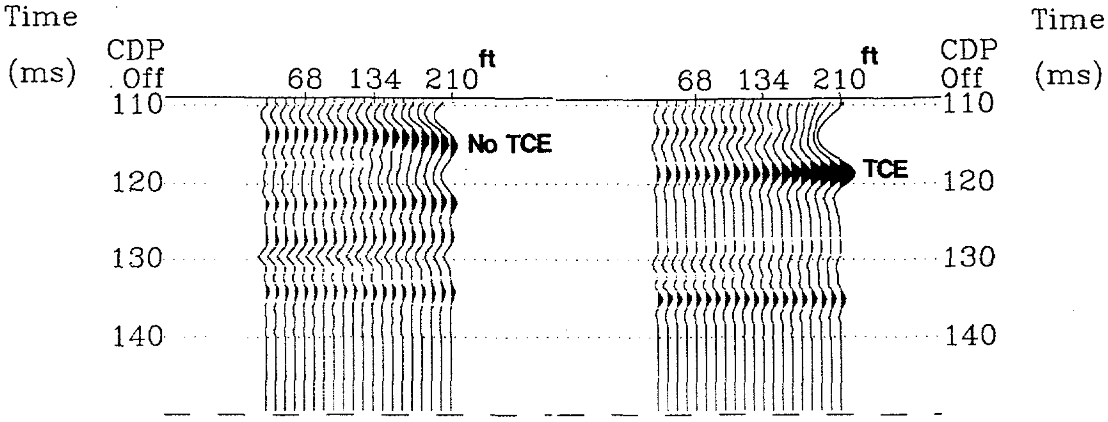

**FIGURE 5** Synthetic CDP gather generated using P-wave and S-wave velocity logs from well MHM-21 and a density log from nearby well MHT-1. Notice that the reflection at 120 ms has a slight increase in amplitude with increasing offset. The synthetic seismogram on the right is the same as on the left, but the P-wave, S-wave, and density values have been replaced using the parameters as in Figures 3-4 to simulate a 10 foot section of TCE saturated sediment. Notice that the reflection at 120 ms has a much greater increase in amplitude with offset as a consequence of the presence of TCE.

The acquisition parameters for seismic line M-1 appear in Table 2. The parameters such as group spacing, near offset, and far offset were based upon the modeling results. The target interval was the "green clay" aquitard at approximately 155 feet depth. The recording offsets were chosen in such a way as to have at least 15 to 20 geophone groups under 22° angle of incidence so that the AVO analysis described above could be performed on the seismic lines.

**TABLE 2** Acquisition parameters for seismic line M-1.

| | |
|---|---|
| Number of channels | 48 |
| Group interval | 2 ft. |
| Shot interval | 2 ft. |
| Near offset | 20 ft |
| Far offset | 114 ft. |
| Nominal CDP fold | 24 |
| Geophone frequency | 40 Hz |
| Energy source | Hammer /8 hits |
| Sample rate | 0.25 ms |
| Record length | 500 ms |

After line M-1 was processed, modifications were made to the basic recording parameters for acquisition of lines M-2 and M-3. For those lines, a 96 channel recording system was used which allowed a greater range of offsets to be recorded. For lines M-2 and M-3 the minimum and maximum offsets were 29 and 219 feet respectively.

## Seismic Data Processing

The seismic data were processed with a standard CDP data processing sequence (Yilmaz, 1987) that included frequency-wave number filtering (F-K or pie slice filtering) to eliminate linear noise trains, spiking deconvolution, and iterative velocity analysis and residual statics application. For display the data were filtered to a 90-275 Hz passband and a five point running mean was applied to enhance the lateral continuity of reflections. To analyze AVO variations near and far offset stacks were generated as well as Smith-Gidlow (1997) fluid factor stacks.

## DIRECT DETECTION OF DNAPL

At the M-Area seepage basin two primary types of DNAPL are present below the water table, trichloroethylene (TCE) and tetrachloroethylene (PCE). The latter being the predominate type of solvent. Water samples taken from well MSB-3D (Figure 1) consisted of a separate phase liquid composed of PCE with a subordinate amount of TCE (Looney, 1992).

In this project two methods were used to investigate any AVO effects caused by the presence of DNAPL. As previously mentioned, the recording geometry was such that 15 to 20 geophone groups were under 22° angle of incidence. If the models were correct, there would not be any significant change in amplitude under 22° caused by the presence of DNAPL. If DNAPL were present, however, a significant amplitude increase would be noted on the far offsets representing angles of incidence over 22°. Method one was range limited stacking. In this method data were gathered and stacked using subsets of the range of offsets to produce a near offset section (Figure 6 top) and a far offset section (Figure 6 bottom). AVO anomalies produced by the presence of DNAPL should show as high amplitudes present on the far offset section, but not on the near offset section. The second AVO analysis technique used was the Smith and Gidlow "fluid factor" stack (Smith and Gidlow, 1987) (Figure 7).

The "fluid factor" stack is derived from the Aki and Richards (1980) approximation of Zoeppritz equations and the Castagna, Batzle and Eastwood (1985) "mudrock line" for 100% water saturated clastic silicate rocks. In this method a series of time and space variant weighting factors are derived from the available P-wave and S-wave velocity data. These weighting factors are applied to the CDP gathers after NMO (normal moveout) corrections and if the model is valid, the CDP stack will be zero for 100% water saturated clastic sediments. Any residual reflections should denote sediments saturated with fluids other than water. In this project, DNAPL would be the only fluid other than water to saturate or partially saturate the sediments.

### Profile M-1 Offset Range Limited Stack

In Figure 6 the upper profile is a near offset stack and the lower profile is a far offset stack. If there are any AVO anomalies, they should be present on the far offset stack and absent on the near offset stack. At shot point (SP) 79 at about 89 ms is an anomaly that was drilled (well MOX-6) and TCE was found to be present. On the near offset stack the anomaly is absent. Another anomaly is at shot point 297 at about 109 ms. This anomaly is adjacent to well MSB-3 which had free phase DNAPL. Another anomaly is at shot point 430 at about 110 ms which is believed to be DNAPL, but is as yet untested.

### Profile M-1 Smith-Gidlow (Fluid Factor) Stack

Profile M-1 is a fluid factor stack based upon the Smith and Gidlow (1987) weighted stack technique. The amplitude anomalies observed on the far offset stack are present. The anomaly observed on the far offset range limited stack at shot point 79 at 89 ms is present as is the other anomalies at shot points 297 at 109 ms and shot point 430 at 110 ms. However, it must be pointed out that any anomaly above 100 ms must be treated with caution, because the fluid factor analysis assumes 100% water saturation. The water table at the M-Area seepage basin occurs at approximately 100 ms; therefore, any anomaly above 100 ms is not at 100% water saturation.

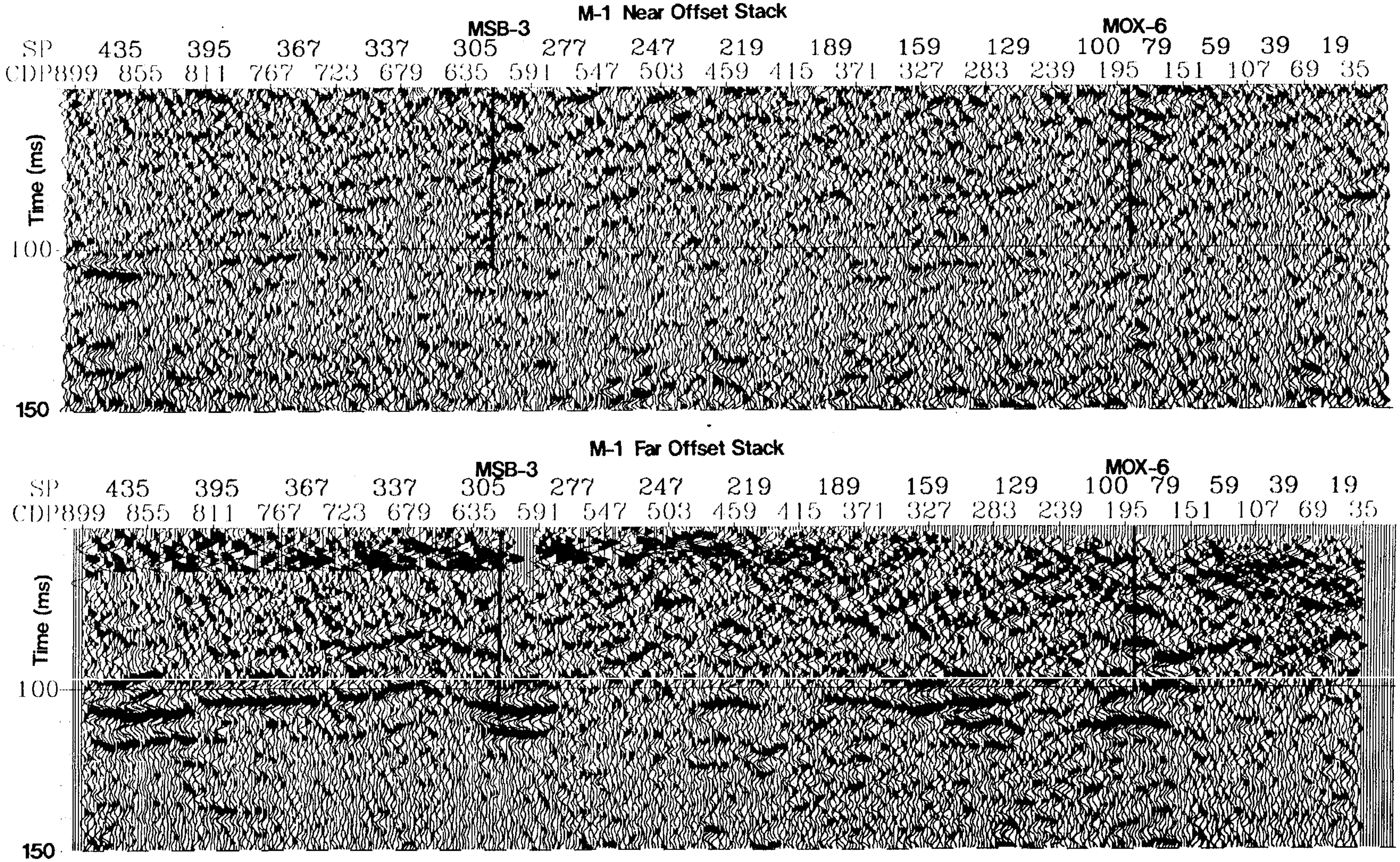

**FIGURE 6** Offset range limited stacks for profile M-1. Near offset stack section top, far offset stack section bottom. The upper section was generated by stacking offsets less than 58 feet. The lower section was generated by stacking offsets greater than 58 feet. High amplitudes that occur only at far offsets should denote the presence of DNAPL. Every second trace is plotted. CDP spacing is one foot.

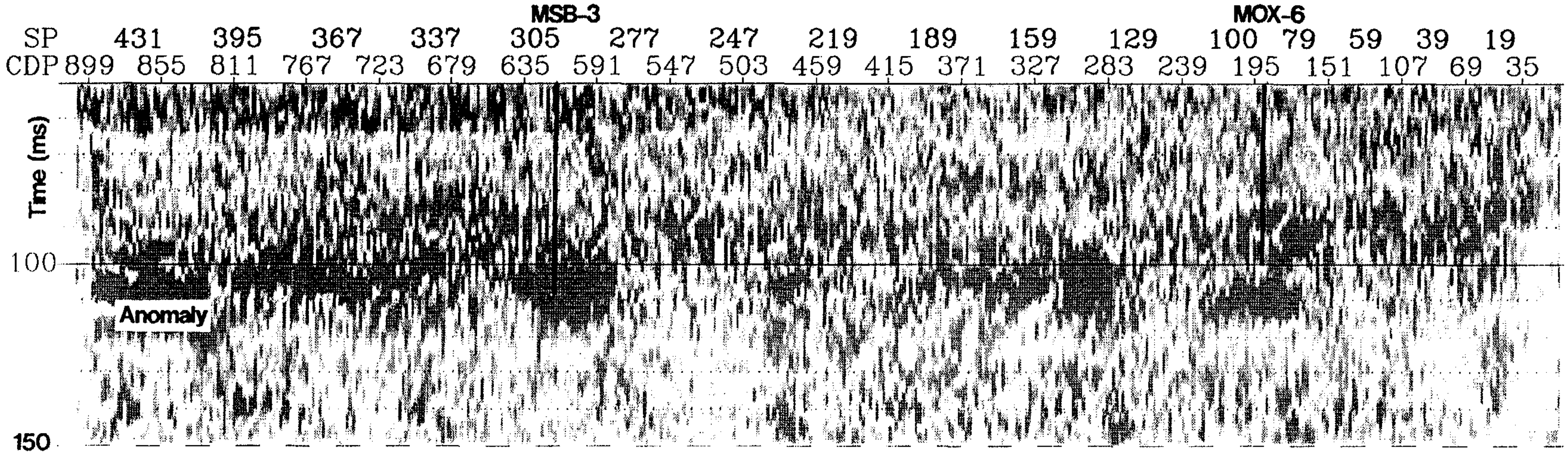

**FIGURE 7** Fluid factor stack of line M-1. AVO anomalies, possibly caused by DNAPL, are indicated. The water table occurs at a depth corresponding to approximately 100 ms time. The amplitude envelope (magnitude of Hilbert transform) is displayed. Every second trace is plotted. CDP spacing is one foot.

## CONCLUSIONS

At the M-Area seepage basin, Savannah River Site, it appears that DNAPLs can be imaged in the subsurface using high-resolution seismic data. Two wells were drilled on anomalies recognized by seismic data and DNAPLs were found at the predicted depth in parts per million (head space data).

Caution must be exercised in applying this technique to other areas. Before any seismic data are acquired, some basic modeling has to be done. The modeling data will determine what is the minimum amount of DNAPL that can be imaged given the geologic conditions for a particular site and provide the necessary data for designing seismic acquisition parameters.

## ACKNOWLEDGMENTS

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# RAPID SITE ASSESSMENT FOR PETROLEUM CONTAMINATED SITES: PERF PROJECT #96-08

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## ABSTRACT

The Petroleum Environmental Research Forum (PERF) is beginning a new project that will focus on Rapid Site Assessment (RSA) issues. The objective of the Program is to develop, apply, and transfer technology and information which will assist in developing rapid, cost-effective approaches to site characterization. The project will be used as a forum for (1) exchanging information about new technologies and frameworks, (2) promoting greater awareness and understanding of rapid site assessment approaches, and (3) advancing regulatory acceptance of the approach.

Currently, five petroleum companies have submitted proposed research contributions. In addition, several European companies, and some U.S. government agencies and national laboratories have indicated an interest in participating. The work required to complete this project will be shared by program participants. This presentation provides an overview of this project. Input from symposium participants is encouraged.

## INTRODUCTION

The Petroleum Environmental Research Forum (PERF) is beginning a new project that will focus on Rapid Site Assessment (RSA) issues relevant to the petrochemical industry. PERF is a research and development joint venture, formed to provide a stimulus to and a forum for the collection, exchange, and analysis of research information relating to the development of technology for health, safety, the environment, waste reduction and system security in the petroleum industry. PERF is a non-profit organization of corporations, engaged in the petroleum industry, that recognize the importance of a clean, healthy environment and are committed to support cooperative research and development. PERF does not itself participate in research projects but provides a forum for Members to collect, exchange, and analyze research information relating to practical and theoretical science and technology concerning the petroleum industry, and a mechanism to establish joint research projects in that field.

PERF Members have initiated or completed more than 50 such joint projects since its inception in 1986. PERF meetings have a decidedly multidisciplinary atmosphere, with attendance by scientists, engineers and managers with backgrounds in chemistry, chemical and environmental

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engineering, geology, microbiology, and other fields. These professionals are guided by the technical challenge to address pollution prevention and safety, as well as a personal concern for the environment.

## PROJECT SCOPE

The objective of the RSA project is to develop, apply, and transfer technology and information which will assist in developing rapid, cost-effective approaches to site characterization. The project will be used as a forum for (1) exchanging information about new technologies and frameworks, (2) promoting greater awareness and understanding of rapid site assessment approaches, and (3) advancing regulatory acceptance of the approach.

The work required to complete this project will be shared by the program participants; however, participants who wish to make monetary contributions may also participate. Current participants in the project are Amoco, Chevron, Exxon, Phillips, and Unocal. The titles of current project contributions are presented below.

Amoco:

(1) Determination of BTX in Air by Hand-Held Gas Chromatography
(2) Comparison o Field Test Kit to Laboratory Analytical Results for the Determination of Soil Contamination Levels
(3) Report on Leaking Underground Storage Tank Site Exploration Technology Assessment: Field Demonstration Project
(4) Study of Refractive Index Change Fiber Optic Sensors
(5) A Cost Effective Means of Delineation and Monitoring of a Groundwater Plume

Chevron:

Environmental Site Assessment Using the R.O.S.T. (Rapid Optical Screening Tool) System at a Former Oil Production Field

Exxon:

(1) Decision guide on when it is cost-effective to consider various existing RSA frameworks for different scenarios
(2) Fact sheets for each framework, describing the process, its applicability, advantages, disadvantages and relative cost

Phillips:

In-Situ, Real-Time Measurements of Contaminants in Soil, Water, in Air

Unocal:

(1) Vadose Zone Rapid Site Assessment using Soil Gas Methods
(2) Rapid Site Assessment Approach to evaluate Natural Attenuation

Additional oil companies are considering participation in this project as well, although formal contribution proposals have not been submitted.

The monetary buy-in option may be used by members of the Network for Industrially Contaminated Land in Europe (NICOLE) who have expressed interest in participating in the project. To date, the only NICOLE member to dedicate money to buy-into the project has been AKZO Nobel. Inclusion of other NICOLE parties will be determined after the contract is signed by the PERF project members and clear objectives and roles are stated for all potential parties.

Other agencies are also becoming involved with the Project in 1998. The USEPA Technology Innovation Office, Oak Ridge National Laboratory, Argonne National Laboratory, and the Army Corp of Engineers are likely project advisors and/or participants (through the signing of a Memo of Understanding). The PERF Project Team is hoping to conduct a joint study with the Army Corps of Engineers, using their SCAPS truck (site characterization and analysis penetrometer system). This system is similar to the R.O.S.T. technology, but has additional capabilities for in-situ analysis of contaminants in ground water.

Further PERF RSA Project activity in 1998 includes discussion and definition of project field work to take place. Ideally, this field work will test and compare new RSA technologies on an already well-characterized petroleum-contaminated site.

The PERF Project Team continues to seek input and guidance from other agencies and laboratories to maximize the value of work spent on this project. Suggestions, comments, and advice are encouraged as the PERF Project Team had a goal to maximize use of existing knowledge and expertise.

For further information or to make comments, please contact Carolyn Johlman with Phillips Petroleum Company at (918) 661-7754 or email at cljohlm@ppco.com.

## References

**www.perf.org**: Source for summary information regarding PERF organization, objectives, and current projects.