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Innovative Characterization Techniques and Decision Support Systems for Ground Water Contamination Projects

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DISCLAIMER

INNOVATIVE CHARACTERIZATION TECHNIQUES AND DECISION SUPPORT SYSTEMS FOR GROUND WATER CONTAMINATION PROJECTS

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ABSTRACT. Ground water contamination projects throughout the world must be approached as individual and unique problems. Many traditional investigation techniques require modification to meet the needs of site-specific situations. Because the age of the science of contaminant hydrogeology can be measured only in a few decades, the field is ripe for innovation. This paper describes the following new technologies:

- At Lawrence Livermore National Laboratory (LLNL), we have developed a new drilling and sampling method, which allows the evaluation of the vertical extent of contamination in a single borehole.
- We are also using new fiber-optic-based chemical analytical sensors that promise to greatly increase the ease of obtaining chemical analyses in the subsurface while greatly reducing costs.
- Because ground water investigations are data intensive, we need the best decision support system information tools to proceed with investigation and cleanup. These tools have three components: a relational database, data analysis tools, and tools for data display.

Depth-Sampling

INTRODUCTION

In investigating ground water contamination in complex alluvial sediments, we must determine the vertical as well as the horizontal extent of the contaminants. In alluvial depositional environments, stream bed deposits, which are usually coarse-grained, high-permeability sediments, may be the result of meandering and braided streams. These deposits carry the bulk of the contamination and may be difficult to define with traditional subsurface investigation techniques, especially in deep, widespread aquifer systems. Identifying the overbank and flood stage deposits, which are usually finer grained materials that retard contaminant flow, is also important for an understanding of contaminant distribution and for planning remediation activities.

Traditional drilling and sampling technologies often utilize a method whereby the drilling proceeds until the drill behavior and examination of cuttings indicate that more sophisticated sampling is required. At that point, the drill rod and bit are withdrawn from the hole; a sampler, such as a split spoon sampler, is sent down the hole on the end of a drive tube; the sampler is driven into the bottom of the hole; and the sample is withdrawn. The drill rod and bit are then re-deployed downhole, and drilling proceeds until the next zone to be sampled is encountered. Once below the water table, the problem of cross contamination of dirty zones and clean zones must be resolved. Therefore, the reliability of the data retrieved is questionable.

We developed a methodology to reduce the number of wells required to characterize a site by providing information necessary to decide how deep to drill and sample and which interval to screen. A number of technologies address this problem, such as cable tool drilling; drilling methods that drive casing behind the drill bit; hollow stem augers for shallow applications; and, new devices that are driven into undisturbed material, then opened to the aquifer, and withdrawn with a water sample intact. At LLNL, we have developed a cost-effective and rapid method of evaluating the vertical distribution of volatile organic compounds (VOCs) in ground water in a complex hydrogeologic environment (Hoffman and Dresen, 1990).

DRILLING AND SAMPLING METHOD

The LLNL method uses a mud rotary drilling system with a wireline punch-coring device. This device has a cutting edge on the drill rod, which stays in the borehole throughout the drilling and sampling operation, acting as a well casing. The drill bit can be deployed or retrieved and replaced with a core barrel on a wireline, which eliminates the time-consuming process of tripping the drill rod and sampling rods into and out of the hole at each sampling location.

When drilling with mud rotary equipment, a mud cake forms along the sidewall of the hole and penetrates the formation materials. The mud cake tends to help hold the hole open and to restrict the flow of water into the hole. However, if the drill has penetrated a contaminated zone, some of the contaminants will become entrained in the drilling fluid and can contaminate the sampler and the sample. To prevent this cross-contamination of the sample, new mud is mixed in a dedicated mud tub, and, when a new water-bearing zone is encountered, the drill bit is removed on a wireline and the new mud is pumped into the drill rod, displacing the old drilling mud through the entire drill rod and part way up the annulus. The cleaned core barrel, lined with clean brass liners, is deployed through the new mud and a 1- to 2-ft coring run is made to collect samples for chemical analysis (Fig. 1). The

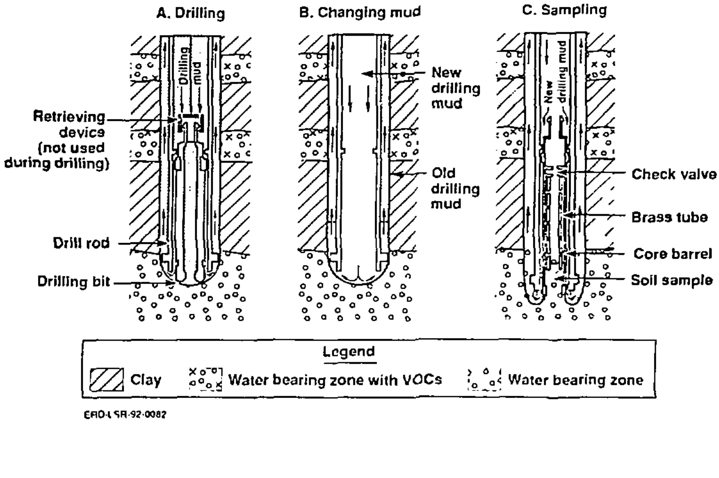

Figure 1. Schematic diagram of the three steps used in depth-sampling.

core barrel is then withdrawn on the wireline, and the core is pushed out of the core barrel. The core is quickly examined, cut at the ends of the brass sleeves, covered with a Teflon sheet, capped with a plastic cap, wrapped in duct tape, and placed on ice.

The cores containing saturated soil samples are submitted to an analytical laboratory for overnight chemical analysis for VOCs. Before the start of the next drilling day, the field geologist supervising the drilling has the appropriate information to make decisions regarding the coming day's drilling. Drilling and sampling continue in this manner until at least one permeable zone beneath the plume is free of contaminants.

At LLNL, we believe that this technology has resulted in a level of information that would have otherwise required at least twice as many boreholes. The degree of detail provided by this methodology is shown in Figure 2.

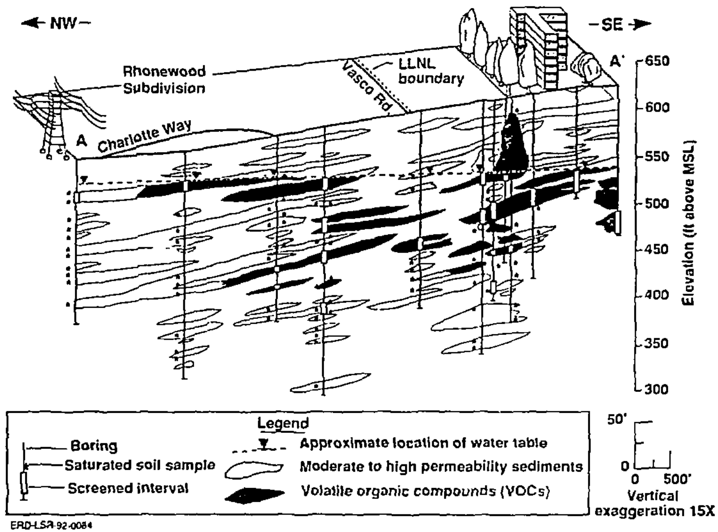

Figure 2. Generalized geologic section showing geologic and chemical complexity in the subsurfaces west of LLNL.

QUALITATIVE AND QUANTITATIVE EVALUATION OF THE METHOD

After comparing the results of the chemical analyses of the saturated sediment samples with chemical analyses of ground water from the well completed in the same zone as the saturated sediment came from, we were quite confident that we had good semiquantitative results. In order to further evaluate the quality of the chemical analyses from the depth-sampling method, we built a device called the bulk thermal desorption chamber (BTDC; Fig. 3). When the analytical laboratory receives the sediment cores, they remove a 20- to 30-gram aliquot of the core for a headspace analysis. The BTDC uses the entire core, still in its brass sleeve, and achieves extraction efficiencies of greater than 94% (Bishop

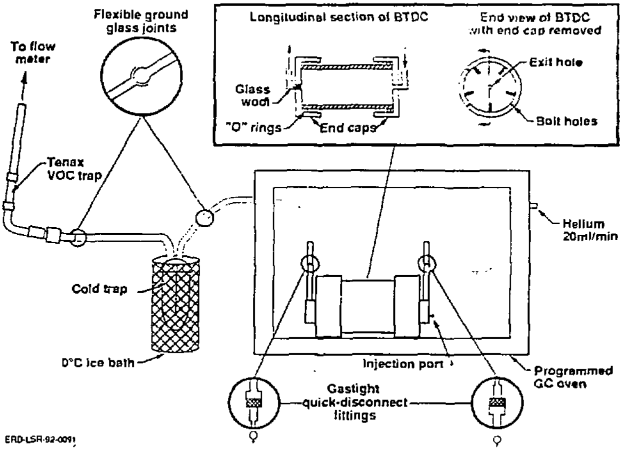

Figure 3. Bulk thermal desorption chamber (Bishop *et al.*, 1990)

et al., 1990). To compare the analyses from the two different methods, 11 samples were analyzed by the BTDC method and by two different analytical laboratories. The comparative analyses shown in Table 1 indicate excellent agreement, increasing our confidence in the depth-sampling method.

TABLE 1. Comparison of bulk thermal desorption chamber (BTDC) to headspace extraction results.

		Concentration PCE			
		Headspace			
Boring	Depth (ft)	Lab-1 (μg/kg)	Lab-2 (μg/kg)	BTDC (μg/kg)	Sediment type
B-518	85	—	15	16	Gravelly sand
	134	19	15	18	Silty sand
B-520	90–92	24	—	28	Silty sand
	95	62	—	61	Gravelly sand
	96	67	—	76	Gravelly sand
	119	4	—	2	Clayey silt
	132–136	16/12	—	16	Sandy gravel
B-521	83	2/3	—	2	Sandy silt
	94	—	5	3	Clayey silt
	98	1	—	2	Clayey silt
	130	—	23	34	Gravelly sand

However, visual examination of the cores revealed that the drilling fluid had displaced at least some of the pore water in the sample. In spite of the fact that the cutting edge of the core barrel extends somewhat ahead of the drill rod, the pressure of the pumped drilling fluid is apparently sufficient to displace some of the pore water in the formation material prior to its entering the core barrel. To evaluate the degree of pore water displacement, we developed a centrifugal pore water extraction chamber (PWEC; Fig. 4). This device receives a core sample in its brass sleeve and contains a catchment space to receive water extracted from the core sample during centrifugation. Because the drilling fluid was made up with water that had a different inorganic chemistry than the ground water, we compared the calcium, sodium, and VOC concentrations of the water taken from the PWEC with the water from the resulting monitor well screened in the same zone as the core sample. The results are shown in Table 2. In this particular core sample, over one-half of the pore water has apparently been displaced by drilling fluid. A number of variables might influence the displacement of pore water, including the hydraulic conductivity of the formation material and the distance that the cutting edge of the core barrel leads the drill rod. We intend to continue these analyses to further define the relationship between the VOC concentrations in the saturated sediment samples and the concentrations of VOCs in ground water from the monitor wells.

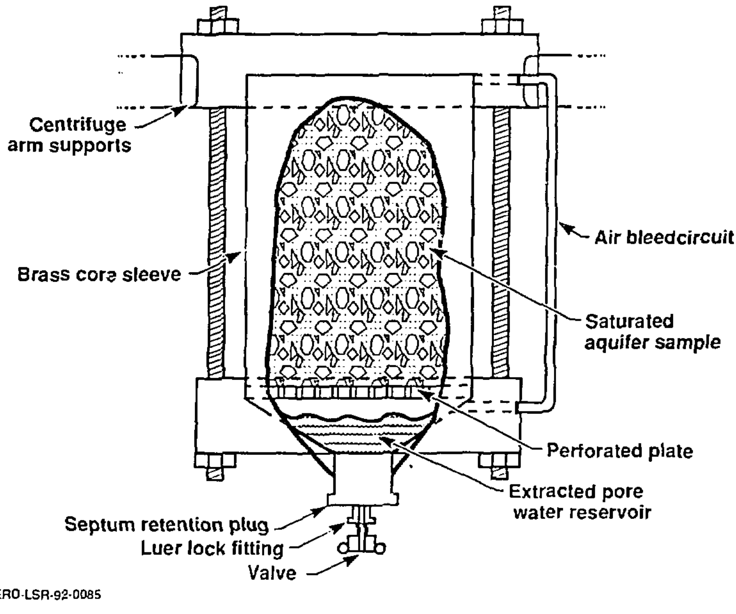

Figure 4. Centrifugal pore water extraction chamber (Bishop *et al.*, 1990)

TABLE 2. Comparison of PCE and cation concentrations in pore water, drilling fluid, and monitor well water (after Bishop *et al.*, 1990).

	Depth (ft)	PCE (ug/L)	Calcium (mg/L)	Sodium (mg/L)
MW-602 monitor well water	90–100	313	66	61
B-602 pore water (PWEC)	93.8	39	32	140
Drilling fluid	—	0	20	190
Percent displacement of pore water	—	88	74	61

Fiber-Optic Chemical Sensors

One of the major costs of ground water investigations and cleanup is chemical analyses. At LLNL, we have been developing and are now field testing a fiber-optic-based optical sensor for quantitative analysis for trichloroethylene (TCE), carbon tetrachloride, and chloroform. The objectives of the LLNL program are to:

- Modify the existing optical sensor technology for the continuous *in situ* monitoring of specific contaminants.
- Develop viable downhole sensor placement technologies.
- Extend the technique to the measurement of other contaminants.
- Deliver the technology in a hand-held device for use in the field.

HISTORY OF THE SENSOR

The optical sensor system is based upon the fact that certain reagents produce colored products in the presence of small amounts of VOCs. In the mid-1980s, the U.S. Environmental Protection Agency (EPA) supported research at LLNL in the development of a fluorescence-based probe for chloroform. This sensor irradiated the reagent with filtered light, causing a fluorescence that could then be measured. The degree of fluorescence was proportional to the concentration of the contaminant. This sensor did not have the sensitivity or reliability necessary for many applications, so the research was discontinued. In 1987, a team of people at LLNL, led by Dr. S. M. Angel, invented a new sensor concept based on the absorption of light by the reagent color change (Angel *et al.*, 1989). This sensor has been demonstrated in the field and is now undergoing advanced field testing and technology development.

SENSOR TECHNOLOGY

When the sensor is placed in the proximity of the headspace of a water sample or in a vapor stream containing the contaminant, the contaminant diffuses through a membrane, contacts the reagent, and produces a colored product. Two optical fibers enter the sensor. One of the fibers carries the incident light, and the other transmits the light reflected off the membrane back to the sensor readout. In the case of TCE, two wavelengths of light are of interest: 540-nanometer (nm) light is absorbed by the color change in the reagent; 640-nm light is also examined because the colored products are transparent to that wavelength and provides an internal standard. The ratio of 540- to 640-nm light at the sensor readout device provides a noise-free measure of 540-nm absorption.

When the analysis begins, the computer attached to the control center of the system monitors the rate of change of absorption, which is proportional to the concentration of the contaminant in the sample. The sensor is also equipped with reagent source and reagent waste tubes. The sensor itself is constructed of a porous membrane tubing, which holds the reagent (Daley *et al.*, 1992) (Fig. 5). When the analysis is complete, the computer controls the injection of new reagent into the sensor and evacuates the old, colored reagent.

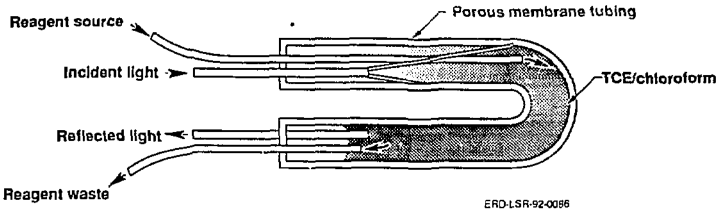

Figure 5. Schematic drawing of the continuous sensor.

SENSOR EVALUATION

The sensor has been evaluated against standards in the laboratory and against duplicate samples analyzed by independent analytical laboratories by U.S. EPA Method 624, purge and trap gas chromatography. All of the analyses agreed very well, and the great majority were within the margin of error claimed by the independent analytical laboratories (Table 3). The sensor also displayed excellent precision in multiple analyses of the same sample (Fig. 6). Similar precision and accuracy were obtained at concentrations down to one part per billion. Using this technology, chemical analyses for certain VOCs can be obtained in the field in the parts-per-billion range in a matter of minutes for a fraction of the cost of traditional analyses.

TABLE 3. Representative data from field calibration study, compiled from TCE measurements from monitoring wells and piezometers at LLNL.

		TCE				TCE	
Well	Date	Fiber (ppb)	GC (ppb)	Well	Date	Fiber (ppb)	GC (ppb)
MW352	2/13/90	44	58	MW357	2/13/90	78	84
P418	2/13/90	54	72	P419	2/13/90	61	66
MW271	3/7/90	86	160	MW364	3/7/90	59	74
MW217	3/5/90	106	86	MW458	3/6/90	33	20
MW365	3/6/90	27	22	MW142	3/6/90	94	140

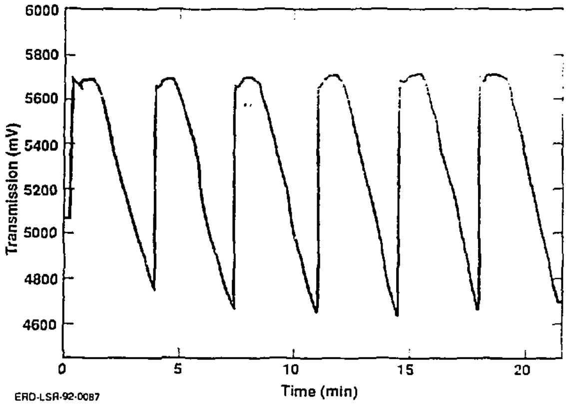

Figure 6. On-demand measurements of headspace above a stirred solution contain 20 ppb TCE (Daley *et al.*, 1992)

SENSOR APPLICATION

Because the sensor currently operates at maximum sensitivity and speed in headspace or in vapor phase analyses, our first deployment was designed for monitoring of soil vapor in an uncased borehole or a well screened in the unsaturated zone. The assembly consists of two packers on either end of the sensor designed to isolate a vertical section of the formation. A screened tube between the packers contains the sensor itself and the reagent delivery system. The delivery system consists of two syringes placed back to back with their plungers linked to an actuator motor. When activated, the syringes operate together, one injecting the new reagent into the sensor and the other withdrawing the used reagent. The packers are inflated and deflated by compressed air, allowing the whole assembly to be moved to different depths within the well (Fig. 7). The light source and detector and the system controller remain at the surface, attached to the sensor assembly by optical fibers and electrical conductors.

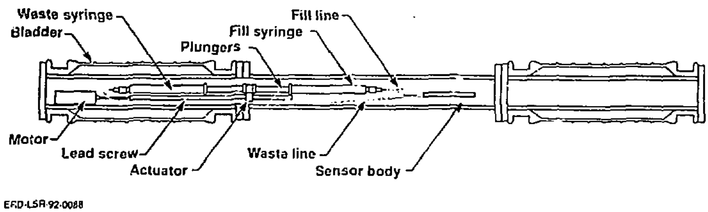

Figure 7. Schematic of the air-actuated well packer assembly containing the fiber-optic sensor and the reagent delivery system.

We constructed a device similar to the well packer assembly (Fig. 7) inside a cone penetrometer. A cone penetrometer is a truck-mounted instrument that drives a steel rod into soft sediments using the weight of the truck as a driver. At appropriate depths in the unsaturated zone, we can obtain an analysis of contaminant concentration in soil vapors (Fig. 8).

Because chemical analyses of water samples below the water table are also of critical importance, we are designing a submersible system that will be deployed in screened wells below the water table. Our current design includes a probe that will extract a sample from the ground water and move it to

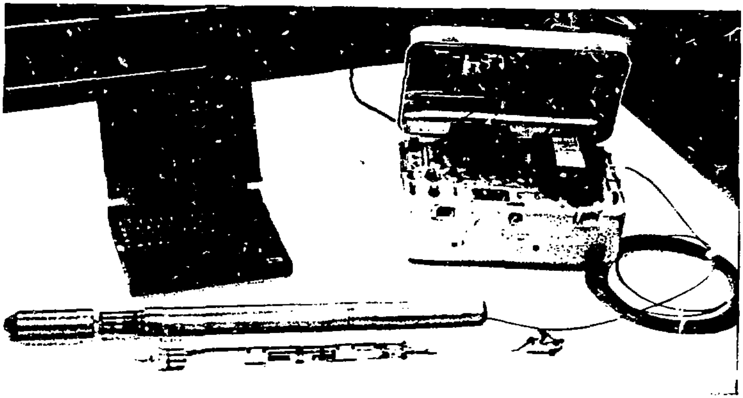

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Figure 8. Photo of the fiber-optic light source and receiver, a notebook size computer to control the system, a cone penetrometer head, and the sensor and reagent delivery system which fits inside the penetrometer head.

a location within the downwell sampler where a headspace can be created at the sensor. Such a system could be moved up and down within a screened well, providing ground water analyses at part-per-billion levels.

Decision Support Systems

INTRODUCTION

In conducting a ground water contamination investigation or cleanup project, whether we have small amounts of data in the early stages of the investigation or very large datasets in a mature project, we must have systems in place that allow us to use the data we have available to make decisions on how to proceed. These decisions included:

- Where to drill the next monitor or extraction well
- Which wells to sample on what schedule.

- Whether to query the analytical laboratory about a potentially spurious analysis.
- How to design the necessary remediation.
- How to manage an extraction well field.
- Whether the cleanup is complete.

A decision support system must contain the necessary tools that will allow us to make the hundreds of daily decisions required in a ground water contamination project, and to increase our chances of making the correct decisions.

COMPONENTS OF THE SYSTEM

There are three components of a decision support system: the database, the data analysis tools, and the data display tools (Fig. 9).

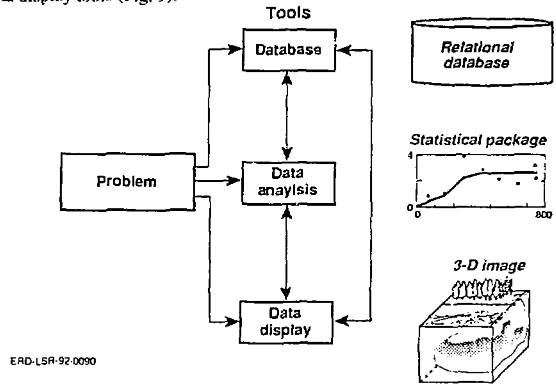


Figure 9. Schematic representation of the components of a decison support system.

- *The Database.* This is where the data are assembled, sorted, and stored so that they can be recalled and used in any manner needed. In any ground water contamination investigation, large amounts of data are collected regarding the subsurface geology, hydrology, and chemistry. The geologic information is derived from geologic logs, interpretation of geophysical investigations; and laboratory analyses of sample porosity, grain size, and mineralogy. Hydrologic information is derived from water level measurements, from measurements and interpretation of pumping tests, and from laboratory analyses of hydraulic conductivities of core samples. Chemical information comes from chemical analyses of ground water samples, soil vapor analyses, analyses of saturated soil samples, and analyses of soil samples from the unsaturated zone. All this information and any other data needed by the project is filtered through a quality assurance/quality control system and a data validation system before it is entered into a relational database (Fig. 10). The relational database allows the storage of each piece of data in a single location in the database without repetition. It also allows us to select a set of parameters and obtain a report of the dataset that matches those parameters.

- *Data Analysis.* In this component, the data can be manipulated and compared, statistical analyses can be applied, and models can be run. Statistical tools can be used to identify trends in contaminant concentrations in various wells or locations of the study area. These trends can then be correlated with ground water gradients and flow directions to help determine sources of the contamination and to guide the location of additional monitor wells to determine the distribution of the contaminants or

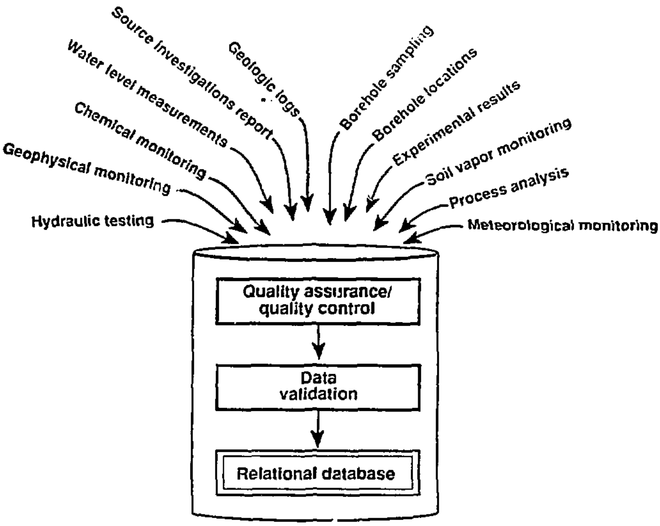


Figure 10. Schematic of the flow of information from various sources through a set of quality filters into the relational database.

extraction wells to improve cleanup efficiency. The statistical analyses can also be used to identify chemical analyses that are outliers. These findings can trigger inquiries to the analytical laboratory regarding spurious results or alter field activities to determine the reasons for the changes in concentration. A continuous feedback loop into the database upgrades the quality of the data and helps validate or reject the outlying analyses.

Interpolation tools are a crucial part of any ground water investigation. Because our known data points are limited to our well locations, we must have the ability to interpolate between the datapoints. This can be done by inspection of the data by scientists who then apply their interpretation of what may exist between the well locations, or we can apply sophisticated mathematical codes that examine the datapoints and supply suggested interpolations. These tools are used to build the necessary numerical grids for ground water flow and contaminant transport computer models. They are also used to supply input to the data display tools. Because the site characterization activities continue through the life of the project and new data are continually entering the database, we continually compare the results of the interpolation tools to the actual data. This helps the interpolation tools to present a more realistic picture and also helps us to continually upgrade the tools as well as our understanding of the subsurface.

The ground water flow and contaminant transport models are dependent on the database and the interpolation tools. These computer codes allow us to apply basic principles of flow and transport, using site-specific data. The results of these models also help us to understand the subsurface environment and active mechanisms of contaminant transport, degradation, dispersion, and diffusion.

Once again, where the model results differ from the field-derived measurements, we alter the assumptions of the model to match the field data, thereby continually improving our understanding of the system. The tools are also used to predict contaminant distribution in the future with and without remediation activities. These predictions allow us to design more efficient monitoring plans and cleanup systems.

Once we are fairly confident that the model output is an acceptable approximation of reality, we can begin to apply tools to help design an optimal cleanup system. At LLNL, we are developing two such tools. The first allows us to work with a map of the site on a computer screen, to move extraction wells around, alter their pumping rates, and superimpose these changes in cleanup system design on the flow and transport field from the models (Canales, 1992). This tool allows us to evaluate a number of different extraction well field designs in a much shorter time frame.

We are also working on an artificial neural network (Rogers and Dowla, 1991). With this system, we provide the neural network with the results of approximately 200 runs of our flow and transport model. Each of these runs may take up to 8 hours of computer time, but we can use multiple computers simultaneously. As a result of observing the outcome of these 200 runs, the neural network learns to predict what the model outcome will be for any given scenario. Once the neural network has learned to make these predictions, it can predict the outcome of a new pumping scenario in a fraction of a second. This allows us to try many more scenarios, as we seek the optimum pumping strategy, in a fraction of the time and cost.

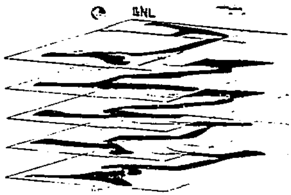
- ***Data Display.*** This component allows the data to be displayed in various lists or as graphics. It can receive its input either from the database or from the data analysis tools. Although the data analysis tools can produce many sophisticated interpretations of data based on numerical equations of basic principles of ground water flow and transport, there continues to be no substitute for the examination of the data by skilled professional ground water scientists and engineers. We can now display the data in a number of ways with different computer codes and on different computer hardware. At LLNL, we display our data in vertical cross sections, horizontal slices, contoured surfaces, and video animation of model outputs (Fig. 11). We can display the data in seven dimensions: the three spatial dimensions, and the dimensions of geology, chemistry, hydrology, and time. By looking at the data displayed in multiple ways, in multiple combinations, from different directions, and in color, scientists are provided with new tools to understand the subsurface environment, to answer many questions, to formulate new questions, and to identify ways in which to proceed with the project.

THE INTEGRATOR

As with the data analysis tools, we must be constantly aware that the input into the data display tools is the data from the database, and must be scientifically defensible. The feedback loop among all three components of the decision support system must always be running in the foreground with emphasis on the quality of the data in the database, and the modification of the various tools when they deviate from reality.

At LLNL, we are also working on a computer code called the INTEGRATOR (Johnson *et al.*, 1992). This code allows us to formulate requests for reports that require input from a number of applications running on different computational platforms. For instance, we may desire to select a portion of the data on the relational database stored on the VAX computer, apply a statistical analysis running on a SUN computer, apply a flow and transport model also running on a SUN, display the output from the model on an IRIS workstation, and control the entire request from a Macintosh computer. This system is a powerful tool for providing decisionmakers with appropriate data, in the appropriate format, and a useful display to ensure the most correct decision.

• Interactive Volume Modeller (IVM)



• SLICE

• Interactive Surface Modeller (ISM)

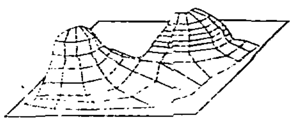


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Figure 11. Examples of different types of graphic data displays, including a three-dimensional representation of TCE deneath the LLNL site, a set of horizontal slices showing changes in buried stream channels with depth (Qualheim and McPherrin, 1992), and wire mesh representation of a surface. Although not shown in this figure, the amount of information is greatly enhanced by the use of color.

Acknowledgments

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