**Subsurface Barrier Validation
With the
SEAttrace™ System
Phase I Topical Report**

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Authors:

Sandra Dalvit Dunn

William Lowry

Robert Walsh

Daniel Merewether

Veraun Chipman

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Karen Cohen

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Science and Engineering Associates, Inc.

3205 Richards Lane, Suite A

Santa Fe, NM 87505

(505) 424-6955

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ABSTRACT

Impermeable subsurface barrier materials and emplacement technologies are being developed to contain high-risk contaminants in soils. These containment technologies are being applied to contaminated sites which are either posing immediate threats to public safety or are too difficult/costly to remediate with current practice. Using techniques derived from mining and construction ground stabilization industries, highly viscous materials and cementitious materials are being injected into soils to form walls and floors of very low permeability media to restrict transport of contaminants to the water table. Since these barriers are applied in high-risk circumstances, knowledge of their emplaced integrity is critical.

Barriers placed in the unsaturated zone pose a particularly difficult verification and monitoring challenge. They cannot be tested with water fill to determine if they are flawed, since doing so would mobilize the contaminants they are intended to contain. Geophysical techniques can image the barrier installation but cannot attain adequate spatial resolution to detect small flaws. Gaseous tracer testing, on the other hand, can detect breaches in barrier structures without risking mobilization of the contaminants, and can, with rigorous analysis, determine both the size and location of the flaws.

The SEAttrace™ system is an integrated, real time gaseous tracer system developed for barrier verification and monitoring in the unsaturated zone. The methodology incorporates gaseous tracer injection inside the contained volume of soil with analysis of tracer arrival at sampling points outside of the barrier walls. Solar powered, remotely accessible, and capable of multimonth standalone operation, SEAttrace™ collects soil gas samples with an automated multipoint soil gas sampling and analysis system, then immediately analyzes this data to locate and size flaws in the barrier construction. Since the approach uses real time analysis to characterize flaws, immediate repair of the barrier may be conducted with the appropriate remedial method. The gas analyzer used by the SEAttrace™ system is also capable of measuring volatile organic compounds in the gas phase, so the system is also well suited for long-term monitoring of the barrier's integrity.

In this effort the soil gas scanning system and data inversion methodology were integrated in a field rugged enclosure for remote operation. The data acquisition/control software and hardware were developed and tested, the inversion methodology was programmed for real time use, and a prototype system constructed for field testing. A mockup barrier was constructed with engineered leaks at known locations.

The test volume consisted of a small-scale barrier with monitoring points both internal and external to the barrier. The shape and the dimensions of the barrier were chosen to be realistic, easily constructed, and capable of allowing multiple leaks to be tested during the same test sequence. A V-shaped trench roughly 5 meters deep and 15 meters long was chosen. The sidewalls and ends of the trench were sloped 45° from horizontal - a slope shallow enough to minimize construction hazards but steep enough that it would be economically viable to use at a real site (the sidewalls meet at a reasonable depth below ground surface). A vertical wall was formed at one end of the trench after the trench had been excavated. This allowed the SEAttrace™ system to be tested in one of

the most typical barrier configurations (a vertical cut-off wall). It also allowed the system to be field tested in a medium that was homogenous (the backfill material between the constructed vertical wall and the excavated sloped wall was well graded).

Five test sequences were completed. The first two sequences were performed in April and May of 1997. Results from these tests showed there were large non-engineered leaks in the barrier, and that the MSA gas analyzer was not capable of operating continuously. The MSA was replaced with a B&K photoacoustic analyzer and the barrier liner was replaced. The remaining three test sequences were performed in September and October of 1997.

Although difficulties were encountered during the execution of this project (problems with the initial mockup barrier installation required removal and replacement of the impermeable liner), the final results showed that the system was capable of locating and sizing leaks in barrier installations. SEAttrace™ was able to find multiple leaks on the barrier, even under adverse conditions including high background concentrations, spatially variable background concentrations, a heterogeneous medium and multiple unanticipated leaks. The very small engineered leak of 1.1 cm diameter was detected. The locations of the leaks that the system found were consistent with time (inversions of sequential leak data sets produced similar results). The calculated location of the engineered leaks was found to be within 0.4 to 1.2 m of the true positions. The single engineered leak that was not affected by another leak was found within 0.4 m of the true position, while leaks near adjacent leaks were found within 1.2 m. The accuracy of the SEAttrace™ system for a barrier where there are few leaks spaced relatively far apart from each other will be more closely reflected by the more accurate results. The calculated radii of the leaks were less accurate. The accuracy of the leak size determination is affected by the forward model used in the SEAIM code, the correlation between leak radius and start time of the leak as seen in the inversion code, and the injection method of the source concentration. The system characterized the leaks as ranging from 10 cm to 17.3 cm in radius, while the actual sizes ranged from 0.5 to 5.1 cm in radius.

It is noteworthy that the technical products of this effort (the integrated monitoring system design and inversion code) were applied at two test barrier installations under a separate contract activity. The Subsurface Contaminants Focus Area, through Sandia National Laboratories, supported this work. Tests were conducted on jet grouted thinwall diaphragm barriers at the Dover Air Force Base Groundwater Remediation Field Laboratory, and a colloidal silica permeation grouted barrier at Brookhaven National Laboratory. The SEAttrace™ approach and hardware systems successfully detected flaws (both intentional and unintentional) in both barriers.

1. INTRODUCTION

The Department of Energy (DOE) is currently developing in-situ barrier emplacement techniques and materials for the containment of high-risk contaminants in soils. These include slurry walls, grout barriers, soil-mixed walls, cryogenic barriers, and other forms of impermeable barriers. Because of their relatively high cost, barriers are intended for use in high-risk circumstances. These include cases where the risk is too great to remove the contaminants, the contaminants are too difficult to remove with current technologies, or the potential for movement of the contaminants to the water table is so high that immediate action needs to be taken to reduce health risks. Consequently, barriers are primarily intended for use in the high-risk sites where few viable alternatives exist to stop the movement of contaminants in the near term. Assessing the integrity of the barrier once it is emplaced, and during its anticipated life, is a very difficult but necessary requirement. Existing surface-based and borehole geophysical techniques do not provide the degree of resolution required to ensure the formation of an integral in-situ barrier.

Many different construction methods and materials are available to create subsurface containment barriers (Rumer and Mitchell 1995). These include but are not limited to:

- slurry trench cutoff walls (soil-bentonite, cement-bentonite, or composite materials used in a continuous trench typically created by a backhoe, clamshell or dragline)
- plastic or diaphragm cutoff walls (typically excavated in panels using a clamshell, dragline or rotary drill)
- thin panel cutoff walls (thin grout wall created with a vibrating beam or a steel sheet pile wall)
- column barriers (vertical, slant, or directional walls created by soil mixing, permeation grouting or jet grouting)
- naturally occurring low permeability geologic formation are often used as the bottom of a barrier containment system

The types of, and potential for, defects in the containment barrier system are dependent on the barrier type and shape, the construction quality control, and the geologic characteristics of the specific site. The configuration of these flaws can be in the form of non-continuous panels at mismatched joints, soil regions with no barrier backfill material due to incomplete emplacement or grouting, open fractures, or thinned areas of the panels. The sources of defects can be grouped into two categories: construction defects and defects due to degradation of the barrier with time.

Construction defects include:

- heterogeneous backfill due to improper mixing, entrapped slurry pockets, or material falling from the trench wall during construction / curing
- inferior quality of the backfill material
- trapped sediments at the bottom of the trench, inadequate excavation of the trench key, or incomplete coupling between the bottom and sides of a barrier
- inadequate bonding between sections of backfill

- inadequate placement between sections of backfill - especially as depth increases
- hydrofracture of the soil during barrier construction

Barrier degradation with time occurs due to the following processes:

- ground freezing and thawing cycles
- wetting and drying cycles in the near surface soils
- desiccation of the backfill material
- chemical incompatibility between the barrier and contaminants
- adjacent ground deformations and backfill stresses

Barrier construction technology has evolved from the construction industry and mining practices, where structural strength is a greater driving criterion than resistance to fluid and contaminant transport. Consequently, validation of these emplacements has been primarily through construction QA practices (grout material balance, surface survey of the installation, materials QA testing, etc.) which do not provide sufficient assurance of emplaced integrity and resistance to contaminant transport.

The most common barrier emplaced to date is the slurry wall, in which a trench is excavated down to an impermeable layer (such as bedrock or clay) and backfilled with a heavy slurry of bentonite and/or grout. These designs are inherently self healing and have historically been applied to contain contaminated groundwater. Testing of these installations is typically accomplished by drawing down the water level inside the barrier to a constant level (referenced to the water level outside of the barrier) and measuring the water flow rate under steady state conditions. The bulk hydraulic conductivity of the barrier can be estimated by this technique, which allows calculation of the contaminant flux from the barrier. A common criterion that has evolved from this practice is a hydraulic conductivity of 10^{-7} cm/s.

Slurry walls cannot treat many applications in the DOE complex because the sites may not be conducive to such emplacements. At the Hanford tanks, for example, barriers are being considered for emplacement beneath the tanks while they are being remediated to contain accidental releases of the tank contents. No confining layer exists at a reasonable depth below the tanks to serve as the floor of a slurry wall installation, and the performance of slurry walls in the vadose zone is uncertain. Consequently, alternate barrier technologies such as jet grouted columns or panels are being considered at many sites, and suitable verification technologies have yet to be developed. Hydraulically testing these installations is not likely, since many of the sites are in the vadose zone. Introducing water to the contained volume may mobilize contaminants otherwise in an immobile state. Geophysical techniques have been tested and have been shown capable of imaging the emplaced barriers, but do not have the required resolution to detect flaws as small as is necessary. Cross borehole electromagnetic surveys, ground penetrating radar, and electrical resistance tomography have successfully imaged barrier material in-situ. In some cases these techniques have detected major flaws, but they are not capable of resolving the types of leaks which would cause the barrier installation to fail its performance criteria. Gaseous tracer testing of barrier installations shows the promise of resolving large and small flaws in barrier walls, so is an attractive approach for conservative verification of

barrier integrity (Heiser 1994; Betsil and Gruebel 1995). Significant research in the use of gaseous tracers, using perfluorocarbon tracers and highly sensitive detection equipment, has been pioneered by John Heiser at Brookhaven National Laboratory.

Science and Engineering Associates, Inc. (SEA) has developed a tracer-based monitoring/verification system for contaminant containment systems. Called SEAtTM, the technology is able to locate and size leaks in subsurface barriers that are in an unsaturated medium. It uses gaseous tracer injection, in-field, real-time monitoring and real-time data analysis to evaluate barrier integrity. SEAtTM currently uses sulfur hexafluoride (SF₆) as the tracer gas, because it is readily detected by field rugged infrared analysis techniques and is a non-hazardous, commonly available gas used as a tracer in ventilation and hydrologic system testing (Wilson and Mackay 1993).

This engineering development effort capitalizes on earlier proof-of-concept tests conducted at the Sandia National Laboratories Albuquerque site (Lowry, et. al., 1996). This program, supported by the Subsurface Contaminants Focus Area, demonstrated that it was possible to monitor gaseous tracer distribution with adequate temporal and spatial resolution to detect leaks. The proof-of-concept tests also showed that a spherical diffusion model could reasonably characterize the leaks using simulated annealing to optimize the data inversion.

The focus of the current effort was to engineer an integrated system to operate autonomously at remote sites, automatically and in real-time characterizing barrier flaws. In this Phase I effort, SEA proposed to do the following:

1. Fully integrate the soil gas monitoring system and the leak identification methodology in a system capable of autonomous operation
2. Evaluate the integrated system under field conditions in a barrier mockup

An integrated SEAtTM system was developed, incorporating real time data acquisition and leak analysis. An engineered thermal enclosure was designed and fabricated which maintained the analyzer and data system at moderated temperatures. The system uses solar photovoltaic power and battery backup to allow operation in remote, unpowered sites. Cellular modem communication allows remote access for data downloads and control system changes.

A new data inversion code was developed that incorporates data screening to optimize calculational time, is capable of searching for flaws in three-dimensional space (the previous version assumed the presence of the barrier wall was a known distance from vapor sampling points), and can operate in real time in the system control computer after gas samples have been collected. Parametric studies and numerical simulations evaluated the code's sensitivity to input parameter variations and real world conditions.

A subscale barrier mockup was constructed in which multiple engineered leaks were located. The system was tested in this facility to determine its ability to accurately locate and size leaks. Five injection sequences were conducted.

This report documents the Phase I accomplishments of this effort.

2. OBJECTIVE

As stated in the contract statement of work, the overall objective of the effort was to “develop and demonstrate an integrated methodology and field system to evaluate the integrity of in situ, impermeable barriers constructed in the vadose zone.” Integrating the soil gas monitoring system with the leak identification methodology included:

- Upgrading and fabricating a new monitoring system capable of automatically providing compositional analysis in real time for enough ports to adequately monitor a full-scale barrier
- Transforming the prototype inverse modeling code into a more generalized code
- Developing a preprocess module to determine if data collected with the monitoring system required analysis with the inversion code

Analytical and numerical simulations were performed to determine the inversion code's sensitivity to model parameters. Once the integrated system was completed, it was tested in a subscale test bed. The test bed demonstrated not only how the system functioned under real conditions, but it also tested the accuracy and repeatability of the SEAttrace™ measurements.

The success criteria stipulate that the system should be capable of determining the leakage characteristics in real time (within six hours of collecting soil gas data), and should be able to detect a leak as small as 10 cm² in area with a positional accuracy of ±50 cm.

3. DESCRIPTION OF THE SEATRACE™ SYSTEM

SEAttrace™ is predicated on the relatively simple and predictable transport process of gaseous diffusion in porous media. Diffusion is an attractive process to utilize for leak detection because the tracer concentration histories measured at locations distant from the source are highly sensitive to both the size of the breach and the distance from the leak source. This sensitivity allows a global optimization modeling methodology to iterate to a leak geometry and location by minimizing errors in a relatively simple transport model. Thus, SEAttrace™ is composed of two distinct functional components: a monitoring system and an optimization code.

A schematic of the SEAttrace™ system is shown in Figure 1. Multiple sample points are located outside the barrier, as well as one or more injection and sample ports inside the barrier. These ports are connected to a stand-alone data acquisition and analysis system. A non-hazardous tracer gas (sulfur hexafluoride) is injected into the barrier, creating a large source volume of the tracer. If the barrier has a breach open to gas phase transport, the tracer will diffuse into the surrounding medium and the exterior sample ports will measure the amount of tracer in the soil gas with time. These concentration histories can then be provided (along with the sample locations, medium properties, and the source concentration) to the global optimization code. The code iterates to find a best-fit solution given the input parameters. This sequence is depicted in the general flow diagram of Figure 2. Components of the integrated system are described in the following sections.

3.1 Sampling and Analysis System

A key feature of the integrated system is its ability to automatically sample and analyze soil gas samples from a large number of sampling locations around the barrier. The SEAttrace™ monitoring system has evolved from earlier SEA designs which automatically measured soil gas pressure and sampled/analyzed soil gas for contaminants and tracer gases. Significant enhancements were made to the system to satisfy the field requirements of this development effort:

- A rigorous, fault tolerant acquisition and control code was written to operate on an embedded PC platform.
- Self checking was incorporated into the software and hardware, to ensure sample manifold integrity, intermediate sample bag integrity, thorough purging of the sampling system between soil gas samples, and also to identify gas sample lines that may be plugged.

3.1.a Soil Gas Scanning System

The general system schematic is shown in Figure 3. The system controller is a low power consumption i486 embedded industrial computer operating at 33 mhz when at full operation. This industrial PC has many features needed for this application: very low power consumption when in the inactive state between sampling operations; fault tolerance through a timer that senses lock-ups and can reboot the computer; and a versatile I/O bus that accommodates a multitude of devices (modems, digital I/O, analog/digital conversion, video displays, etc.) Communication with the analog/digital converters and gas analyzer is accomplished through standard RS232 and RS485 serial lines. A cellular-capable modem is attached to the computer through its native PC/104 bus. Cellular communication is enabled for defined periods of the day so that the computer can be accessed remotely to change operational parameters and download data.

The computer activates sampling sequences at defined times of the day, controls the sampling operation, and stores the analysis data. Two types of operations are executed. One is simply measuring the soil gas pressure at the sampling locations, and the other is the complete sampling and analysis of soil gas composition at each port. After the soil gas analysis data has been collected, the control code passes the data to the inversion code for leak characterization, which then returns the leak information for storage. The system developed for this project is capable of sampling up to 64 sample lines in the soil. Typical time requirements for the different operations are:

- Soil gas pressure measurement: 6 minutes
- Soil gas sampling and analysis: 8 hours
- Inversion code operation after completion of the soil gas analysis: 20 minutes

The sampling manifold consists of an array of small, low power electric solenoid valves controlled by a corresponding array of relays (see Figures 4 and 5). An individual solenoid valve to the common manifold connects each sample line. A DC sample pump draws the gas sample through the valve into the manifold, and transfers it to an intermediate Tedlar sample bag. The pump internal to the gas analyzer then pulls a sample from the bag. The use of the intermediate sample bag is required because the flow rates attained through the sample line are too low to satisfy the gas analyzer flow requirements. This configuration allows purging and acquisition of the next sample in the sequence while the gas analyzer is evaluating the previous sample.

Purging of the sample manifold and lines occurs prior to acquisition of the next sample, using a network of solenoid valves and the sampling pump. Complete purging of the gas analyzer filter chamber is ensured by analyzing a sample of gas obtained from the interior of the instrument enclosure. If that sample shows concentration of the tracer gas above a predefined level, the system is purged again until the criteria is satisfied. Atmospheric gas samples are analyzed both before and after a sampling run to ensure total system purge.

3.1.b Gas Analyzer

The gas analyzer used in this system is the Innova Instruments Model 1302 photoacoustic analyzer (former Bruel & Kjaer Model 1302). This is an infrared absorption device capable of quantifying the presence of up to five compounds (plus water vapor) in the soil gas. Photoacoustic analysis occurs by capturing a sample of the soil gas inside a chamber, pulsing the gas with a very precisely filtered infrared source at a wavelength corresponding to a unique absorption band of the compound, and sensing the magnitude of the absorbed energy by a set of microphones. This device is capable of cost effective, reliable measurements in environments unsuitable for most other instruments. The unit has an operating temperature range of 5 to 40°C with a temperature influence of ± 10 percent of the detection threshold per °C. Performance reliability of the analyzer is ensured by a series of self tests. In the course of this project several other analysis techniques were considered and this device was found to be the most mature and field ready. Early in the project a non-dispersive infrared (NDIR) analyzer was purchased (MSA Model 7000 LIRA analyzer) and installed in the system. This unit is relatively inexpensive (\$7000 vs. \$35,000 for the photoacoustic analyzer) and potentially capable of sensing the sulfur hexafluoride tracer gas with sufficient accuracy for SEAtace™ applications. It is also a flow through device, which could operate at the low flow rates resulting from the long tubing runs present in the typical barrier verification application (hence negating the need for an intermediate sampling bag). This flow-through design allowed much shorter sampling times. However, when placed in the field, this instrument required daily recalibration due to a combination of the minor temperature variations present in the field instrument enclosure and the need to turn the analyzer off between sample periods to conserve power. This was unacceptable, and required reconfiguring the sampling plumbing to incorporate an intermediate sample bag, recoding the control software, and physically installing the photoacoustic analyzer in the enclosure.

Gas chromatographs were also considered. They were ruled out because of the difficulties in satisfying their operating environment requirements. They require an inert carrier gas flow that necessitates a very large gas source for long-term operation (several weeks unattended). The units we evaluated also could not operate for these extended time periods without frequent calibration by the operator, which made their integration with the system difficult. To collect the soil sample, solenoid valves in a manifold system sequentially isolate up to 64 sample ports. Soil gas samples are drawn into an intermediate tedlar sample bag using a diaphragm pump. The B&K uses its own pump to draw the sample from the tedlar bag into its test chamber. The tedlar bag, the manifold and its associated tubing, and the tubing from the SEAtace™ system to the subsurface port are purged prior to sample collection.

SEAtace™ performs numerous diagnostic tests to assure continuous sample quality. To assure gas samples are not diluted by leaks in the system's plumbing, the manifold and tedlar bag are always kept at a slight overpressure. A vacuum test is performed on the manifold before each gas analysis sequence is initiated to determine if there are any leaks in the plumbing. To assure adequate purging between measurements, an atmospheric sample is analyzed at the beginning and end of each sequence. The pressure and temperature in the manifold are monitored to assure these parameters are

within the hardware's specified operating ranges. Monitoring the pressure of the intermediate sample bag while collecting a sample can be indicative of the integrity of the sample bag, pump, and pressure sensor. Finally, any errors recorded by the B&K analyzer are collected and stored.

3.1.c Power and Environmental Control.

Stand-alone operation was a goal of this development project because at many remediation sites power is not accessible, and when it is, it is frequently unreliable. Protection from the elements was also crucial, as was moderating the temperature rise encountered due to the internal heat generation of the system components (the gas analyzer is the greatest contributor to the thermal load, at nominally 100 Watts during its operation). In the early stages of this project a company was contacted with expertise in designing and fabricating instrument enclosures for remote applications (Zomeworks Corporation, Albuquerque, NM). A design was proposed which would integrate remote power, protection from the elements, and thermal control in an integrated enclosure. Called the Cool Cell, this system satisfies the enclosure thermal performance requirements through use of a large water heat sink and a passive cooling cycle. A 30-gallon reservoir is located near the top of the enclosure. During operation of the heat generating components (and also during the day due to heat gain by solar exposure) the water will absorb heat energy and moderate the temperature rise inside the enclosure. At night, a passive thermosyphon action initiates in the circulation loop. The water reservoir is connected to a radiator on the top of the enclosure with a supply and return line (see Figure 6). During the day circulation of water through the loop is prevented because the radiator water is at a temperature higher than that in the reservoir, and insufficient density gradients exist to induce natural thermosyphon circulation. At night, however, the radiator will cool below the reservoir temperature, resulting in a density gradient that causes recirculation of the water as heat is rejected from the radiator. If the temperature of the water in the reservoir drops below 40° F, the temperature/density relationship of water is such that thermosyphon action will no longer occur at night. Hence, in the winter the system tends to retain the generated heat instead of rejecting it, which helps maintain the instruments at temperatures above freezing. Temperature data is plotted in Figure 7 showing the heat rejection and temperature moderating effect of the Cool Cell design.

The solar electric portion of the system is a conventional photovoltaic panel/gel cell battery system. It is designed to provide 30 Watts of continuous power, using four solar panels and eight batteries. An integral charge controller prevents both overcharging and discharging of the batteries to unacceptable levels. The assembled system is shown in Figure 8.

3.2 Data Inversion Methodology

Once concentration history data has been collected, it must be analyzed if any tracer gas was detected outside the barrier. This type of posttest analysis is typically performed by manually trying to match field results to results from forward diffusion

models through an iterative process. This is a time consuming, artful process as the leak geometry, dimensions, and location are variable, the medium properties are often not well characterized, and the source concentration is variable. To overcome the difficulties of manual analysis, SEAtTM uses a global optimization technique to effectively search multidimensional "space" to simultaneously find the best fit solution based on all of the input parameters.

3.2.a General Methodology

The general methodology of this approach rigorously searches for a set of parameters that will best characterize the leak. It requires a diffusion model that calculates concentration histories from the multiparameter "space." These calculated concentrations are compared to the measured concentrations using an objective function. For this project, the objective function was defined as the sum of the squares of the differences between the predicted and measured tracer concentrations. A stochastic method is then employed to minimize the objective function, thus finding a best fit to the data given a range of defined parameters. The stochastic method chosen is called Simulated Annealing (Ouenes 1992). The technique selects points from the given input ranges for each parameter at random. Using these values, the objective function is evaluated. The process is repeated, the two values for the objective functions are compared, and the code chooses which is more accurate. This point is remembered and the process repeated with a new set of parameter values. The parameter values are chosen using a probability distribution that relies on the objective function of previous points in a complex way. The accuracy of the results is dependent on how well the chosen leakage model matches the monitoring data, the number and ranges of the unknown input parameters, and how the model parameters physically interact with one another. Appendix A describes the methodology in detail.

Presently SEAIM utilizes a single one-dimensional spherical diffusion model (see Figure 9). The model assumes the following:

- A constant source concentration is maintained inside the barrier
- The flux exiting the leak is not restricted by diffusion through the leak (a function of the barrier thickness, source concentration, and the leaks dimension and flow properties)
- The region of the barrier under evaluation is a plane surface
- The medium outside the barrier is homogenous (e.g., that the diffusivity of the tracer gas through the soil pores is constant)
- It neglects gravity, advective flow of the tracer, and adsorption/desorption of the tracer

While this diffusion model is simplistic, to a first-order it is realistic. If the area of the barrier wall is much greater than the area of the leak, at some distance from the leak the gas will approach spherical diffusion regardless of the true geometry of the leak. Additionally, the barrier wall will act as a flat no-flow boundary and the medium that the

tracer gas is diffusing into can be assumed to be semi-infinite. The partial differential equation describing this transient process is:

$$\frac{\partial c}{\partial t} = \frac{D}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c}{\partial r} \right)$$

where c is the concentration at radial position r and time t . The controlling parameter in this process is the diffusivity of the tracer in the soil gas, D , which is inclusive of the effects of porosity and soil tortuosity. If the barrier is well constructed (e.g., there are only a limited number of breaches in the barrier walls), the mass of tracer gas that can be injected into the internal pore volume of the barrier will be very large when compared to the mass of tracer gas that can diffuse through the leak area(s). Thus, the barrier will serve as an infinitely large reservoir of tracer gas at a fixed concentration (once the injected tracer gas has been completely injected and reached a state of equilibrium). Boundary conditions can be set as:

$$c(r_0, t) = c_0 \text{ at } t \geq 0 \text{ and } c(r, t) = 0 \text{ at } t \geq 0$$

Solving the differential equation results in a straightforward expression of:

$$c(\underline{p}; x, t) = \frac{r_0}{r} c_0 \operatorname{erfc} \left(\sqrt{\frac{(r-r_0)^2}{4D(t-t_0)}} \right), \quad r > r_0, \quad t > t_0$$

where

$$r^2 = (x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2,$$

$y_0 = ax_0 + b$ (the barrier surface is a plane described by $y = ax + b$),

(x_0, y_0, z_0) is the location of the leak,

(x, y, z) is the location of the sampling point,

t_0 is the time that the leak began, and

r_0 is the constant radius of the leak after time t_0 .

In the inversion code, the size and location of the leak and the time the leak began are treated as unknowns; the source concentration and diffusivity can be treated as either variables or constants, and the location of the sampling ports, with respect to the barrier, are assumed to be known. A range of values (search limits) must be input for each variable.

3.2.b Inversion Code Design and Testing

The inversion code, called SEAIM, was designed to be a general tool for inverse modeling. Improvements from the prototype include the ability to search for the leak in a volume rather than a plane and the ability to accommodate future developments in the forward model. Appendix B lists the requirement specifications and general design document for the inverse model software. Programming of the code, which was completed in FORTRAN, was a significant effort. After the code was completed, it was thoroughly tested against the earlier prototype code. Once it was determined that the two codes yielded similar results given the same input parameters, a series of benchmark

studies was performed to gain further insight into the performance characteristics and abilities of the code with the forward model described in the previous section. These studies examined the ability of SEAIM to return accurate estimates of the model parameters for various settings of parameters and locations of leaks. A total of 18 separate studies were performed. They are discussed in detail in Appendix C.

To summarize the results of the benchmark study, SEAIM was able to return accurate estimates of the x_0 , y_0 , and z_0 model parameters (the location of the leak in space). The radius of the leak, r_0 , and the source concentration were strongly coupled, and exerted influence on each other. In general, SEAIM was able to return reasonable estimates (normally within a factor of three) for the leak radius and the source concentration. The diffusivity of the soil, D , was usually estimated within an acceptable range. Note that this parameter may be measured at a site, so it may be possible to fix D within the inversion.

In an effort to understand the inversion code's sensitivity to model parameters, a parametric study was conducted. For each parameter studied, it was allowed to vary while all the other model parameters were set at their true values. The shape of each of these plots is particularly important. In order for the inversion algorithm to be able to accurately find the desired value of the model parameter, there must be a well-defined minimum or trough in the vicinity of the answer. The resulting plots are shown in Figures 10 through 16.

As can be seen, for x_0 , y_0 , and z_0 in particular, there is a very pronounced minima at the location of the true value for the model parameters. Note that for y_0 , the double minima are present due to the search range specified and the fact that the simulated monitoring point array was planar in nature. This resulted in two identical answers, one on either side of the monitoring array. This result demonstrates the necessity to either avoid planar monitoring point configurations or define the search range to avoid the incorrect minima (i.e., define the search range to be toward the barrier from the monitoring point location). Because the search range over these parameters are typically bounded to within several meters of the actual leak location, the inversion algorithm has a very defined minima on which to converge. Model parameters r_0 and D likewise have very well defined minima at the location of the true values. The source concentration, c_0 , however, has very broad minima. The implications here are that there are many values of c_0 in the vicinity of the true value that may be chosen by the inverse algorithm. And finally, the start-time model parameter, t_0 , also has a very broad minima, which accounts for the inability of the inverse algorithm to determine an accurate value for t_0 .

While the design of the code allowed solution for seven parameters (x_0 , y_0 , z_0 , r_0 , D , c_0 , t_0), it is important to recognize that accurate solution for the leak location (x_0 , y_0 , z_0) and radius (r_0) are important and the other parameters are less significant.

There are some limitations of the inversion methodology. As mentioned previously, the accuracy of the code results is dependent on how well the chosen leakage model represents reality. This issue is discussed in detail in section 4. Numerical Modeling. Additionally, code results are very dependent on user supplied input, in particular, the search ranges. If the search range for any parameter is defined so that the inversion code is using values close to one of the boundary values, code results are

meaningless. E.g., if the search range for the x coordinate is input as $-12 \leq x \leq -8$ and the code is systematically returning values of $-8.2 \leq x \leq -8$, the overall results are probably inaccurate. There is presently no post processor with the SEAtree™ system that looks for this affect, so the user must review the system's results manually. Thus, while the real-time calculations will often be sufficient, some off-site processing will likely be needed to ensure accurate leak characterization. This is especially true when the results have significant ramifications of barrier integrity that have large cost or regulatory impact.

Appendix D lists the instructions for using the SEAIM code.

3.2.c Variations on the Forward Model

A major assumption made in the formulation of the one-dimensional spherical model, which will not be correct in a thick barrier (greater than 5 or 6 inches), is that the flux exiting the leak is not restricted by diffusion through the leak. Figure 17 graphically depicts how barrier thickness will effect the resulting tracer concentration in the medium outside the barrier. The amount of tracer that can diffuse through a leak is a function of the barrier thickness, source concentration, and the leak's dimension and flow properties. Of these parameters, the ratio of the leak area to the barrier thickness is the most important. The smaller this number is the greater the exiting flux will be restricted.

Realizing that many of the construction techniques for barriers result in barriers that are between one and three feet thick, some effort was expended under the Sandia contract to formulate a diffusion model which would account for the thickness of the barrier.

The problem was addressed in two parts: a) the leak, and b) the medium outside the barrier. A separate solution was developed for each part of the problem. Numerical modeling of the two regions was performed with a finite difference numerical simulation code, T2VOC. T2VOC is capable of modeling three-phase (gas, aqueous, NAPL), three-component (water, air, VOC), nonisothermal flow and transport through porous media (Falta, Pruess, Finsterle, and Battistelli 1995).

The Leak. T2VOC runs suggested that the hole in the barrier acts as a conduit, allowing diffusion of gas from the source concentration within the barrier, C_o , to a much lower concentration in the soil immediately outside the barrier, C_{exit} . A one-dimensional model describing this geometry can be described by the following governing equation.

$$\frac{1}{R} \frac{\partial^2 (RC)}{\partial R^2} = \frac{1}{D} \frac{\partial C}{\partial t}$$

Using the boundary and initial conditions of:

$$C = C_o \quad @ \ z = 0 \text{ and } t > 0$$

$$\begin{aligned} C &= C_{\text{exit}} & @ z = L_h \text{ and } t > 0 \\ C &= 0 & @ t = 0 \text{ and } 0 \leq z \leq L_h \end{aligned}$$

The equation can be solved to provide the following equations for concentration profiles and mass fluxes:

$$\begin{aligned} C(x, t) &= C_o + (C_{\text{exit}} - C_o) \frac{z}{L_h} - \frac{2}{L_h} \sum_{m=1}^{\infty} e^{-D\beta_m^2 t} \frac{\sin(\beta_m z)}{\beta_m} \\ q''(x, t) &= \frac{D(C_o - C_{\text{exit}})}{L_h} \left[1 + 2 \sum_{m=1}^{\infty} e^{-D\beta_m^2 t} \cos(\beta_m z) \right] \end{aligned}$$

where:

$C(x, t)$ = the concentration within the leak at a given distance from the leak entrance and time;

C_o = source concentration

C_{exit} = concentration at the exit of the leak

L_h = thickness of the barrier

$q''(x, t)$ = flux through the leak

D = diffusivity within the leak

Results from T2VOC showed that steady state conditions were reached very quickly (fractions of hours) within the leak. If only steady state conditions are of concern, the above equations can be reduced to:

$$\begin{aligned} C(x) &= C_o + (C_{\text{exit}} - C_o) \frac{z}{L_h} \\ q''(x) &= \frac{D(C_o - C_{\text{exit}})}{L_h} \end{aligned}$$

These equations were able to match results from T2VOC within $\pm 10\%$ if C_{exit} was assumed to be equal to $\frac{1}{2} C_o$. This assumption will need to be validated in the future with other parametric runs.

Medium outside the barrier: The region outside the barrier can best be described as 1-D spherical diffusion of the flux moving through the leak into a semi-infinite medium of effective diffusivity D_m . Such a process can be described by the following governing equation:

$$\frac{1}{R} \frac{\partial^2 (RC)}{\partial R^2} = \frac{1}{D} \frac{\partial C}{\partial t}$$

subjected to boundary conditions:

$$\begin{aligned} C &= 0, & @ \ t = 0 \text{ and } 0 \leq R \leq \infty \\ -D \left(\frac{\partial C}{\partial R} \right) &= q'' & @ \ R = R_h \text{ and } t > 0 \\ C &= 0 & @ \ R = \infty \text{ and } t > 0 \end{aligned}$$

Using several transformations and employing the Laplace transformation technique, the solution to this set of equations was obtained to be:

$$C(R, t) = \frac{q'' R_h^2}{DR} \left[\operatorname{erfc} \left(\frac{R}{\sqrt{4Dt}} \right) - e^{-H^2 R^2 / 4D} \operatorname{erfc} \left(H \sqrt{Dt} + \frac{R}{\sqrt{4Dt}} \right) \right]$$

This equation predicts that very close to the leak exit, the concentrations reach a steady state value very quickly. Thus in anything but highly transient phenomena, the equation can be reduced to:

$$C(R, t) = \frac{q'' R_h^2}{DR} \left[\operatorname{erfc} \left(\frac{R}{\sqrt{4Dt}} \right) \right]$$

where:

$C(R, t)$ = the concentration within the leak at a given radial distance from the leak exit and time;

q'' = steady state flux through the leak

R_h = radius of the leak

R = radial distance from the leak

D = diffusivity in the medium outside the leak

T = time

While it was outside the scope of this contract to incorporate the flux limited model into the SEAIM code, work was performed to more thoroughly validate the model.

4. NUMERICAL MODELING

The objectives of the modeling effort were to further validate the flux limited forward model and to better understand how typical field conditions differ from the ideal model(s) which are used in the inversion code. A version of the Lawrence Berkeley National Laboratory TOUGH code, T2VOC, was used to model the diffusive transport processes. T2VOC is a finite difference simulator capable of multicomponent, multiphase heat and mass transport in porous media (Falta, Pruess, Finsterle, and Battistelli 1995).

4.1 Validation of the Flux Limited Forward Model

All the problems run used the radial 2-D mesh (with minor changes) which was set-up and validated for work under the Sandia contract. Required changes included adjusting the modeled volume to reflect a realistic minimum volume for an actual barrier (roughly 1000 cubic meters). This was done by turning off nodes around the perimeter of the mesh. The mesh allowed for a small injection node in the center of the volume. A schematic of the mesh is given in Figure 18.

The baseline case had a constant source concentration of 0.304 kg/m^3 (50,000 ppm), a barrier thickness of 0.6 m (2 ft), and a leak radius of 0.152 m (6 in). The source volume was enclosed (e.g., a capped barrier was modeled). The medium (inside and outside the barrier) was homogeneous with a porosity of 30%, an effective diffusivity of $3.5\text{e-}6 \text{ m}^2/\text{s}$, a water saturation of 5% and a permeability of $9.87\text{e-}12 \text{ m}^2$. The barrier was homogenous with a very low porosity (1%) and permeability $9.87\text{e-}14 \text{ m}^2$. The leak through the barrier was cylindrical and on the center axis of the grid. All of the boundaries were no flow (zero diffusive transport).

The preliminary T2VOC calculations performed to develop / validate the flux limited diffusion model included varying the barrier thickness and leak radius within the baseline T2VOC model, and comparing the resulting concentrations with those predicted from the analytical model. Results were very promising, showing the analytical model was able to accurately predict the concentrations for distances 1m or greater from the leak if the correct exit concentration for the leak was known. For the T2VOC model initially used in the testing, this concentration could be assumed to equal one-half the source concentration. Figure 19 shows a typical comparison between the analytical and numerical model. Under this contract, the relationship between the source and exit concentration was studied further. It was determined that changing the effective diffusivity would effect the exit concentration. Over the three order of magnitude range of effective diffusivities tested, the ratio of the exit to source concentration varied from 0.7 to 0.5. Figure 20 plots the effective diffusivity versus the concentration ratio. As the effective diffusivity increases the concentration decreases. This will result in lower calculated concentrations in the medium, i.e., as the effective diffusivity increases the resistance to diffusion decreases resulting in smaller concentration gradients. The tracer gas will move further into the medium with time, but the resulting concentrations will be smaller in magnitude. A best fit of the data resulted the relationship of:

$$C_{\text{exit}}/C_0 = 0.7 - 5.714D$$

4.2 Effects of a Non-Constant Source Volume

Unlike the model assumption, the concentration of the tracer gas inside the barrier will not be constant. Injection of the gas at specific points will create concentration gradients within the barrier. If there are leaks in the barrier, the gas will begin to diffuse into the surrounding medium before an equilibrium condition is reached inside the barrier. Even if the leak does not begin until after a quasi-equilibrium condition is reached, if the mass of tracer in the barrier is small relative to the mass that diffuses out of the barrier (through leaks or into the atmosphere, if the barrier is uncapped), the source concentration will be depleted with time. As the mass of the tracer gas is a function of the pore volume and the concentration, it is possible for even a large barrier (volume wise) to have only a relatively small mass of tracer gas.

To address how a non-constant source concentration will effect the concentration profiles outside the barrier, the following problems were modeled. Results are summarized after each model description.

4.2.a Tracer Injection into a Capped Barrier with an Existing Leak

The baseline case for this model work was the same as that discussed above, with the exception that the tracer gas was injected into the source volume over a 5-hour period. Results showed an initial pulse of tracer gas diffusing through the leak creating higher concentrations in the medium than seen in the baseline case. Figure 21 shows calculated concentration histories at three distances from the leak for the baseline case. Figure 22 shows the same information for the injection case. These higher concentrations began to slowly decay within 24 hours and asymptotically approached the values seen in the baseline case within a month of the injection. The results were explained by viewing the concentration of the tracer within the barrier. The injection of the gas into a point source created spherical diffusion from the injection point out into the source volume. When the concentration front reached the barrier it could not continue to expand in that direction except through the leak. The concentration at the barrier wall (the leak entrance) increased very rapidly, causing a pulse of tracer to diffuse through the leak. As the tracer began to equilibrate within the barrier, the concentration at the leak entrance began to diminish, causing less tracer to diffuse through the leak and the subsequent decay in the tracer concentration in the medium. The tracer within the barrier required almost 5 days to equilibrate. The magnitude of the increased concentration in the medium was a function of how close the injection port was to the leak, and how quickly the concentration in the source volume equilibrated. As the distance from an injection port to a leak is unknown, the solution to the problem lies in forcing the source concentration to rapidly equilibrate. A model simulating multiple injection ports throughout the barrier resulted in medium concentration profiles within 10-15% of the baseline case within one week of injection (Figure 23).

To determine how an initial pulse of tracer diffuses through a breach into the surrounding medium would effect SEAtTM results, results from the baseline and the two injection cases were inverted. The calculated position of the leak was very close to the actual position in all three cases. The calculated leak radius (in the case where a single injection mode was modeled) was larger than either the actual leak radius or the leak radius calculated in the other cases. This was expected due to the much higher concentrations seen in the medium in the single injection case.

4.2.b Tracer Injection into an Un-capped Barrier with an Existing Leak

This simulation used the baseline case with the exception of having one surface of the source volume be a zero concentration rather than a no-flow boundary emulating exposure to surface air. Results showed that the source concentration rapidly diminished, causing the measured concentrations in the medium to be significantly less than in the baseline case. The model was then executed with tracer gas continuously injected in the source volume. While the concentration could be maintained in this manner, the amount of gas that required to be injected makes this approach expensive. Consequently, capping the barrier with a temporary, inexpensive plastic sheet has been used to conserve tracer gas.

4.3 Advective Movement of the Tracer Gas

For the medium outside the barrier, conditions will likely be different than the model assumptions. Most geologic formations are not homogeneous, and in addition to molecular diffusion, there are several advective forces that can influence the movement of the tracer gas. These advective forces include density, pressure and temperature. Depending on the molecular weight and concentration of the tracer, gravity will influence the isopleths

The tracer gas of choice (sulfur hexafluoride), has a molecular weight of 146 gm/gm mole. At the concentrations anticipated to be measured at the monitoring ports (several hundred to several thousand ppm), it was thought that transport of the gas due to gravity could possibly be on the same order of magnitude as that of molecular diffusion. Because the gravitational force is directional, elliptical rather than spherical isopleths would develop. This would result in the code predicting the leak location to be lower than it actually is. It should be noted that gravity will also effect the distribution of the tracer gas inside the barrier. Because the source concentration (10,000 to 50,000 ppm) is much higher than the anticipated concentrations at monitoring ports, the effect will be much more pronounced inside the barrier. However, because the inversion code treats the source concentration as an unknown, the density induced gradient within the barrier is of little consequence to the SEAtTM system (the gradient will not cause the source concentration to be non-constant). A conservative estimate at how gravity will effect the measured concentrations can be viewed by turning the two-dimensional cylindrical mesh on edge and adding gravity along the axis of the leak. This was done using the baseline model. Results are shown in Figure 24. The overall magnitude of the measured concentration in the medium is larger than for the baseline case. This was found to be

predominantly the result of the concentration gradient established within the source volume, not gravity. The true influence of gravity was determined by comparing the resulting concentrations in two cells the same radial distance from the leak (one cell on the leak axis, the other near the surface of the barrier). The difference in the measured concentrations in these cells indicates how non-spherical the resulting isopleths were due to gravity. It was found that there was only a small difference (less than 15%), as shown in Figure 25. As such, it was determined that given the anticipated concentrations in the medium, gravity will not significantly influence the results of the system.

Temperature and pressure gradients in the medium will also contribute to the transport of the tracer gas. These gradients are dependent on the depth of the barrier below ground surface and changing atmospheric conditions. For barriers near the ground surface (10m or less), these transport mechanisms may be important. Initial calculations have shown that temperature gradients are cyclical on a yearly period, and have a significant time lag with depth below ground surface. If temperature changes to the soil and the gases' properties are ignored, the advective motion of the tracer due to the gradient is small compared to molecular diffusion and gravity. Pressure gradients may be important if the heterogeneity of the medium is such that the barometric pumping of the soil gas results in something other than a cyclical motion of the tracer. It is also possible that the geometry of the barrier could cause preferential movement of the tracer during the inhalation / exhalation cycles of air into the medium. The effects of barometric pumping were not evaluated.

4.4 Heterogeneous Soil Properties

Molecular diffusion is sensitive to heterogeneities of the medium. Layers of very low porosity (regions of high saturation, clay layers, etc.), regions in which pore spaces are not well connected, and areas where fracture flow is dominant can all impact the system results. Layers having different effective diffusivities will alter the shape of the isopleths in the medium. The greater the deviation from spherical isopleths, the less accurately the forward models used with the SEAttrace™ system will represent the data. It is important to note that the results of the system will only be effected by a layered medium if the ports used to calculate the properties of a breach are in different layers. Since SEAttrace™ solves for leak characteristics locally (using a search area of 2 to 3 m in radius), this will not typically be the case.

Heterogeneous effects were modeled using a three-dimensional rectangular mesh. The model nodalization was based on a realistic but conservative layered medium (see Figure 26a and 26b). Three cases were modeled. One is a baseline case with homogeneous soil gas diffusivity, adjusted for porosity and tortuosity, of $4.64\text{e-}6 \text{ m}^2/\text{s}$ (the diffusivity of SF_6 in free air is $7.03\text{e-}6 \text{ m}^2/\text{s}$). The barrier is modeled as a 1m thick slant wall with a very low diffusivity ($4.64\text{e-}9 \text{ m}^2/\text{s}$), extending up to the surface. An impermeable sheet to conserve tracer covers the top of the barrier. The initial concentration inside the barrier is 100,000 ppm SF_6 in soil air, and the leak is equivalent to a 9 cm diameter hole in the barrier. The resulting concentration contours at 1, 7 and 30 days are shown in Figure 27 through 29. Note the stair-stepped shape of the

concentration profiles near the barrier, an artifact of the nodalization. Gravity is active in this simulation, drawing the isopleths downward slightly.

The second simulation considered a layered system, with a horizontal layer of soil of 1/5 the diffusivity of the baseline value extending downward from just below the leak (soil above the leak same as the baseline case). This contrast in diffusivity could be due to granular material of finer pore size or higher moisture content. Contours are plotted in Figures 30 through 32. Note that the isopleths are not significantly distorted at the interface of the two soil types.

A third simulation was conducted with an inclusion near the leak representing a 1 m³ rock of diffusivity equal to the barrier wall material. The concentration distributions shown in Figures 33 through 35 show the effects of this perturbation.

The SEAIM code analyzed the output of the T2VOC simulations to determine the impact of the modeled heterogeneity on the code's ability to characterize the leaks. These results are summarized in Table 1. The simulations ranged in locating accuracy from 0.4 to 1.0 m, and estimated the leak sizes to be 20.3 to 34.5 cm diameters (with actual sizes ranging from 1.1 to 10.16 cm). Given the sampling port locations indicated in Figure 26, the SEAIM code actually solved more accurately for the layered case than the homogeneous case. This is suspected due to gravitational effects, which would be most pronounced in the homogeneous case and less in the layered case (where the low diffusivity layer below the leak would restrict downward transport). The soil permeability was modeled as 1 Darcy (1e-12 m²).

5. FIELD TEST

5.1 Test Objectives

The key issues in determining the success of any subsurface containment system include how accurately the system can determine leak location and size, how small a leak can be detected, how quickly a leak can be detected, and how cost effective the system is.

The first two parameters, determining leak location and size, are dependent on the forward model used with the system and the accuracy of the input data for the system. Presently, as discussed previously, the code is limited to a one-dimensional spherical diffusion model.

While this diffusion model is simplistic, determining the location of the leak has been found to be insensitive to the majority of the assumptions made in developing the inversion model. As long as the isopleths are spherical (e.g. gravity is not a significant factor in the tracer movement and the medium diffusivity is homogenous), and the location of the monitoring ports are well known, SEAttrace™ can accurately predict the location of a leak with the forward model. Predicting the size of the leak is more difficult. To accurately calculate the leak size, not only must the isopleths be spherical, but also must all of the other assumptions used in deriving the forward model be true.

The remaining parameters (how quickly a leak can be detected, how small a leak can be detected, and the cost effectiveness of the system), are all dependent on how rapidly the tracer gas moves into the surrounding medium, how close the monitoring ports are spaced, and the lower detection limit and accuracy of the gas analyzer.

All of these issues are complex, and could not be adequately addressed in the scope of the test. Rather the test objectives were defined such that specific factors could be isolated and studied. These objectives included:

- determining how the barrier thickness and the leak radius effect the exit flux
- determining how the leak geometry effects the isopleths
- testing how well SEAttrace™ can define multiple leaks on the barrier and how the location of the leaks effects the systems results
- determining if SEAttrace™ can accurately locate a leak given an existing background concentration of the tracer in the medium
- testing how different tracer gases effect the systems results

5.2 Test Design

For the field test to meet its objectives, it needed to mimic typical site conditions as closely as possible. Because there is no one specific barrier type or material that will always be used, possible defects from any of the commonly used barriers had to be considered.

Heterogeneous backfill will result in lenses of higher conductivity material within the barrier. These lenses could be small (centimeters) due to improper mixing, or fairly

large (meters) due to slurry pockets or collapse of wall soil. The increase in hydraulic conductivity could easily be several orders of magnitude or more. A backfill material that does not meet required specifications may result in unacceptable performance of the barrier, resulting in planar contaminant flow through the barrier. The backfill may be unacceptable due to insufficient uniformity or gradation of the material, or insufficient quality of the water used in mixing the backfill. Trapped sediments at the bottom of the excavated trench, inadequate excavation of the trench or panel key, or incomplete coupling between a constructed bottom and sides of a barrier will all allow flow of contaminants beneath the wall. Flow could be limited to a small area, as with an inadequate tie of a single panel into the bottom of the barrier, or it could be extended over a significant length of the joint. Inadequate bonding between sections of backfill could result in a vertical strip of material with increased flow properties, as would inadequate placement between backfill panels. Finally, hydrofracture of the soil during grout injection could result in an incomplete formation of a panel, leaving an area of material with increased flow properties.

Degradation of the barrier after completion may result from freeze/thaw cycles, wet/dry cycles, desiccation of the backfill, and chemical incompatibility between the barrier material and the contaminant it is designed to contain. This degradation would result in planar leakage through the barrier.

For the field test, it was assumed that three types of leaks needed to be evaluated: windows (areas small relative to the overall size of the barrier); cracks (defects much larger in one direction than the other); and planes (areas large relative to the overall size of the barrier). It was further assumed that all the defects would have significantly increased flow characteristics (characteristics similar to the surrounding native soil) compared to the rest of the barrier.

The test volume consisted of a small-scale barrier with monitoring points both internal and external to the barrier. The shape and the dimensions of the barrier were chosen to be realistic, easily constructed, and capable of allowing multiple leaks to be tested during the same test sequence. A V-shaped trench roughly 5 meters deep and 15 meters long was chosen (Figure 36). The sidewalls and ends of the trench were sloped 45° from horizontal - a slope shallow enough to minimize construction hazards but steep enough that it would be economically viable to use at a real site (the sidewalls meet at a reasonable depth below ground surface). A vertical wall was formed at one end of the trench after the trench had been excavated. This allowed the SEAttrace™ system to be tested in one of the most typical barrier configurations (a vertical cut-off wall). It also allowed the system to be field tested in a medium that was homogenous (the backfill material between the constructed vertical wall and the excavated sloped wall was well graded).

The size of the barrier has very little influences in the effectiveness of the SEAttrace™ system. However, there were some practical issues that had to be addressed. As the surface area of a containment system increases, more monitoring/injection ports are required. The current monitoring system is capable of consecutively measuring a total of 64 ports. This number of ports easily provided adequate coverage for the chosen design. Additionally, the depth of the deepest monitoring port will typically be slightly greater

than the length of the barrier wall. Monitoring ports will often be emplaced with push techniques, whose accuracy in location decreases with distance. SEAtaceTM results are dependent on knowing the exact location of the monitoring ports. Given the geometry of the field test barrier, the maximum depth of any port was less than 25 feet — easily accomplished in most soils with direct push technologies. To minimize the costs associated with port emplacement and assure accuracy of the port locations for the test, ports were placed through the trench walls after the trench had been excavated and before it was backfilled.

Leak locations and dimensions on the barrier panels were chosen based on results of one-dimensional simulations. Appendix E discusses the calculations. Ports were spaced on 2 meter intervals on a plane parallel to and 0.75 meters from the barrier panels. Rows of ports were offset 0.4 meters (1' 3 3/4") from one another. This spacing allowed for a reasonable spacing between ports if they had been installed from the surface, as well as minimized the distance a leak could be from any point on the barrier to its closest monitoring port.

The leak locations which were originally chosen are superimposed over the port locations in Figure 37 (the schematic shows the panels from a line of site perpendicular to the panels, as opposed to a typical cross-sectional view). Table 2 lists the leak radius and corresponding wall thickness along with other pertinent information of each defect. The port locations chosen allowed for a great deal of flexibility to accommodate actual field conditions. It is important to note that the design of the test allowed for each leak to be closed. Thus, not all leaks were used with each test sequence. During the initial tests on the barrier, several non-engineered flaws were discovered near the bottom of the barrier. During subsequent repair of the barrier several of the valve assemblies were destroyed. Additionally, during the repair of the barrier two new engineered leak were added to the barrier. A description of this leak and its location is given in Table 2.

Leaks were chosen to cover a wide variety of geometries, with the baseline leak defined as a 5.1 cm (2 in.) radius leak 0.6 m (2 feet) thick. The effect of barrier thickness was to be tested by comparing the baseline leak with leaks of the same diameter but different lengths (0 and 1.2 meters, 0 and 4 feet respectively). The effect of leak radius was to be tested by comparing the baseline leak (81 sq. cm.) with leaks larger (180 and 1100 sq. cm.) and smaller (5 and 45 sq. cm.). Finally, the effect on leak location was to be tested by comparing results from baseline leaks located in the center of a barrier wall and on a joint of the barrier.

5.3 Construction

The geometry and dimensions of the excavated trench are depicted in Figure 36. Figure 38 shows a cross sectional view of the completed experimental set-up. The trench was excavated using a trackhoe. Inspection of the trench afterward revealed three distinct geologic layers. The upper layer (approximately one third of the total depth) was an alluvial deposit; the middle layer (approximately one third of the total depth) a clay layer, and the bottom third was a dense but highly fractured shale. After excavation a vertical cut-off wall was constructed at one end of the trench. The wall was framed in place. Its

main purpose was to support the membrane during backfill, although it also afforded an opportunity to test leaks on a vertical wall section.

As soon as the trench was completed, holes for the exterior monitoring ports were emplaced perpendicular to the walls using a K-V Associates hand held penetrometer on the east, west and south panels of the barrier. Holes were roughly 1" in diameter and 2' deep. Three-quarter-inch PVC pipe was used to keep the holes open until the points were surveyed and the ports emplaced. Ports were connected to the monitoring system via 1/8 inch o.d., 1/16 inch i.d. polyethylene tubing. The annulus around the ports/tubing was backfilled with a bentonite/sand mixture. The mixture was chosen such that the holes would not be a leak path for the tracer gas. Tubing was routed up the trench walls to a 4" diameter PVC pipe that extended around the perimeter of the trench. The pipe protected the tubing from ultraviolet light.

As soon as the ports were installed, the trench was sprayed with a 3-4" layer of gunnite concrete (Figure 39). The gunnite stabilized the trench walls, held the flanges for the valves (part of the engineered leaks) in place, and provided a smooth surface for the membrane to lay against. The trench was then lined with a 30-mil high-density polyethylene geomembrane, which formed an impermeable boundary to the tracer gas. After the liner was in place, the valves were attached to the flanges (Figure 40 depicts a typical valve assembly, Figure 41 shows an installed assembly) and the barrier was backfilled. A well graded sand/soil mixture (crusher fines) was used to backfill the entire volume behind the framed vertical wall and from the bottom of the barrier to above the valve assemblies of the barrier interior, Figure 42. Native material was used to finish backfilling the trench. While the trench and the area behind the vertical (north) wall was being backfilled, a PVC pipe manifold was installed to allow easy removal of the tracer gas from the barrier interior, interior monitoring ports were added near each valve and exterior monitoring ports were added on the north panel. After the backfill was completed, the trench area was covered with a surface seal (plastic sheeting) to prevent excessive loss of the tracer to the atmosphere and water infiltration. Sandbags were used to hold the surface seal in place. Finally, two injection ports were installed in the center of the barrier to a depth of 10 ft bgs. Figure 43 is a photo of the completed test facility.

During the initial tests on the barrier, several non-engineered flaws were discovered near the bottom of the barrier. The fill material in both the barrier interior and in the area behind the vertical (north) wall was removed. To minimize damage to the barrier, only the upper portion of the soil was removed with a trackhoe. The remainder was removed with a suction truck. Inspection of the liner showed areas at the north and south ends of the bottom of the barrier where the seams of the liner were not closed. Repair of the liner was not possible and it was removed. Environmental Liners, a company based on making and installing landfill liners, was hired to install a new geomembrane. The geomembrane chosen was a 30 mil plasticized polyvinylchloride (PVC). It was much more flexible than the original liner, and was installed as a single piece of material. Custom boots were used to prevent leakage between the valves and the liner. After the liner installation was complete, the barrier and was refilled with a trackhoe. The fill material was not compacted. Upon completion of the backfill, a geomembrane was used to cover the barrier. The surface seal was covered with a 2-3" layer of native material for protection. Four injection ports were installed in the interior of

the barrier to a depth of 8 ft using the K-V penetrometer. Monitoring ports for the north panel were also installed with the K-V penetrometer.

Prior to the repairs on the barrier being completed, it was discovered that rodents or rabbits had damaged much of the tubing. All of the tubing from ports on the west wall and almost half of the tubing from ports on the south wall had been severed. The protective pipe was removed and the tubes were repaired. The majority of the ports could be identified from the location of the tubes as they exited from behind the gunnite. However, there were 4 pairs of tubes that were grouped. The port associated with each of these tubes could only be narrowed down to two choices. Review of the carbon dioxide elevations measured at the ports and comparison to elevations measured prior to tubing damage was used to identify these ports.

5.4 Test Execution

Five test sequences were completed, with successful results on the last two. The first two sequences were performed in April and May of 1997. Results from these tests showed there were large non-engineered leaks in the barrier, and that the MSA gas analyzer was not capable of operating continuously. The MSA was replaced with a B&K photoacoustic analyzer and the barrier liner was replaced. The remaining three test sequences were performed in September and October of 1997. The selection of the tracer gases chosen for these tests was driven by the type of analyzer (innova model 1302 photoacoustic analyzer) used in the system). Both carbon dioxide and sulfur hexafluoride are readily sensed with the photoacoustic device. Carbon dioxide was tested because it is a very inexpensive gas, however, its presence in the subsurface was found to be in large enough quantities, and variable enough, to render it unsuitable for barrier testing. Sulfur hexafluoride was used for the balance of the testing because it is well characterized for tracer applications, easily analyzed with the photoacoustic analyzer, and relative easy to gain regulator approval to inject into the subsurface. A brief description of each test sequence is given below:

Test Sequence 1: The primary objectives of the first test sequence were to proof-test the new scanning system, test the overall integrity of the barrier, and determine the viability of using CO₂ as a tracer gas. The scanning system was moved to the site and background data was collected over a one-week period. Once the performance of the scanning system was verified, all of the engineered leaks were closed and CO₂ was injected into the barrier via a single injection port to achieve an equilibrium source concentration of 25,000 ppm. Data was continuously collected over the next several days. Analysis of the data showed no significant increase in the measured concentration of CO₂ in the surrounding medium during this time. The smallest diameter valve on each panel was opened. Analysis of the data collected over the next week showed no change from the original background concentration. Larger diameter valves were sequentially opened in time. Throughout the duration of the test, there was no change in the measured concentrations of CO₂ in the medium.

Test Sequence 2: The second test sequence was identical to the first sequence with the exception that SF₆ was used as the tracer gas rather than CO₂. Background data was collected over several days. Analysis of this data revealed the MSA analyzer was unable to measure the calibration gas (1000 ppm of SF₆) accurately with time. Initial speculation was that the temperature within the cool cell was increasing enough over the length of an analysis period that it altered the calibration of the analyzer. Subsequent testing and discussion with the vendor concluded that unless the analyzer was manually recalibrated immediately prior to each test sequence and that the external temperature of the analyzer was maintained to within several tenths of a degree, it would be unable to measure the tracer gas with any accuracy. As such, it was unusable with the system. To complete the test, it was decided to use the scanning system to automatically collect samples, and then to analyze them manually using a B&K photoacoustic gas analyzer. The engineered leaks were closed and SF₆ was injected into the barrier via a single injection port to achieve an equilibrium source concentration of 100,000 ppm. Data collected subsequently showed there were at least two non-engineered leaks in barrier. Both were at the bottom of the barrier, one near the south wall the other near the north wall. Concentrations of the tracer gas at the exterior monitoring ports were beyond the range of the analyzer within 15 hours of injecting the tracer. Given the magnitude of the tracer gas diffused into the medium from these non-engineered leaks coupled with the calibrated analysis range of the analyzer, any possibility of finding the engineered leaks was eliminated. Discussion with the CTM resulted in postponing further tests until the barrier could be re-excavated and repaired, and the SEAtaceTM system could be altered to use the B&K analyzer.

Test Sequence 3: After repairs were completed on the barrier and the scanning system was reconfigured to incorporate the B&K photoacoustic gas analyzer, the background concentration in the medium was measured for several weeks. This period was also used to test the scanning system, and to verify the port assignments (tubing from ports on the West and South panels of the barrier were severed by rabbits while the barrier was being repaired. While all of the tubes were repaired, there were several ports which could not be individually identified based on location of the tubing as it appeared from behind the barrier. These ports were identified using the measured carbon dioxide concentrations in the medium). In general, the scanning system worked very well, continuously recording two scans of data a day. Each scan required over eight hours to complete, which taxed the designed power load of the system. During extended periods of low solar gain, a few scans were not initiated.

Tracer gas (SF₆) was injected into the barrier September 19, 1997 (Julian day 261.5). A total of 8.2 pounds of tracer was added to the barrier. This amount of gas was calculated to provide a constant source concentration of 8-10,000 ppm within the barrier. The gas was to be injected equally between four injection ports whose locations were chosen such that each port would provide tracer to approximately one fourth of the total barrier volume. The total amount of tracer to be injected was transferred to a small gas cylinder. The amount of gas to be injected into each port was to be controlled during the injection by weight difference of the cylinder. Problems during the injection led to the

entire amount of gas being injected through the two northern most ports (ports were approximately 2 m from the north wall). As predicted in the T2VOC modeling, the tracer diffused to the nearest barrier surfaces (the north wall and the bottom of the barrier) where it increased in concentration until the gas could diffuse into the southern end of the barrier. This created a much higher than anticipated source concentration for some period of time in regions of the barrier near the injection port. Had the barrier been tight this would not have affected the experiment. However, several non-engineered leaks at the bottom of the barrier in the region where the concentration was very high resulted in a pulse of tracer diffusing from the leaks into the surrounding medium. The amount of tracer that diffused from these leaks was large enough that all of the monitoring ports saw an increase in tracer concentration. Figures 44 through 48 depict the measured concentration histories by panel. As soon as the non-engineered leaks were discovered, engineered leaks were opened on each panel in hopes that the amount of tracer diffusing through the leaks would be high enough to be seen over the gas diffusing from the bottom of the barrier. Three and one-half days after injection (Jday 265) the 3" diameter, 2' long valve on the west panel, the 4" diameter, 2' long valve on the east panel, and the 4" diameter, 2' long valve on the south panel, were opened. Gas could also diffuse through a 7/16" hole in the north wall. As early as Jday 266.5, an increase greater than would be expected just due to the non-engineered leaks at the bottom of the barrier was observed in the concentration measurements in ports near the valve on the west panel. The percentage of the concentration due to the opened valve and that due to non-engineered leaks could not be determined. While the elevated concentration at the port remained throughout the test, it never became pronounced enough to clearly define the leak. Figures 49 through 52 show the data represented as contour plots for various time slices throughout the test sequence. The contour plots were created by "unfolding" the panels of the barrier about the bottom of the barrier. They assume the ports on each panel are on a plane. To better understand how the concentrations at the ports varied due to the injection of the tracer, the background concentration initially measured in the medium was subtracted from the raw data. Figures 53 through 57 show the resulting concentration histories by panel while figures 58 through 60 show contour plots of the data for several times.

Data analysis with the inversion code was performed on the data that was adjusted for the initial background concentration. Results were found to be the same as those for test sequence 4, and will be discussed with that sequence.

Test Sequence 4: After it was determined that no additional engineered leaks would be seen from test sequence 3, those valves were closed (with the exception of the single valve on the west panel) and others opened. On Julian day 273 the 1" diameter valve was opened on the north panel, the 15" diameter, 2' long valve on the east panel was opened, and on the south panel the 4" diameter, 1' long valve was activated. Data was recorded for a week. There was no obvious increase in any ports near any of the valves during this time. (It should be noted that most of the ports near the 15" diameter, 2' long valve were severed and thus could not be measured.) As such, the analysis of this test was grouped with that from test sequence 3. Concentration histories of the raw and adjusted data are shown in figures 44 through 48 and 53 through 57. Contour plots of the

raw and adjusted data for several times during the test period are shown in figures 61 through 63.

The inversion analysis found 7 distinct leaks. Of these, the only engineered leak the code was able to discern was the 3" diameter, 2' long leak on the west panel (near port 39). However, the code predicted the leak to be much lower on the panel and further north than it actually was, 2 meters from the known valve location. This was not surprising, as the concentrations measured at the ports used to predict the leak location were a combination of the true leak and the non-engineered leak which was located below and to the north of the engineered leak. Table 3 lists the calculated average location and radius of each leak over all the test periods.

Test Sequence 5: The final test sequence was conducted using a series of pulse injections near the center of each panel. A pulse injection near the panel wall allowed for a short term, high source concentration to exist near the panel wall without significantly increasing the overall concentration in the barrier. Thus monitoring ports near the non-engineered leaks at the bottom of the barrier did not see increased tracer concentration. Prior to the injection, the existing concentrations in the medium were allowed to either equilibrate, or begin to decrease. The injections were performed October 7, 1997. Five engineered leaks were opened at the time of the injection. Monitoring ports near four of these leaks recorded an increase in the tracer concentration. Data analysis showed, and on-site inspection confirmed, that tubing to the monitoring ports near the fifth leak had been severed. Because of the combination of high existing background concentrations and non-engineered leaks on this panel (the east panel), the engineered leaks could not be seen. As with the data collected in tests 3 and 4, the recorded background concentration in the medium at the time of injection was subtracted from all data recorded throughout the test prior to the data being sent to the inversion code. Figures 64 through 67 plot the adjusted concentration histories by panel. Figures 68 through 73 show the same data represented as contour plots for various time slices. The contour plots were created by "unfolding" the panels of the barrier about the bottom of the barrier. They assume the ports on each panel are on a plane. Inversion of the data yielded a total of nine leaks, four engineered and five non-engineered. The found locations of the leaks match the contour plots fairly well, although the inversion code is capable of finding leaks which the contour plots don't see. Also, the contour plots are only a two-dimensional representation of three-dimensional data. As such, they are only as accurate as the assumptions used to create them, and can be somewhat misleading, as evidenced by the contours shown on the South panel. The calculated average location and radius of each leak over the test period is given in Table 3. The engineered leaks were typically found to within 1m or better of their true position. The 3" diameter leak on the West panel was found most accurately, within 0.3 m. It is important to note that this was the only leak far enough away from any non-engineered leaks such that none of the ports used to predict the leak location saw increased concentrations from another leak. The accuracy of the system seen for this leak will be typical given a barrier which is essentially sound, e.g., a barrier where there are few leaks, spaced relatively far apart from each other. The engineered leaks on the North panel were close enough to affect each other (e.g., to have the measured concentrations at the monitoring ports be a combination from both leaks). Additionally, there was a non-

engineered leak in close proximity to the engineered leaks. The remaining engineered leak, on the South panel, was found by the inversion code to be further down on the panel than it actually was. This was caused by a non-engineered leak (near port 11) near this leak but lower in the barrier. Figures 74 and 75 are a graphical representation of the data in three dimensions. As seen in the figures, the calculated position of each of the leaks with time was very consistent. While the accuracy of the calculated position of the non-engineered leaks is unknown, the calculated positions from tests 3 / 4 and 5 can be compared for those leaks that were found in both test sequences. For leaks away from the large non-engineered leaks at the bottom of the barrier (found in test 3 / 4 but not seen in test 5 because of the injection method), the calculated leak positions were very close (0.2 meters or closer) between the test sequences. For the non-engineered leak near the bottom of the barrier, the position calculated in tests 3 / 4 was lower down on the barrier panel. As discussed earlier, this is an artifact of the increase in tracer concentrations at the monitoring ports from other nearby leaks. As such, the position calculated from test 5 will be more accurate. Figure 76 shows the calculated leak locations between the different test sequences.

5.4 Summary of Test Results

While the field test of the scanning system was not completed under the desired, well-controlled environment, the overall results were good and the test objectives were met. SEAttrace™ was able to find multiple leaks on the barrier, even under adverse conditions including high background concentrations, spatially variable background concentrations, a heterogeneous medium and multiple unanticipated leaks. The very small engineered leak of 1.1 cm diameter was detected. The locations of the leaks that the system found were consistent with time (inversions of sequential leak data sets produced similar results). The calculated location of the engineered leaks was found to be within 0.4 to 1.2 m of the true positions. The single engineered leak that was not affected by another leak was found within 0.4 m of the true position, while leaks near adjacent leaks were found within 1.2 m. The accuracy of the SEAttrace™ system for a barrier where there are few leaks spaced relatively far apart from each other will be more closely reflected by the more accurate results. The calculated radii of the leaks were less accurate. The accuracy of the leak size determination is affected by the forward model used in the SEAIM code, the correlation between leak radius and start time of the leak as seen in the inversion code, and the injection method of the source concentration. The system characterized the leaks as ranging from 10 cm to 17.3 cm in radius, while the actual sizes ranged from 0.5 to 5.1 cm in radius.

The scanning system functioned primarily as designed, automatically collecting and reducing the data. The extensive data analysis used to remove the effects of background concentrations required analysis after the tests on a desk-top computer. The system did, however invert data automatically during the last test injection sequences. Automatic inversion required 20 to 30 minutes after all gas composition data was collected.

Several changes need to be made to make using the system less cumbersome and more reliable. Over the course of the test periods, some scans were skipped due to

inadequate power during extended periods of limited solar exposure, and transporting the system proved to be awkward and expensive. Future systems should include a backup generator to cover periods of low power, and should be trailer mounted. Finally, the system should be able to monitor concentrations of the tracer gas within the barrier, which is typically in the 10,000s (beyond the range of the calibration used to accurately measure the concentrations outside of the barrier). This could be done either by diluting the sample with atmospheric air or by reconfiguring the SEAttrace™ code so that it is able to utilize the dual range capability of the B&K analyzer.

The inversion code was thoroughly tested during the field experiment, and encountered many situations which would not be typically encountered at a site. To increase the accuracy of the results calculated in the field under very adverse conditions changes need to be incorporated into the pre- and post-processors for the code. These include:

1. real time checking of the defined search ranges used in predicting the leaks
2. the ability for each leak to have different search bounds for source concentration, radii, start time and medium diffusivity
3. the ability for the code to determine the most suitable nearest neighbors in real time
4. comparison of calculated leak characteristics with time (would aid in 1-3 above)
5. to report the average of some number of the best answers for each run rather than just the single best fit answer
6. to intelligently check for bad data (ports reading atmosphere or behaving in some other way that's not reasonable, as well as zero readings that are clearly erroneous)

Finally, the most complete verification of barriers would include multiple injection steps. The initial injection should be a low (1-5,000 ppm) constant concentration throughout the barrier interior to check for large leaks. If leaks are found from the initial injection, pulsed injections near suspect areas (based on concentration histories) or where leaks were not found could be used to find small leaks or help define multiple leaks in a given area. Pulsed injections would increase the detail of SEAttrace™ results without flooding the medium with the tracer and without significantly increasing the source concentration. If no leaks were found after the initial injection, the source concentration would gradually be increased until either the barrier is verified as being tight or until leaks are seen. This stepped injection scheme requires more labor (and therefore additional cost) but ensures a more complete verification.

6. LESSONS LEARNED

The difficulties experienced during the field test phase provided valuable experience that will be applied to subsequent barrier testing activities. Following is a summary of field techniques and processes that are critical to the operation of the system:

Knowledge of the vapor sampling port locations is critical to the accuracy of the leak location system. It is also difficult to achieve. Since diffusion from a discrete source is typically a spherical process, the concentration gradient is highly dependent upon the radial distance from the source. Positional accuracy on the order of centimeters is desired. This accuracy can be attained using borehole deviation logging tools, or emplacement systems such as cone penetrometers that incorporate tilt meters in their tips.

Protection of sample tubing from damage is crucial. At the field tests in northern New Mexico an excessive amount of rodent damage occurred which rendered many of the sample tubes unusable. Long-term damage due to ultraviolet radiation also can cause tubes to fail. Protection of the tubing inside sealed plastic pipe prevents these types of damage as well as that due to foot and vehicular traffic.

Injection of the tracer gas must occur in slow, controlled, and staged steps. Initial injection at a low concentration allows detection of relatively large flaws, if they exist, without flooding the gas analyzer. This also prevents too large of a background concentration to accumulate in the soil outside of the barrier for subsequent testing. Subsequent testing at higher tracer concentrations, achieved by pulse injections near the barrier walls, allows monitoring for successively smaller leaks.

Tracer injection ports should be spaced to avoid challenging the barrier wall with a high concentration dynamic pulse of tracer gas for the initial injection. Ports should be evenly spaced throughout the barrier interior if possible, and not located closer to the barrier wall than to each other. If the barrier is proven to be tight through several stepped injections in which the concentration of the entire volume of the barrier is increased, no additional testing needs to be done. If, however, leaks are found upon the initial injection, pulsed injections near the barrier walls that did not exhibit signs of leakage, would need to be performed.

In general, the monitoring system operated as desired. Several changes (both hardware and software) will be incorporated in the next phase to facilitate its operation:

Use of remote control software to allow remote changes to the inversion code and its control files. The current control program does allow remote access and limited changes to the operation (sampling times, etc.) but does not allow wholesale changes of the input files or the main executable. Currently available remote control software allows this, and needs to be tested on the system's control computer to ensure compatibility with the control and inversion software.

Enhancements in the inversion software will screen and flag data for blocked lines and damaged tubes. Tube damage can be detected by evaluating the CO₂ content of the soil gas. Ambient air CO₂ is typically between 400 and 500 ppm, while soil gas CO₂ is much higher (usually above 1000 ppm). Tube blockage can be detected with a more accurate sample flow measurement. Evaluating these parameters in real time, and ignoring

tubes with questionable integrity, can increase the accuracy and effectiveness of the inversion process.

Cellular access is sometimes erratic. Alternatives, such as satellite communication, should be evaluated, although their costs may be prohibitive.

7. APPLICABILITY, USAGE COSTS, AND LIMITATIONS

The SEAttrace™ methodology, and gaseous tracer testing in general, is applicable to the verification of barrier structures emplaced above the water table. It is particularly well suited to emplacements at sites where the entire barrier is located in the unsaturated zone and it is not safe or practical to test the barrier's integrity hydraulically. The technique can assess the integrity of any impermeable barrier type. Sampling array emplacements can be accomplished by either conventional drilling or direct push techniques. Vapor sampling lines can potentially be several hundred feet deep in the soil (SEA has successfully operated its sampling systems with 300 to 400 ft. of sample lines). It is unlikely that a barrier can be emplaced deeper than the SEAttrace™ system can monitor, since the constraints on accurate barrier emplacement increase with depth.

SEAttrace™ is capable of locating flaws with positional accuracy of 0.5 to 1.0 m. If the purpose of SEAttrace™ testing is to assist remediation of barrier flaws, this positional accuracy is sufficient to guide regrouting techniques to patch the holes in the barrier. The system can detect flaws from very small (centimeters in diameter) to very large.

Costs of SEAttrace™ verification activities at barrier sites of various magnitudes (characterized by the square footage of barrier wall tested) have been estimated based on SEA experiences at Dover Air Force Base and Brookhaven National Laboratory field tests. If the SEAttrace™ monitoring system is purchased and dedicated to the site (approximately \$100K), the costs shown in Table 4 are estimated. These include the total cost of installation, operation, and data analysis/reporting. Note that the unit cost, indicated as dollars per square foot of barrier wall area, is highly dependent on the scale of the barrier. Ultimately, for the "large" typical barrier of 100 ft. by 100 ft. in area, the unit costs would be about \$8.45/ft². This considers that the monitoring system is dedicated to the site and remains as a long-term monitoring system (the gas analyzer used in SEAttrace™ is capable of quantifying up to five hydrocarbons simultaneously). If the system were not needed for long-term monitoring, it could be leased for a short term, reducing the unit cost to about \$7/ft².

Gaseous tracer testing of barriers is not an instantaneous process, requiring time for the tracer to diffuse through leaks (the smaller the leak, the longer the time required to conduct the measurement). The time required to conduct a tracer based measurement is as follows:

1. One week to install vapor sampling ports
2. Three days to complete instrument checkout, collect background data, and inject the initial tracer pulse
3. Two days for tracer to distribute throughout barrier and start appearing at outside monitoring ports.
4. Four days to complete initial tracer test
5. Six additional days to ramp up internal tracer concentration and monitor for additional leaks

SEAtace™ cannot, obviously, be used to detect leaks below the water table, although the presence of flaws in barriers above the water table can be indicative of similar irregularities below the water table. Gaseous tracer testing in general is susceptible to errors due to the moisture halo that may result from moisture from the grout moving out into the soil. This residual moisture may temporarily block up the soil pores sufficiently to inhibit the diffusion of tracer gas out through the flaw. This effect should diminish as the residual moisture wicks out into the soil.

The SEAtace™ approach estimates the size and location of flaws. Classical performance specifications of barrier performance are in the form of bulk hydraulic conductivity, not the size of the flaw. Leak size can be related to this performance specification if material properties are assumed (the hydraulic conductivity of the native soil), but this is not an immediately determined relationship. Regulatory acceptance will require correlation of the leak geometry and the hydraulic conductivity performance specification.

8. CONCLUSIONS

The overall objective of the effort was to develop and demonstrate an integrated methodology and field system to evaluate the integrity of in situ, impermeable barriers constructed in the vadose zone. An autonomous, remotely accessible, automatic monitoring and analysis system was designed and fabricated. It was thoroughly tested under field conditions, and was able to function as designed throughout the test period. Data inversion software was developed with enhanced capabilities over the previous prototype version, and integrated with the monitoring system for real time operation. Analytical simulations were performed to determine the inversion code's sensitivity to model parameters. Numerical simulations were performed to better understand how typical field conditions differ from the ideal model(s) which are used (or have been developed for use) in the inversion code and to further validate the flux limited forward model developed for use with the system. Results from the analytical and numerical assessment of the inversion code showed that the SEAttraceTM approach could locate leaks within 0.4 to 1.2 m. Leak size determination was less accurate, but produced results within a factor of 3 to 8 for leaks in the 2.5 to 10 cm diameter range. The smallest engineered leak in the test, 1.1 cm diameter, could be located but its size estimate was high by a factor of 30. Data analysis was performed automatically after each gas scan was completed, yielding results in less than thirty minutes, although the bulk of the results reported required post test data analysis to remove effects of high background concentrations.

The field test of the integrated system was problematic, primarily due to unanticipated, unintentional leaks formed in the impermeable liner. The test facility constructed to proof the system was ambitious, initially having 11 engineered leaks of various dimensions that could be independently operated. While a great deal of care went into the construction of the facility to assure there would be no undesired leaks, the primary barrier to diffusion (a 30-mil high density polyethylene membrane) failed. The unanticipated leaks were large enough that tracer gas diffusing from them masked the designed leaks. The test facility was re-excavated and a new membrane installed. Initial tests of this barrier showed that it also leaked near the bottom of the barrier. However, careful control of the subsequent tracer gas injections, coupled with extensive data analysis to minimize the effects of the high background tracer gas concentrations, allowed leak characterization to be completed successfully.

The proposed Phase II demonstration for this project is a double wall, jet grouted coffer dam at the Dover Air Force Base Groundwater Remediation Field Laboratory. This barrier will be constructed of multiple thin wall panels (nominally 6" to 10" thick) installed to form a vertical right circular cylinder, approximately 30 ft. in diameter. The barrier will be keyed into a clay layer at the 45 ft. depth, forming the bottom of the barrier.

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Figure 1. Schematic of a SEAttrace™ system installation.

Figure 2. General sequence of SEAttrace™ system operational flow.

Figure 3. General monitoring system schematic.

Figure 4. Sampling and analysis system.

Computer and
gas analyzer →

Solenoid array →

Solenoid relays →

Figure 5. Control computer, gas analyzer, and solenoid valve system (prior to replacement of the NDIR analyzer with the photoacoustic analyzer).

Day time operation:
heat is absorbed in water reservoir,
no thermosyphon action

Night time operation:
heat is radiated to night sky
through thermosyphon action

Figure 6. Instrument enclosure passive thermal control system.

Figure 7. Record of internal enclosure and ambient air temperature showing the moderating effect of the passive thermal control system.

Figure 8. Monitoring system enclosure, showing the solar panels and sample tubing connection plate.

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Figure 10. Error functional versus model parameter x_0 , where all other parameters are held to their true value.

Figure 11. Error functional versus model parameter y , where all other parameters are held to their true value.

Figure 12. Error functional versus model parameter z , where all other parameters are held to their true value.

Figure 13. Error functional versus model parameter r , where all other parameters are held to their true value.

Figure 14. Error functional versus model parameter t , where all other parameters are held to their true value.

Figure 15. Error functional versus model parameter C , where all other parameters are held to their true value.

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Figure 20. Effective diffusivity versus the concentration ratio for the flux limited forward model.

Case 1

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Case 5

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Case 9

Figure 23. Calculated concentration histories at three distances from the leak for a case identical to the baseline with the exception that the injection of the tracer gas into the source volume through multiple ports is modeled.

Figure 24. Calculated concentration histories at three distances from the leak for a case identical to the baseline with the exception that gravity is modeled.

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Figure 29. Contour plot of the calculated isopleths for the baseline, homogenous case after 1 month (30 days).

Figure 30. Contour plot of the calculated isopleths for the layered, heterogeneous case after 1 day.

Figure 31. Contour plot of the calculated isopleths for the layered, heterogeneous case after 1 week.

Figure 32. Contour plot of the calculated isopleths for the layered, heterogeneous case after 1 month (30 days).

Figure 33. Contour plot of the calculated isopleths for the the boulder simulated within an otherwise homogenous medium case after 1 day.

Figure 34. Contour plot of the calculated isopleths for the the boulder simulated within an otherwise homogenous medium case after 1 week.

Figure 35. Contour plot of the calculated isopleths for the boulder simulated within and otherwise homogeneous medium case after 1 month (30 days).

Figure 36. Schematic of the constructed test facility.

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Figure 40. Typical assembly of an engineered leak used at the test facility.

Figure 41. Installation of an engineered leak installation (18 inch diameter valve simulating a 2 ft. thick barrier wall).

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Figure 45. Measured concentration histories for ports on the west panel of the field test barrier for test sequences 3, 4 and 5.

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Figure 50: Contour plot of the raw concentration data measured on Julian day 266.5, during test sequence 3. The maximum concentration contour is 10,000 ppm, near port 63. Note that information from the south, east and west panels was combined in creating the contours for these panels. Ports for the north panel were not referenced to the same datum as the other panels, thus contours for this panel are created using only the ports on the panel.

Figure 51: Contour plot of the raw concentration data measured on Julian day 269.0, during test sequence 3. The maximum concentration contour is 6,000 ppm, near port 63. Note that information from the south, east and west panels was combined in creating the contours for these panels. Ports for the north panel were not referenced to the same datum as the other panels, thus contours for this panel are created using only the ports on the panel.

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Figure 56: Concentration histories for ports on the north panel of the field test barrier for test sequences 3 and 4 after the background concentrations has been removed.

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Figure 58: Contour plot of the adjusted concentration data recorded on Julian day 266.5, during test sequence 3. The maximum concentration contour is 10,000 ppm, near port 63. Note that information from the south, east and west panels was combined in creating the contours for these panels. Ports for the north panel were not referenced to the same datum as the other panels, thus contours for this panel are created using only the ports on the panel.

Figure 59: Contour plot of the adjusted concentration data recorded on Julian day 269.0, during test sequence 3. The maximum concentration contour is 6,000 ppm, near port 63. Note that information from the south, east and west panels was combined in creating the contours for these panels. Ports for the north panel were not referenced to the same datum as the other panels, thus contours for this panel are created using only the ports on the panel.

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Figure 63: Contour plot of the adjusted concentration data recorded on Julian day 279.0, the end of test sequence 4 and immediately prior to the injection of the tracer gas for test sequence 5. The maximum concentration contour is 1,000 ppm, near ports 63, 41 and 4. Note that information from the south, east and west panels was combined in creating the contours for these panels. Ports for the north panel were not referenced to the same datum as the other panels, thus contours for this panel are created using only the ports on the panel.

Figure 64: Concentration histories for ports on the west panel of the field test barrier for test sequence 5 after the background concentrations have been removed.

Figure 65: Concentration histories for ports on the south panel of the field test barrier for test sequence 5 after the background concentrations have been removed.

Figure 66: Concentration histories for ports on the east panel of the field test barrier for test sequence 5 after the background concentrations have been removed.

Figure 67: Concentration histories for ports on the north panel of the field test barrier for test sequence 5 after the background concentrations have been removed.

Figure 68: Contour plot of the raw concentration data measured on Julian day 280.5, during test sequence 5. The maximum concentration contour is 1250 ppm, near port 63. Note that information from the south, east and west panels was combined in creating the contours for these panels. Ports for the north panel were not referenced to the same datum as the other panels, thus contours for this panel are created using only the ports on the panel.

Figure 69: Contour plot of the raw concentration data measured on Julian day 281.5, during test sequence 5. The maximum concentration contour is 1000 ppm. Note that information from the south, east and west panels was combined in creating the contours for these panels. Ports for the north panel were not referenced to the same datum as the other panels, thus contours for this panel are created using only the ports on the panel.

Figure 70: Contour plot of the raw concentration data measured on Julian day 283.0, during test sequence 5. The maximum concentration contour is 1500 ppm, near port 2. Note that information from the south, east and west panels was combined in creating the contours for these panels. Ports for the north panel were not referenced to the same datum as the other panels, thus contours for this panel are created using only the ports on the panel.

Figure 71: Contour plot of the adjusted concentration data recorded on Julian day 280.5, during test sequence 5. Contours show 4 clearly defined, individual leaks. Note that information from the south, east and west panels was combined in creating the contours for these panels. Ports for the north panel were not referenced to the same datum as the other panels, thus contours for this panel are created using only the ports on the panel.

Figure 72: Contour plot of the adjusted concentration data recorded on Julian day 281.5, during test sequence 5. Contours show multiple individual leaks. Measured concentrations at the ports on the north panel are clearly a function of multiple leaks in close proximity. Note that information from the south, east and west panels was combined in creating the contours for these panels. Ports for the north panel were not referenced to the same datum as the other panels, thus contours for this panel are created using only the ports on the panel.

Figure 73: Contour plot of the adjusted concentration data recorded on Julian day 283.0, during test sequence 5. Note that information from the south, east and west panels was combined in creating the contours for these panels. Ports for the north panel were not referenced to the same datum as the other panels, thus contours for this panel are created using only the ports on the panel.

Figure 74. Results of the various leak positions as determined by the SEAIM code with time for test sequence 5, for the south, west and east panels of the barrier.

Figure 75. Results of the various leak positions as determined by the SEAIM code with time for test sequence 5, for the north panel of the barrier.

Figure 76. Comparison of the leak locations predicted by the SEAIM inversion code for tests 3, 4 and 5.

Figure 77. Potential barrier installations and monitoring configurations.

Table 1. Calculated characteristics of a leak by the inversion code SEAIM using concentration histories predicted with T2VOC given a homogeneous medium, a medium having two geologic layers, and a medium with a large rock near the leak.

	position			radius (m)	start time (sec)	concentration (ppm)	diffusivity (mg/m ³)	Dist from leak (m)
	X (m)	Y (m)	Z (m)					
Time = 24 hours (1 day)								
homogeneous run	28.85	20.93	-2.31	5.18E-02	1.7E+04	8.7E+04	4.5E-06	1.0
layered run	28.06	20.93	-2.44	2.95E-03	2.5E+04	5.2E+04	9.5E-06	0.6
rock run	28.37	21.04	-2.78	8.18E-03	1.6E+04	9.6E+04	6.1E-06	0.3
Time = 168 hours (7 days)								
homogeneous run	27.30	21.05	-3.63	1.51E-03	1.4E+04	4.7E+04	6.9E-06	1.0
layered run	27.98	21.07	-2.71	3.48E-03	6.1E+03	5.2E+04	4.7E-06	0.4
rock run	27.39	21.00	-3.50	2.36E-03	1.5E+04	3.5E+04	3.8E-06	0.9
Time = 720 hours (30 days)								
homogeneous run	27.74	20.97	-3.23	3.28E-03	2.3E+04	7.4E+04	1.8E-05	0.5
layered run	27.43	21.09	-3.40	4.80E-03	2.5E+04	6.5E+04	3.3E-06	0.8
rock run	27.48	21.07	-3.49	3.65E-03	9.4E+03	5.1E+04	4.2E-06	0.8

Table 2. Properties of the engineered leaks installed in the field test mock barrier.

Leak no.	Panel	Location depth, relative to panel	width, relative to panel	Leak shape	Available for test sequences:	Leak radius		Leak diameter		Leak area		Barrier thickness	
						(in)	(cm)	(in)	(cm)	(sq. in.)	(sq. cm.)	(ft)	(m)
1	east	center	closest to north panel	cylinder	1-5	7.5	19.1	15	38.2	176.7	1140.1	2	0.6
2	east	center	center	cylinder	1-5	2	5.1	4	10.2	12.6	81.1	2	0.6
3	east	center	closest to south panel	cylinder	1-5	2	5.1	4	10.2	12.6	81.1	4	1.2
4	south	center	center	circle	1-5	2	5.1	4	10.2	12.6	81.1	0	0
5	south	center	center	cylinder	1-2	2	5.1	4	10.2	12.6	81.1	2	0.6
6	south	center	center	cylinder	1-5	2	5.1	4	10.2	12.6	81.1	2	0.6
7	west	center	center	cylinder	1-2	3	7.6	6	15.2	28.3	182.4	2	0.6
8	west	closer to south panel	center	cylinder	1-5	1.5	3.8	3	7.6	7.1	45.6	2	0.6
9	north	center, horizontal	center	rectangular box	1-2	0.5(a)	1.3(a)	25.0(b)	63.5(b)	12.5	80.6	2	0.6
10	north	near bottom	corner of north and west panels	cylinder	1-2	2	5.1	4	10.2	12.6	81.1	2	0.6
11	north	center	center	cylinder	1-2	0.5	1.3	1	2.6	0.8	5.1	0	0
12	north	center	closest to west panel	circle	3-5	0.21875	0.555625	0.4375	1.2	0.15033	0.96987	0	0
13	north	center	closest to east panel	circle	3-5	0.5	1.27	1	2.6	0.785398	5.067075	0	0

Table 3. Results of the mock barrier field tests.

		TRUE POSITION OF VALVES					TEST 3/4					TEST 5						
		x (m)	y (m)	z (m)	r (m)	r (in)	x (m)	y (m)	z (m)	r (m)	r (in)	Dist from true position of leak (m)	x (m)	y (m)	z (m)	r (m)	r (in)	Dist from true position of leak (m)
Non-engineered; east panel	Closest Port	2					10.7	3.3	-3.4	0.3	12.8		10.7	3.2	-3.5	0.1	5.1	
	std dev						0.9	0.6	0.6	0.4	16.5		0.7	0.6	0.6	0.1	5.4	
Non-engineered; east panel	4						9.6	3.9	-4.7	0.5	19.3							
	std dev						0.9	0.5	0.2	0.6	24.4							
Non-engineered; sw corner of bottom	11						4.3	4.4	-3.8	0.2	9.8		4.1	5.1	-3.0	0.4	14.5	
	std dev						0.3	0.5	0.5	0.4	14.2		0.6	0.2	0.7	0.3	13.1	
4" diameter, 1' long leak; south panel	18	3.3	5.0	-2.4	0.1	2.0							2.9	5.3	-3.4	0.2	6.7	1.2
	std dev												0.3	0.3	0.6	0.2	6.0	
Non-engineered; south panel near surface	23						0.3	9.6	-1.2	0.3	10.7		0.2	9.4	-1.1	0.2	6.8	
	std dev						0.6	0.7	0.8	0.3	13.5		0.5	0.6	0.6	0.2	7.9	
3" diameter, 2' long leak; west panel	39	8.3	7.7	-2.6	0.0	1.5	9.4	6.4	-3.7	0.4	15.2	2.0	8.4	7.8	-2.9	0.1	5.0	0.4
	std dev						0.1	0.2	0.5	0.4	14.9		0.1	0.5	0.5	0.2	6.7	
Non-engineered leak; bottom	41						9.8	4.9	-4.2	0.2	8.4							
	std dev						0.2	0.3	0.1	0.2	6.9							
Non-engineered leak	42												13.2	8.6	-2.1	0.1	3.8	
	std dev												0.4	0.6	0.6	0.1	5.4	
1" diameter, 6" long leak; north panel	47	6.8	0.2	-2.2	0.0	0.5							7.1	0.1	-1.7	0.1	4.1	0.6
	std dev												0.1	0.3	0.1	0.1	5.1	
Non-engineered leak; north panel	48												7.1	0.6	-3.1	0.1	5.4	
	std dev												0.1	0.3	0.1	0.2	6.0	
7/16" diameter, 0' long leak; north panel	53	4.5	0.2	-2.4	0.0	0.2							5.5	0.6	-2.5	0.2	6.8	1.0
	std dev												0.3	0.4	0.2	0.2	7.8	
Non-engineered leak; bottom	63						8.5	4.6	-4.4	0.1	5.5							
	std dev						0.1	0.1	0.2	0.2	6.6							

Table 4. Estimated usage costs of SEAttrace system.

Scale of Barrier:	Small (10 X 20 Ft.)	Medium (30 X 60 Ft.)	Large (100 X 100 Ft.)
Approximate Barrier Wall Sq. Footage	840 Ft.²	7,500 Ft.²	42,000 Ft.²
Vapor Point Installation Cost	\$16 K	\$22 K	\$60 K
Mobilization, Travel, Tubing Hookup, & Monitor System Checkout	\$15 K	\$20 K	\$25 K
Monitoring System	\$100 K	\$100 K	\$120 K
Tracer Gas	\$8 K	\$12 K	\$20 K
Design, Tech. Support, & Data Reduction	\$40 K	\$50 K	\$130 K
Total	\$179 K	\$182 K	\$355 K
Unit Cost Per Barrier Wall Area	\$213/Ft.²	\$24.30/Ft.²	\$8.45/Ft.²

APPENDIX A THE INVERSION METHODOLOGY

Inverse modeling is used to reverse calculate flow and transport processes in an effort to understand unknown properties and flow conditions. This can be accomplished with numerical or analytical techniques, depending upon the complexity of the process and the detail required in the final result.

For this application a numerical method was chosen which would allow near real time assessment of recorded gas data. Consequently, the solution method chosen is readily programmed for use on a portable personal computer, which also performs the role of controlling data acquisition, archiving data, and reporting/transmitting the results.

The estimation of the size and location of a leak from measured concentration histories is an inverse problem of multiphase flow in porous media. From measured tracer concentrations C_{ik} taken at locations, $\underline{x}_i = (x_i, y_i, z_i)$ and times t_{ik} one seeks estimates for a set of parameters $\underline{p}$ that characterize the leak.

The inverse problem requires a leakage model

$$c(\underline{p}; \underline{x}, t)$$

that solves the forward problem; that is, it maps each point $\underline{p}$ from a multiparameter space into a set of predicted concentration histories. For example, an idealized leakage model for a vertical barrier surface described by $y = a + bx$ is

$$c(\underline{p}; \underline{x}, t) = \frac{r_0}{r} c_0 \operatorname{erfc} \left(\sqrt{\frac{(r - r_0)^2}{4D(t - t_0)}} \right), \quad r > r_0, \quad t > t_0$$

where

$$\begin{aligned} r^2 &= (x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2, \\ y_0 &= a + bx_0, \end{aligned}$$

(x_0, y_0, z_0) is the location of the leak, t_0 is the time that the leak began, r_0 is the constant radius of the leak after time t_0 , c_0 is the uniform tracer concentration within the hemisphere of radius r_0 after time t_0 , D is the uniform diffusivity of the medium, and $\operatorname{erfc}(\bullet)$ is the complement of the error function. In the idealized case at least the first four parameters are unknown. In a realistic application the model may be more complex, perhaps a finite element model, and there may be many unknown parameters.

The inverse problem can be cast in the form of a nonlinear global optimization problem. The objective function to be minimized may be taken as the sum of the squares of the differences between predicted and measured tracer concentrations:

$$E(\underline{p}) = \sum_{i,k} [c(\underline{p}; \underline{x}_i, t_{ik}) - C_{ik}]^2$$

The problem is made difficult by the fact that there may be more than one set of parameter values for which E achieves the minimum.

No algorithm can solve a general, smooth global optimization problem in finite time. This fact has led to the use of stochastic methods, some of which are called Simulated Annealing (SA). An SA method has solved an inverse porous flow problem to obtain relative permeability and capillary pressure as a function of water saturation (Owens 1992). SEA has developed an SA method for estimating subsurface barrier leak size and location. This work is discussed below.

The simplest stochastic method for global optimization is to repeatedly select points in the parameter space at random, using a uniform probability distribution. The objective function is evaluated at each point; the minimum value and the point with the minimum value are remembered, all other information is discarded. Even with a large sample of points, the Pure Random Search method may not find the global minimum, but it probably will come close. As the sample increases, the probability of success converges to 1.

SA methods are similar to Pure Random Search. Points are selected at random and the best point is remembered. The difference is that an SA method does not use a uniform distribution to select points in the parameter space. Instead, the probability distribution depends in a complex way on the objective function of previous points.

In an SA method the probability distribution for the next point is centered around a particular point in parameter space, which we call the base point, by analogy to a base camp. As we shall see, the base point need not be the best point found so far. One way in which various SA methods differ from each other is in the exact form of the probability distribution.

The rule for determining the base point is responsible for the name "Simulated Annealing." If the objective function is smaller at the next point than it was at the base point, then the base point is moved to the new point. If the objective function is larger, we take a chance on moving the base point; we "roll the dice." If the objective function is much larger at the next point, the probability of moving the base point is less, because that probability is given by the following expression:

$$e^{-\Delta E/T}$$

This is analogous to the physical annealing process, where ΔE is the difference in energy states and T is proportional to the temperature. When T is relatively large, there is a good possibility that the base point will climb out of a local minimum to look for other minima. If T is small, the base point is more likely to avoid "uphill" steps. In an SA method, the temperature is reduced as the process proceeds, just as in physical annealing.

SA methods not only differ in the form of the probability distribution used to select the new point, they also differ in the cooling schedule.

To select the next set of parameter values to be tested, each parameter is selected independently, using a probability distribution proportional to

$$e^{-W|p_j - q_j|/(M_j - m_j)}$$

where p and q are the new point and the base point, respectively, $[m_j, M_j]$ is the interval of allowed values of p_j , and W is a shape constant. This is a relatively simple probability distribution that satisfies the requirements that the probability density be positive over all possible parameters values and that the density be a maximum at the base point.

In a previous SA algorithm for an inverse porous flow problem, the “temperature” was periodically reduced by a factor between 0.7 and 0.95 (Owens 1992). Other studies suggest that the temperature should be proportional to

$$E(\underline{p}_b) - E_o$$

where $\underline{p}_b$ is the most recent base point and E_o is an estimate of the minimum value for E . In order to assure that T converges to zero even when E_o is underestimated, the present algorithm uses

$$T = V \frac{E(\underline{p}_b) - E_o}{\ln(n + 1)}$$

where n is the number of points for which E has been evaluated and V is a constant. The value for E_o is based on the fractional measurement errors e_i at the various monitors; that is,

$$E_o = \sum_i e_i^2 \left(\sum_k C_{ik}^2 \right)$$

For the calculations reported here, V was set to 100. With this choice, the probability of accepting a point that would “double” the error is about 98.6 percent for $n=1$ and about 86 percent for $n=2000$.

An SA algorithm needs a stopping rule, which tends to be problem-dependent. The present algorithm stops a search when $E(\underline{p}) \leq E_o$ or after a fixed number of evaluations N .

In order to estimate the uncertainty in the result, several sequences are run, each starting from the same initial $\underline{p}$ but using a different sequence of random numbers. Because of this repetition, it is reasonable to use a relatively small value of N for each search.

This iterative methodology was incorporated into a Fortran code developed to run on a standard personal computer. Tests with simulated soil gas concentration histories from a one-dimensional spherical diffusion model were conducted to demonstrate the methodology.

APPENDIX B

REQUIREMENTS SPECIFICATION AND DESIGN DOCUMENT FOR THE INVERSION CODE

Purpose of the Software

The SEAtTM concept is based on injection of a tracer gas into the barrier-contained volume; with the ground outside of the contained volume being monitored for indication of leaks. If tracer gases were detected, the SEAIM software would use the measured concentration histories to estimate the size and location of the leak. To accommodate anticipated further developments, SEAIM is a general tool for inverse modeling.

Purpose and Contents of This Document

This document contains the requirements for Version 1 of SEAIM.

Scope of SEAIM

The SEAIMsystem includes two separate software subsystems. The SEAIMCLC subsystem receives data from the measurement and recording portion of SEAt. It does not invoke itself; it is initiated by the user or by a SEAtTM management module or other management software residing on the same computer.

The SEAIMIO subsystem interacts with the user for preparation of input and for display and printing of results. The management software or the user must manage file naming, archiving, and retrieval. SEAIM always uses the same temporary file names.

Terminology

This specification uses general terms in place of some of the specific language that would be appropriate to the SEAtTM application. Space and time variables are examples of the general term "independent variables." "Scalar dependent variable" is a generalization of the tracer gas concentration history.

REQUIREMENTS

1. Software Requirements

- 1.1. SEAIM 1 shall consist of the two subsystems, SEAIMCLC and SEAIMIO.
- 1.2. Both subsystems shall run under MS-DOS and shall be capable of independent operation on the same or separate platforms.
- 1.3. SEAIM 1 shall have documented quality assurance reviews that trace the development of the software from these requirements through design, implementation, and verification and validation.
- 1.4. The quality assurance documentation shall include the mathematical foundation of the algorithm contained in these requirements.

2. Requirements for Library of Models

- 2.1. SEAIMCLC shall contain a library of models, each capable of evaluating its scalar dependent variable, c , at a given set of values of its independent variables and given values of its model parameters.
- 2.2. Each model in the library shall be associated with a unique model identifier.
- 2.3. The input to each model shall be (a) values of its model parameters and (b) sets of values of its independent variables.
- 2.4. The output from each model shall be the values of its scalar dependent variable that correspond to the sets of values of its independent variables.
- 2.5. Each model in the library shall be associated with a list of its model parameters and a list of its independent variables.
- 2.6. For any model in the library, each of its model parameters shall be associated with an identifier that is unique among identifiers for that model. [Note that identifiers for independent variables are neither required nor prohibited.]
- 2.7. Each model parameter shall be associated with an indication of whether its uncertainty shall be reported as a standard deviation or as an error factor. [The error factor for an uncertainty distribution is the value at the 95th percentile divided by the median of the distribution.]
- 2.8. The library of models shall include the model for ideal spherical diffusion with constant source, as specified in Requirement 8. {Note that no other models are required.]

3. Overall Processing Requirements

- 3.1. SEAIMCLC shall be capable of direct evaluation of a model and capable of inverse modeling.

- 3.2. The default mode of operation shall be inverse modeling.
- 3.3. SEAIMCLC shall verify input data as necessary to assure graceful termination.
- 4. Requirements for Direct Evaluation of a Model.
 - 4.1. For direct evaluation, SEAIMCLC shall read a Direct-Evaluation Input File and write a Direct-Evaluation Output File.
 - 4.2. A Direct-Evaluation Input File shall contain the following:
 - 4.2.1. an identifier for the input set;
 - 4.2.2. an indicator that specifies direct modeling;
 - 4.2.3. a model identifier;
 - 4.2.4. a set of pairs, each consisting of a parameter identifier and a value for that model parameter; and
 - 4.2.5. sets of values for the model's independent variables. [Note that there is neither requirement for nor prohibition against (a) use of independent variable identifiers or (b) simplified input of repeated values of independent variables.]
 - 4.3. A Direct-Evaluation Output File shall contain the following:
 - 4.3.1. the date and time that SEAIMCLC was invoked;
 - 4.3.2. the content of the Direct-Modeling Input that was read;
 - 4.3.3. if an input error was detected, a clear explanation of the input error;
 - 4.3.4. if a processing error was detected, values of all variables at the time the processing error was detected, and
 - 4.3.5. if no error was detected, the time that processing was completed; and
 - 4.3.6. if processing was completed, then for each set of values of the model's independent variables, the value of the dependent variable according to the model.

5. Requirements for inverse modeling
 - 5.1. For inverse modeling, SEAIMCLC shall read a Model Input File, a Dependent-Variable Input File, and an Algorithm Input File and write an Inverse-Modeling Output File..
 - 5.2. A Model Input File shall contain the following:
 - 5.2.1. a model identifier and
 - 5.2.2. a set of triplets, each consisting of a parameter identifier and minimum and maximum values for that model parameter.
 - 5.3. A Dependent Variable Input File shall contain the following:
 - 5.3.1. a header for the input set [Note that SEAIMCLC is not responsible for verifying that the header is unique.] and
 - 5.3.2. any number of Dependent Variable Data Points, each consisting of a value for each of the model's independent variables, a value for the dependent variable, and the absolute uncertainty for the value of the dependent variable. [Note that there is neither requirement for nor prohibition against (a) use of independent variable identifiers or (b) restriction to and simplified input for patterns of repeated absolute uncertainties or repeated values of independent variables.]
 - 5.4. An Inverse-Modeling Output File shall contain the following:
 - 5.4.1. the date and time that SEAIMCLC was invoked,
 - 5.4.2. the content of the Model Input File and the Dependent-Variable Input File;
 - 5.4.3. if an input error was detected, a clear explanation of the input error;
 - 5.4.4. if no input error was detected, default values for the parameters of the method described in Requirement 9 and any replaced values;
 - 5.4.5. if a processing error was detected, values of all variables at the time the processing error was detected, and
 - 5.4.6. if no error was detected, the time that processing was completed;
 - 5.4.7. if processing was completed, estimates of the values of the model parameters, with uncertainties, calculated by the method described in Requirement 9 [Note that output of intermediate results is neither required nor prohibited.]; and
 - 5.4.8. if processing was completed, then for each input Dependent Variable Data Point, the value of each of the model's independent variables, and the value of the dependent variable according to the model, using the estimated values of the model parameters.

- 5.5. An Algorithm Input File shall contain changes, if any, to default values of the parameters of the method described in Requirement 9.
6. External Interface Requirements
 - 6.1. The interface for transfer of data from the SEAtTM system to SEAIMCLC shall consist of a Model Input File, a Dependent-Variable Input File and an Algorithm Input File.
 - 6.2. Each of the three interface files shall be in ASCII format and comma delimited in a manner compatible with the Lotus spreadsheet software.
7. Internal Interface Requirements
 - 7.1. Direct-Evaluation Input Files, Direct-Evaluation Output Files and Inverse-Modeling Output Files shall be in ASCII format and comma delimited in a manner compatible with the Lotus spreadsheet software.
8. User Interface Requirements
 - 8.1. SEAIMIO shall include a user-interface module for creating Direct-Evaluation Input Files, Model Input Files, Dependent-Variable Input Files and Algorithm Input Files and for processing Direct-Evaluation Output Files and Inverse-Processing Output Files.
 - 8.2. The user interface module shall have the look and feel of a spreadsheet application. [Note that there is no requirement to validate input and detect errors, but the software should do so as convenient.]
 - 8.3. The values of the dependent variable from the Direct-Evaluation Output File (Requirement 3.3) shall be easily copied into the Dependent-Variable Input File (Requirement 4.3.2).
 - 8.4. All of the contents of the output files shall be identified and easily found.
9. Requirements for Model for Ideal Spherical Diffusion With Constant Source
 - 9.1. The model for ideal spherical diffusion with constant source, ISDCS, shall have the following independent variables:
 - 9.1.1. three Cartesian spatial coordinates, x, y, and z and
 - 9.1.2. time, t.

- 9.2. The ISDCS model shall have the following model parameters:
- 9.2.1. three Cartesian coordinates of the source location, x_0, y_0, z_0 ;
 - 9.2.2. the radius of the source, r_0 ;
 - 9.2.3. the start time for the source, t_0 ;
 - 9.2.4. the strength of the source, c_0 ; and
 - 9.2.5. the diffusivity of the medium, D .
- 9.3. The ISDCS model shall evaluate its scalar dependent variable, c , in accordance with the formula

$$\frac{r_0}{r} C_0 \operatorname{erfc} \left(\sqrt{\frac{(r - r_0)^2}{4D(t - t_0)}} \right),$$

where r is determined by the formula

$$\sqrt{(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2},$$

- 9.4. Uncertainty for t_0 shall be reported as a standard deviation. Uncertainties for all other ISDCS model parameters shall be reported as error factors. [Note that the ISDCS model must also satisfy Requirements 1.2 through 1.7.]
10. Requirements for Inverse Modeling Method
- 10.1. The parameter of the inverse modeling method shall be the following;
 - 10.1.1. the number of independent searches, S ;
 - 10.1.2. the maximum number of iterations in each search, N ;
 - 10.1.3. the “temperature” constant, V ; and
 - 10.1.4. the probability density shape constant, w .
 - 10.2. SEAIM shall perform S independent searches for a best set of model parameters and output the average value found for each model parameter and the standard deviation or error factor of these values.
 - 10.3. For each search, the best set of model parameters shall be the set that minimizes E , the sum of the squares of the differences between the dependent variables in the Dependent Variable Input File and the dependent variables calculated by the selected model.
 - 10.4. Each search shall terminate when the value of E is less than E_0 , the sum of the squares of the uncertainties in the dependent variables in the Dependent Variable Input File, or when N sets of model parameters have been evaluated, whichever comes first.

- 10.5. The base-camp set of model parameters shall initially be the arithmetic or geometric means of the limits of each parameter. Arithmetic means shall be used for parameters with uncertainties reported as standard deviations; geometric means shall be used for parameters with uncertainties reported as error factors.
- 10.6. If the most recent set of model parameters has a value of E less than the lowest previous value, E_s , then that set of parameters shall become the base-camp set. Otherwise a random number shall be chosen, and the most recent set of parameters shall become the base-camp set with probability

$$\exp\left[\frac{(F-E)}{T_s}\right] \text{ where } T_s \text{ is } \frac{V(E_s - E_o)}{\ln(n+1)} \text{ and } n \text{ is the number of sets of}$$

parameters evaluated during the current search.

- 10.7. Each set of model parameters in a search shall have its parameters selected randomly by the Simulated Annealing algorithm of Requirement 9.10.
- 10.8. If a model parameter has its uncertainty reported as a standard deviation, then the parameters in Section 9.10 have the following definitions:
 - 10.8.1. q is the value of that parameter in the base-camp set,
 - 10.8.2. m is the minimum value for that parameter as specified in the Model Input File,
 - 10.8.3. M is the maximum value for that parameter as specified in the Model Input File, and
 - 10.8.4. p is the selected value for that parameter.
- 10.9. If a model parameter has its uncertainty reported as an error factor, then the parameters in Section 9.10 have the following definitions:
 - 10.9.1. q is the natural logarithm of the value of that parameter in the base-camp set,
 - 10.9.2. m is the natural logarithm of the minimum value for that parameter as specified in the Model Input File,
 - 10.9.3. M is the natural logarithm of the maximum value for that parameter as specified in the Model Input File, and
 - 10.9.4. p is the natural logarithm of the selected value for that parameter.
- 10.10. The Simulated Annealing algorithm shall be as follows [not required to be a separate module, but minimum coupling is desirable]:
 - 10.10.1. set g to $1 - \exp[-w(q-m)/(M-m)]$
 - 10.10.2. set h to $1 - \exp[-w(M-q)/(M-m)]$;
 - 10.10.3. if g = 0, set Q to 1, otherwise set Q to $1/[1+(h/g)]$;
 - 10.10.4. select random R uniformly from the interval [0,1]

10.10.5.if $R < Q$, set p to $\frac{q + (M - m) \ln[(Rg / Q) + (1 - g)]}{w}$,

10.10.6.otherwise set p to $q - \frac{(M - m) \ln\{[(1 - R)h / (1 - Q)] + (1 - h)\}}{w}$.

APPENDIX C: BENCHMARK STUDY OF THE INVERSION CODE

To gain further insight into the performance characteristics and abilities of the SEAIM software, SEA has performed a series of benchmark studies. These studies examined the ability of SEAIM to return accurate estimates of the model parameters for various settings of parameters and locations of leaks. A total of 18 separate studies were performed, which are discussed below.

Benchmark #1:

In this benchmark, the ability of SEAIM to find acceptable estimates for model parameters was studied using five leaks of different radii. The results of this benchmark indicated that SEAIM was capable of returning accurate estimates for the position of the leak and the diffusivity of the soil, but was unable to arrive at reasonable estimates for the radius of the leak, the start time or the source concentration.

Benchmark #2:

In this benchmark, the values of x_0 , y_0 , and z_0 were fixed at the values found in benchmark #1 and each of the five cases were re-run to see if fixing these values lead to an improvement in the other model parameters. The results of this benchmark indicate that fixing x_0 , y_0 , and z_0 at the values from the previous run yielded no improvement in the final answer.

Benchmark #3:

In this benchmark, the ability of SEAIM to return accurate values for the model parameters when setting the diffusivity, D , and/or the source concentration, c_0 , at fixed values was investigated. A single leak radius was used for this benchmark. The results of the benchmark indicate that fixing these parameters did not prevent SEAIM from obtaining reasonable estimates for the position of the leak, but did not yield any improvement in the estimates of leak radius or start time.

Benchmark #4:

In this benchmark, the ability of SEAIM to return accurate values for the model parameters when the source concentration, c_0 , is fixed at its true value was examined for the five leak radius test cases. The results of the benchmark indicate that fixing c_0 at its true value leads to improvement in the estimate for the radius of the leak, but no improvement in the start time.

Benchmark #5:

In this benchmark, the ability of SEAIM to return accurate values for the model parameters when the source concentration, c_0 , is set to 1 was examined for the five leak radii test cases. The results of the benchmark indicate that this value of c_0 does not adversely affect the position estimate, but does significantly affect the radius of the leak.

Benchmark #6:

In this benchmark, the ability of SEAIM to return accurate values for the model parameters when the exponential value used to compute the error functional is increased from two to six was examined. This was found to yield no improvement in the results of the inversion.

Benchmark #7:

In this benchmark, the ability of SEAIM to return accurate values for the model parameters when the exponential value used to compute the error functional is increased from two to six and the source concentration, c_0 , is fixed at its true value was examined. This was found to yield no improvement in the results of the inversion.

Benchmark #8:

In this benchmark, the ability of SEAIM to return accurate values of the model parameters when the exponential value used to compute the error functional is increased from two to six and the source concentration, c_0 , is fixed at 50% higher than its true value was examined. This was found to yield no improvement in the results of the inversion.

Benchmark #9:

In this benchmark, the ability of SEAIM to return accurate values of the model parameters with choice of Simulated Annealing parameter "w," the probability distribution weighting constant, was examined. The results of this benchmark indicate no preferential choice of "w."

Benchmark #10:

In this benchmark, the ability of SEAIM to return accurate values of the model parameters when the source concentration, c_0 , is fixed at 50% of its true value is examined. This was found to yield no improvement in the results of the inversion.

Benchmark #11:

In this benchmark, the ability of SEAIM to return accurate values of the model parameters when the source concentration, c_o , is fixed at 0.4% less than its true value is examined. This was found to yield no improvement in the results of the inversion.

Benchmark #12:

In this benchmark, the ability of SEAIM to return accurate values of the model parameters when the source concentration, c_o , is fixed at 2% of its true value is examined. This was found to yield no improvement in the results of the inversion.

Benchmark #13:

In this benchmark, the ability of SEAIM to return accurate values of the model parameters when the source concentration, c_o , is fixed at 20% of its true value is examined. This was found to yield no improvement in the results of the inversion.

Benchmark #14:

In this benchmark, the ability of SEAIM to return accurate values of the model parameters when the start time of the leak is fixed at various values. This was found to yield no improvement in the results of the inversion.

Benchmark #15:

In this benchmark, the ability of SEAIM to return accurate values of the model parameters for leaks at various points within the monitoring array is examined. The results of this benchmark indicate that if the leak is within the bounds of the monitoring array, then the inversion is capable of accurately locating the leak. If the leak is outside the bounds of the monitoring array, then the accuracy of the position is dependent upon the distance away from the monitoring array.

Benchmark #16:

In this benchmark, the ability of SEAIM to return accurate values of the model parameters for leaks at various points within the monitoring array when the source concentration is fixed at 30% greater than the true value is examined. This benchmark yielded the same results as benchmark #15.

Benchmark #17:

In this benchmark, the ability of SEAIM to return accurate values of the model parameters when the start time of the leak is fixed at 0 is examined. This was found to yield no improvement in the results of the inversion.

Benchmark #18:

In this benchmark, the ability of SEAIM to return accurate values of the model parameters when the leak is at various distances from the monitoring point array is examined. This was found to yield no improvement in the results of the inversion.

4.6.11
12.10.1

APPENDIX D

INSTRUCTIONS FOR USING THE INVERSION CODE

Field Version

As currently implemented, the SEAIM analysis software is a single FORTRAN subroutine which is executed using the statement

Call SEAIM

There are no arguments used in the call statement. SEAIM requires that four files be present in order to execute, [name].loc, [name].dat, [name].bnd, and INPUT.INV. The required format for these files are outlined at the end of this appendix.

Upon execution, SEAIM first opens the file INPUT.INV and reads in the unique header for this inversion operation. SEAIM then generates a file named STATUS.INV. This file contains number codes and messages relating to execution of SEAIM. SEAIM then continues to read in the information contained in INPUT.INV and to open the necessary files. If the headers in the files are inconsistent with the header in INPUT.INV, then a 0 is written to the STATUS.INV file and execution stops. Otherwise, execution continues. SEAIM calls SEARCH to evaluate the input data and determine the number of leaks that may be present. SEARCH is described below. SEAIM is currently set up to detect up to 15 independent leaks, but will only invert 1 leak at a time and only if that leak is independent of any other leaks. The independence of leaks is based on the nearest neighbor information contained in the INV.LOC file. If the first leak found and a subsequently found leak are determined to be nearest neighbors to each other, then an error code is written to STATUS.INV along with the message "Interacting Leaks Detected." This error forces SEAIM to terminate execution. Otherwise, SEAIM performs an inversion on the first leak detected. The inversion is performed using the Simulated Annealing algorithm coupled with a 1 dimensional spherical diffusion model. "Fit" of a forward modeled data set to measured data is determined using an L2 norm of the measured and calculated data. Only nearest neighbors to the leak are used to calculate the L2 norm. Once the inversion is completed, the results are written to the file RESULTS.INV, which has the following format.

* ****
: :
: :
: :

```

1.000000
test
19961122
5      5000      100.000000      6.000000
1
082755.400
13
2.914572      7.869996E-02
-2.471794E-03  7.141535E-02
-3.465280      1.289104E-01
6.382923E-01  3.065359
-5.937828      3.220284E+08
3114.138000    2.805969
1.000000E-04   1.000000
7193830.000000
082938.018

```

The first line is the SEAIM version number. Line 2 is the unique header used to identify the inversion run. Line 3 is the data on which the inversion was requested. Line 4 contains the four simulated annealing parameters. Line 5 is the number of leaks identified. Line 6 contains the time at which the inversion was started. Line 7 contains the number of the monitoring point identified as closest to the leak. Line 8 contains the estimate for x_0 and its uncertainty. Line 9 contains the estimate for y_0 and its uncertainty. Line 10 contains the estimate for z_0 and its uncertainty. Line 11 contains the estimate for r_0 and its standard deviation. Line 12 contains the estimate for start time t_0 of the leak, and its uncertainty. Line 13 contains the estimate of leak concentration and its standard deviation. Line 14 contains the estimate for soil diffusivity and its standard deviation. Line 15 contains the relative error value for this set of model parameters. Line 16 contains the stop time of the inversion. This file, along with STATUS.INV, is stored by the control software, as they are overwritten by subsequent executions of SEAIM.

Office Version

The office version of the SEATrace SEAIM inverse analysis software is executed by typing SEAIM and pressing return at the command prompt. The first choice that the user is given is whether to execute a forward or an inverse calculation. Enter an "F" to perform a forward calculation, or an "I" to begin an inverse calculation. Both options will be discussed below:

X_o - X coordinate of the leak (m)
 Y_o - Y coordinate of the leak (m)
 Z_o - Z coordinate of the leak (m)
 R_o - Radius of the leak (m)
 T_o - Start time of the leak (seconds)
 C_o - Concentration of tracer gas in the leak
 D - Diffusivity of the soil (m^2/s)

The code then prompts for whether a monitoring point location exists or if the monitoring point coordinates are to be entered. Entering a "Y" indicates that the file is already built, and SEAIM then prompts the user for the name of the file, which is assumed to be of the form [name].loc. Entering an "N" indicates that there is no file, and the information must be entered by hand. The code prompts the user for the number of monitoring points, which must be less than 100. SEAIM then prompts the user for the X, Y, and Z coordinates of each of the monitoring points. Once all the monitoring point coordinate information has been entered, either through the external file or from the keyboard, SEAIM requests that the number of times after the leak has started at which the model will be evaluated be entered. Next, SEAIM requests the actual times, in hours, at which concentrations will be calculated. Once this measurement time information has been entered, SEAIM allows the user the choice of adding a 10% experimental error to the data. To do this, the user enters a "Y" or an "N" to skip this. Once this is done, SEAIM evaluates the forward model and writes the output to external files, DIR_IN.DAT and DIR_OUT.DAT. DIR_IN.DAT contains all the input information which was used to set up the model and perform the evaluation. An example of the contents of DIR_IN.DAT are shown below.

Forward Model Header

```
1
x0 = 3.000000
y0 = 0.000000E+00
z0 = -3.000000
r0 = 1.000000E-02
t0 = 0.000000E+00
c0 = 50000.000000
D = 1.000000E-04
1 3.0000 1.0000 -3.0000 10.0000
```

Line 1 contains a header for the run. Line 2 contains the number of the forward model used. Lines 3 - 9 contain the values of the forward model parameters that were used. Starting in Line 10, the monitoring point coordinates and the times at which data was modeled are output. Each line contains 5 values. Value 1 is the number of the monitoring point, value 2 is the x coordinate of the monitoring point, value 3 the y coordinate and value 4 the z coordinate. Value 5 is the time at which the concentration is to be computed.

The contents of file DIR_OUT.DAT are shown below

SEAIM Version = 1.000000

Data set header =

Date of Execution = 25-Nov-96

Start Time = 11:07:16

Stop Time = 11:07:16

Model Parameters are:

```
x0 = 3.000000
y0 = 0.000000E+00
z0 = -3.000000
r0 = 1.000000E-02
t0 = 0.000000E+00
c0 = 50000.000000
D = 1.000000E-04
```

Independent variables and concentrations are:

(Loc X(m) Y(m) Z(m) T(hours) C(ppm))

1 3.000 1.000 -3.000 10.000 356.082

Line 1 contains the current version number for SEAIM. Line 2 contains a data set header. Line 3 is the data on which execution of the forward model took place. Lines 4 and 5 are the start and stop times, respectively, of the forward model. Lines 6-13 contain the values of the model parameters used. Starting at Line 14, the calculated concentration values are printed out. Each line contains 6 values. Value 1 is the monitoring point number, Values 2-5 are the coordinates of the monitoring point and the time at which the concentration was computed, and value 6 is the calculated concentration.

Inverse Analysis: For inverse analysis of data that has been acquired in the field, SEAIM assumes that several files are present on the computer prior to execution. The first file is a monitoring point locations file, named [name].loc, the second file is the data file, [name].dat, and the third file is the [name].bnd file, which is only required if the SEARCH algorithm is to be used. To begin inverse analysis of a measured data set, enter an "I" at the prompt. SEAIM then provides the user with a list of the forward models which may be used. The models are selected by entering the number corresponding the desired model. For example, 1 signifies the 1-D Spherical Diffusion model. Once the forward model has been selected, SEAIM then prompts the user for the name of the monitoring point locations file, [name].loc, and the name of the concentrations data file, [name].dat. When these names have been entered, SEAIM opens the files and reads in the information contained in them. The code then prompts the user as to whether the SEARCH option should be used. If the user selects "Y", then SEARCH is used to scan the input data, determine the presence of any leaks and identify the monitoring point which is closest to each of the leaks detected. The SEARCH algorithm also reads information from the bounds file discussed above and assigns search ranges to X_0 , Y_0 , and Z_0 . The initial guess for X_0 , Y_0 , and Z_0 are set at the coordinates of the identified nearest monitoring point. SEARCH returns the number of leaks found and the number of the monitoring point closest to each leak. For the desktop version, SEAIM is set to invert only 1 leak at a time. So, the user is provided with a list of the leaks detected and asked to select which leak to invert. Once the number of the leak has been entered, SEAIM prompts the user for an upper limit on the concentration and an estimate of the diffusivity of the soil. For leak radius, r_0 , SEAIM assumes that the radius will be between 1 mm and 1m, with an initial guess of 1cm. For start time, the upper bound is set at one second before the earliest measurement of the input data set was taken, and the lower bound is set at 5 days prior to this time. The initial guess is set at the midpoint between these bounds. The lower bound on concentration is set at 1, and the initial guess is set at one-half the upper bound. Since diffusivity can be measured fairly accurately at a site, it is considered constant. Once this information is entered, the user is shown the simulated annealing algorithm parameters as set, and asked if they are satisfactory or if they should be changed. In general, these parameters should not be changed. By entering an "N," the inverse process begins.

If the user, however, chooses not to use SEARCH, then the inversion run is set up in a different manner. For this case, the user is prompted to enter an estimate, an upper bound and a lower bound for each of the model parameters. The user may fix a parameter

at a particular value by entering the same value for estimate, upper, and lower bound. Once the search criteria for the model parameters have been entered, the user is prompted to enter the number of the monitoring point closest to the potential leak location. For this reason, it is recommended that a data set first be analyzed using SEARCH, to generate estimates of leak location and nearest monitoring points, then analyzed without SEARCH. Upon entering the number of the nearest monitoring point, SEAIM provides the user with the currently set simulated annealing parameters. The user has the option of changing these, but it is recommended that they be left as they are set. Enter an "N" to begin the inversion process.

Once the inversion process has been completed, SEAIM writes the file INV_OUT.DAT. This file contains the results of the inversion process. An example of the output file generated when the SEARCH algorithm is used is shown below:

```
SEARCH found      1 leak(s)
leak #      1 is closest to monitoring point      13
This point has the coordinates:
X =      3.000000
Y =      1.000000
Z =     -3.000000
```

```
SEAIM Version =      1.000000
```

```
Data set header =
```

```
Date of Execution = 26-Nov-96
```

```
Start Time = 08:22:53
```

```
Stop Time = 08:24:38
```

```
Simulated Annealing used as inversion algorithm
```

```
Number of independent searches =      5
```

```
Number of iterations per search =      5000
```

```
Annealing temperature constant =      100.000000
```

```
Probability weighting constant =      6.000000
```

The best model parameters are:

X0 = 3.154039 uncertainty = 4.392812E-02
Y0 = 1.003715E-01 uncertainty = 9.565159E-02
Z0 = -3.322851 uncertainty = 1.411776E-01
r0 = 1.192572E-01 standard deviation = 4.651033

T0 (hrs) = -42.868990 uncertainty = 6.385521E+09
c0 = 15684.490000 standard deviation = 5.001647
D = 1.000000E-04 standard deviation = 1.000000

Sum of Squared Residuals = 5638261.000000

Loc	X(m)	Y(m)	Z(m)	T(hrs)	C(meas)	C(calc)
1	1.000	1.000	-1.000	24.000	262.972	367.702
2	1.000	1.000	-2.000	24.000	422.859	496.186
3	1.000	1.000	-3.000	24.000	510.996	593.012
4	1.000	1.000	-4.000	24.000	422.859	568.748
5	1.000	1.000	-5.000	24.000	262.972	449.873
.						
.						
.						
.						

The output file is fairly self explanatory. The parameters of interest are the best estimates for each of the model parameters and the sum of squared residuals value, which is a measure of how "good" the answer is. Below is shown an example of the output file when the SEARCH algorithm is not used:

SEAIM Version = 1.000000

Data set header =

Date of Execution = 26-Nov-96

Start Time = 08:29:02

Stop Time = 08:30:46

Simulated Annealing used as inversion algorithm

Number of independent searches = 5

Number of iterations per search = 5000
 Annealing temperature constant = 100.000000
 Probability weighting constant = 6.000000

The best model parameters are:

X0 = 3.115735 uncertainty = 3.516909E-02
 Y0 = 6.575295E-02 uncertainty = 7.982842E-02
 Z0 = -2.983639 uncertainty = 1.232772E-01
 r0 = 9.342650E-02 standard deviation = 4.364409

T0 (hrs) = 2.109262 uncertainty = 1.148897E+07
 c0 = 26473.100000 standard deviation = 5.740205
 D = 7.850450E-05 standard deviation = 3.297858

Sum of Squared Residuals = 1030083.000000

Loc	X(m)	Y(m)	Z(m)	T(hrs)	C(meas)	C(calc)
1	1.000	1.000	-1.000	24.000	262.972	325.586
2	1.000	1.000	-2.000	24.000	422.859	483.666
3	1.000	1.000	-3.000	24.000	510.996	564.689
4	1.000	1.000	-4.000	24.000	422.859	478.907
5	1.000	1.000	-5.000	24.000	262.972	320.571
.						
.						
.						
.						

SEARCH Algorithm

The SEARCH algorithm was developed to provide the user with a method for examining the data, determining the presence of leaks, and generating initial estimates for the location of each detected leak. The algorithm is based on the same assumption as the forward model used for inversion, mainly 1-D spherical diffusion. This assumption dictates that the monitoring point closest to the leak will have a higher concentration at a given time than its neighbor points, which are the monitoring points which are closest to the point being tested. SEARCH examines the input concentration data for each time sequence independently. The measured concentration value at each monitoring point is compared to the concentrations at each of its nearest neighbors, as specified in the

[name].loc file. If the concentration at the monitoring point is greater than the concentrations at each of its nearest neighbors, then that point is classified as being nearest to a leak, and the coordinates of that monitoring point are used as the initial basecamp guess for the inversion process. The file [name].bnd is opened and scanned until the number of this monitoring point is detected. At this point, the bounds on the X, Y and Z search region corresponding to this monitoring point are loaded.

Required File Formats

The following files are used by the two versions of SEAIM.

Monitoring Point Information File: [name].loc: This file is created by SEA once a monitoring system has been installed at a site. If monitoring points are added or removed at a later date, this file must be modified to account for these changes but otherwise the file does not need to be modified. The name of this file is of the form [name].loc, where name relates to the site, such as SANDIA1 or LANL2. The format for this file is shown below:

Test

25

1	1.0	1.0	-1.0	0.
2	1.0	1.0	-2.0	0.
3	1.0	1.0	-3.0	0.
4	1.0	1.0	-4.0	0.
5	1.0	1.0	-5.0	0.
6	2.0	1.0	-1.0	0.
7	2.0	1.0	-2.0	0.
8	2.0	1.0	-3.0	0.
9	2.0	1.0	-4.0	0.
10	2.0	1.0	-5.0	0.
11	3.0	1.0	-1.0	0.
12	3.0	1.0	-2.0	0.
13	3.0	1.0	-3.0	0.
14	3.0	1.0	-4.0	0.
15	3.0	1.0	-5.0	0.
16	4.0	1.0	-1.0	0.
17	4.0	1.0	-2.0	0.
18	4.0	1.0	-3.0	0.
19	4.0	1.0	-4.0	0.
20	4.0	1.0	-5.0	0.

```

21 5.0 1.0 -1.0 0.
22 5.0 1.0 -2.0 0.
23 5.0 1.0 -3.0 0.
24 5.0 1.0 -4.0 0.
25 5.0 1.0 -5.0 0.
1 3 2 6 7 0 0 0 0 0
2 5 1 7 3 6 8 0 0 0
3 5 2 8 4 7 9 0 0 0
4 5 3 5 9 8 10 0 0 0
5 3 4 9 10 0 0 0 0 0
6 5 1 11 7 2 12 0 0 0
7 8 2 6 12 8 1 3 11 13
8 8 3 7 13 9 2 4 12 14
9 8 4 8 14 10 3 5 13 15
10 5 5 9 15 4 14 0 0 0
11 5 6 12 16 7 17 0 0 0
12 8 7 11 17 13 6 8 16 18
13 8 8 12 18 14 7 9 17 19
14 8 9 13 19 15 8 10 18 20
15 5 10 14 20 9 19 0 0 0
16 5 11 17 21 12 22 0 0 0
17 8 12 16 22 18 11 13 21 23
18 8 13 17 23 19 12 14 22 24
19 8 14 18 24 20 13 15 23 25
20 5 15 19 25 14 24 0 0 0
21 3 16 17 22 0 0 0 0 0
22 5 17 21 23 16 18 0 0 0
23 5 18 22 24 17 19 0 0 0
24 5 19 23 25 18 20 0 0 0
25 3 19 20 24 0 0 0 0 0

```

The first line is a 20 character header. Line 2 contains the number of monitoring locations at the site, and is an integer value. In this example, there are 25 monitoring points. Following line 3 is a group of monitoring point coordinates, the group being of size equal to the number of monitoring points. Each line contains 5 values, monitoring point number, x coordinate, y coordinate, z coordinate and coordinate uncertainty. The next group of lines, equal to the number of monitoring points, is a set of nearest neighbors for each monitoring point. Each line contains 11 values, the first being the monitoring

point number, the second being the number of nearest neighbors, and the remaining 9 being the numbers of the monitoring points considered as the nearest neighbors. For example, if only 3 nearest neighbors are specified, then columns 3, 4, and 5 will contain non-zero numbers and the rest will be zeroes. Monitoring point 25, for example, is specified to have only 3 neighbors, and the monitoring point numbers for these 3 neighbors are 19, 20 and 24. This set of information is also generated by SEA once a monitoring system is installed. The SEAIM code is currently set to handle a maximum of 100 monitoring point locations.

Measured Concentration Data File: [name].dat

The measured concentration data file contains the measured values taken by the gas analyzer. The file name is of the form [name].dat, where the name relates to the site, such as SANDIA1 or LANL2. The file has the following format:

Test

2		
1	24	262.972
2	24	422.859
3	24	510.996
4	24	422.859
5	24	262.972
6	24	422.859
7	24	818.619
8	24	1135.906
9	24	818.619
10	24	422.859
11	24	510.996
12	24	1135.906
13	24	1866.366
14	24	1135.906
15	24	510.996
16	24	422.859
17	24	818.619
18	24	1135.906
19	24	818.619
20	24	422.859
21	24	262.972
22	24	422.859

23	24	510.996
24	24	422.859
25	24	262.972
1	30	343.777
2	30	515.49
3	30	607.865
4	30	515.49
5	30	343.777
6	30	515.49
7	30	924.238
8	30	1245.792
9	30	924.238
10	30	515.49
11	30	607.865
12	30	1245.792
13	30	1979.664
14	30	1245.792
15	30	607.865
16	30	515.49
17	30	924.238
18	30	1245.792
19	30	924.238
20	30	515.49
21	30	343.777
22	30	515.49
23	30	607.865
24	30	515.49
25	30	343.777

The first line in the file is a 20 character header. Line 2 contains an integer value representing the number of time sequences to be used for inversion. For example, if data was acquired starting at time $t = 3$ hrs and then at time $t = 6$ hrs, then the number of time sequences is 2. Following this line are the actual data for each time sequence. The inversion code requires that all monitoring ports be present in each sequence. The first value on each line is the monitoring point number, the second number is the time at which the monitoring point sample was acquired (in hours) and the third value is the concentration of tracer gas measured. In the above example, data was acquired from 25 monitoring points at times $t=24$ hrs and $t=30$ hrs. Monitoring point concentration values

which are considered in error should be set to zero, but must still be included in the data set. The SEAIM code is currently set to read in a maximum of 125 time sequences.

Search Bounds Data File: [name].bnd

This file is envisioned to exist on the system in a read-only format. The file is created by SEA once a monitoring system has been installed at a site. The name of this file is of the form [name].bnd, where the name relates to the site, such as SANDIA1 or LANL2. The format of this file is shown below:

Test

```
1 10 0 .5 -.5 0 -10
2 10 0 .5 -.5 0 -10
3 10 0 .5 -.5 0 -10
4 10 0 .5 -.5 0 -10
5 10 0 .5 -.5 0 -10
6 10 0 .5 -.5 0 -10
7 10 0 .5 -.5 0 -10
8 10 0 .5 -.5 0 -10
9 10 0 .5 -.5 0 -10
10 10 0 .5 -.5 0 -10
11 10 0 .5 -.5 0 -10
12 10 0 .5 -.5 0 -10
13 10 0 .5 -.5 0 -10
14 10 0 .5 -.5 0 -10
15 10 0 .5 -.5 0 -10
16 10 0 .5 -.5 0 -10
17 10 0 .5 -.5 0 -10
18 10 0 .5 -.5 0 -10
19 10 0 .5 -.5 0 -10
20 10 0 .5 -.5 0 -10
21 10 0 .5 -.5 0 -10
22 10 0 .5 -.5 0 -10
23 10 0 .5 -.5 0 -10
24 10 0 .5 -.5 0 -10
25 10 0 .5 -.5 0 -10
```

The first line in this file contains a 20 character header. The number of lines after the first line is equal to the number of monitoring points at the site. Each line contains 7 values. The first value is the monitoring point number, the remaining values represent maximum and minimum bounds on X, Y and Z search regions. The sequence is Xmax Xmin Ymax Ymin Zmax Zmin. This file is used by the SEARCH algorithm implemented in SEAIM to automatically detect a leak and generate an initial guess and search bounds on X, Y and Z for use in the inversion process.

SEAIM Field Version Execution Instruction File: [name].inv

This file is only used by the field version of SEAIM. The SEAIM execution instruction file is generated by the data acquisition system controlling software. This file contains all information necessary for the field version of SEAIM to perform an inverse analysis on a set of data. This file is the first opened by SEAIM, and any extra information desired to be added into the file will require modification of the main code. Currently the file is required to be named INPUT.INV, but this may be changed. Below is the file format currently required.

```

test      ! Header for inversion problem
1         ! Forward model ID
test.loc  ! Monitoring point location file
test.dat  ! Measured concentrations data file
0.0       ! Background concentration value
test.bnd  ! Search region bounds
.01       ! Initial guess for r0
1         ! Upper bound for r0
.001      ! Lower bound for r0
11.000    ! Initial guess for T0
11.999    ! Upper bound for T0
-12.0     ! Lower bound for T0
30000     ! Initial guess for c0
60000     ! Upper bound for c0
1         ! Lower bound for c0
.0001     ! Initial guess for diffusivity
.0001     ! Upper bound on diffusivity
.0001     ! Lower bound on diffusivity
5         ! Number of independent searches
5000      ! Number of iterations per search
100.0     ! Temperature constant
6.0       ! Probability density shape constant

```

```

0      ! Key to let X,Y, or Z be fixed
2      ! Number of nearest monitoring point to leak
1      ! Number code for model parameter to fix
0.     ! value at which model parameter is fixed

```

Note: The comments (! and text) after each value are provided for ease in interpretation by the user, and are not required for actual field implementation.

Line 1 is a 20-character (maximum) header which is assigned by the control software and is unique to all 4 files required for inversion. SEAIM checks the header on each of the remaining 3 files to ensure consistency, and returns an error code in the output file STATUS.INV if the same header is not found in all 3 files. Line 2 is an integer value representing the model ID number. Currently a model ID value of 1 is required. Line 3 contains the monitoring point location file name of not more than 12 characters. Line 4 contains the concentration data file name of not more than 12 characters. This is the name of the file containing the measured concentrations which shall be used in the inversion. Line 5 contains a real value representing a background or baseline value of concentration, below which a concentration should be considered 0.0. Line 6 contains the search bounds file name of not more than 12 characters and which contains the information necessary to set up the search bounds. Line 7 is a real number representing the estimate for the radius of the leak, r_0 , and is currently set at 0.01m. Line 8 is a real number representing the upper bounds on the radius of the leak and is currently set at 1.0m. Line 9 is a real number representing the lower bounds on the radius of the leak and is currently set at 0.001m. Line 10 is an initial guess for the concentration of the tracer gas at the leak, and is currently set at 75% of the concentration behind the barrier. Line 11 is an upper bound on the tracer gas concentration at the leak, and is set at the concentration behind the barrier. Line 12 is a lower bound on the tracer gas concentration at the leak, and is set to 1 (real). Line 13 is an estimate of the diffusivity of the soil at the site. Line 14 is an upper bound on the estimate of the diffusivity. Line 15 is a lower bound on the estimate of the diffusivity. Currently these values are fixed at the measured values at the site. Line 16 represents the number of independent searches that the inversion algorithm will perform, and is currently set to 5 (integer). Line 17 represents the number of iterations per search, and is currently set to 5000 (integer). Line 18 represents the temperature constant, V , used by the inversion algorithm, and is currently set to 100.0. Line 19 represents the probability density shape constant, w , used by the inversion algorithm, and is currently set to 6.0. Line 20 contains an integer number allowing either X, Y, or Z, or all three, to be fixed at values. The default value is 0, meaning that none of the parameters are fixed. If the value is 1, then 1 parameter will be fixed. If the parameter is 2 or 3, then either two of the parameters or all three of the parameters, respectively, will be fixed. If the value is 0, then no further information is read from the file. However, if the value is non-zero, then the next line, line 21, contains the monitoring point number of the nearest neighbor to the leak. After reading in the number of the nearest neighbor, a group of 2 values is read in for each number of parameters that is fixed. For example, if only 1 parameter is fixed, then the next 2 lines contain the parameter to be fixed (1=x, 2=y, or 3=z) on the first line, and the second line contains the value at which the parameter is to

be fixed. To illustrate this further, consider how the x parameter is fixed. Line 20 will contain the value 1 (only 1 parameter fixed), line 22 will contain the value 1 (x parameter fixed) and line 23 will contain the value at which x is to be fixed. If 2 parameters are to be fixed, say x and z, then line 20 will contain the value 2, line 22 will contain the value 1, line 23 will contain the value at x is fixed, line 24 will contain the value 3, meaning z, and line 25 will contain the value at which z is to be fixed. In general, the use of fixed parameters will not be part of the standard operating procedure for the field version of SEAIM.

APPENDIX E

DESIGN CALCULATIONS FOR THE TEST FACILITY

Leak locations and dimensions on the barrier panels were chosen using results from a one-dimensional spherical diffusion model:

$$C(r, t) = \frac{(C_o - C_{exit})r_o^2}{Lr} \operatorname{erfc}\left(\frac{r}{\sqrt{4D(t-t_o)}}\right), r > r_o, t > t_o$$

where:

r is the distance from the leak center,

C is the concentration for a given r and t

D is the effective diffusivity of the tracer through the soil pores

t_o is the time that the leak began,

r_o is the constant radius of the leak after time t_o

C_o is the constant source concentration

C_{exit} is the concentration at the exit of the leak, and

L is the thickness of the barrier

Like the one-dimensional spherical model used in the inversion code, this model assumes a constant source concentration inside the barrier and a constant diffusivity of the tracer gas through the medium outside the barrier. It also neglects both advective flow and adsorption/desorption of the tracer. Unlike the model used in the inversion code, this model assumes that the leak impedes diffusion into the medium. In determining the impedance, the model assumes a constant diameter leak through the barrier with flow properties equal to the surrounding medium and a constant concentration at the leak exit equal to zero (found to be valid for barriers 1' thick or greater). The model is valid for steady-state conditions. It was used in the calculations because it is more conservative in its prediction of resulting concentrations in the medium for a given leak area.

For these field test calculations, input ranges for the analytical model were as follows:

- Source concentration: 45,000 ppm (273,150 mg/m³)
- Leak radii of 1.27, 2.54, 3.81, 5.08, and 19.5 centimeters (0.5, 1, 1.5, 2, 3, and 7.5 inches, respectively)
- Barrier thickness of 0.15, 0.61, and 1.22 meters (.5, 2, and 4 feet, respectively)
- Soil diffusivities of 1e-6, 5e-6, and 1e-5 m²/s (the measured diffusivity at the Sandia site was 1e-5 m²/s).

Test duration of 1,2,3 and 4 weeks.

A lower detection limit of 30 ppm was assumed for the gas analyzer.

Given these conditions, it was determined that for a four week test duration all combinations (with the exception of the three smallest diameter holes combined with the lowest diffusivity and the thickest barrier) could readily be detected with the SEAtace™ system to distances of at least 1.5 meters from the leak. With a standard 0.61 m (2 feet) thick barrier, a diffusivity of $1\text{e-}6\text{ m}^2/\text{s}$, and a four week test duration all but the smallest diameter leak could be detected to distances of at least 1.5 meters from the leak. Figure E1 shows typical results from the calculations. Using 1.5 meters as the maximum distance a leak could be from its nearest monitoring port, a grid of port locations was calculated. As shown in Figure E2, ports were spaced on 2 meter intervals on a plane parallel to and 0.75 meters from the barrier panels. Rows of ports were offset 0.4 meters ($1' 3 \frac{3}{4}''$) from one another. This spacing allowed for a reasonable spacing between ports if they had been installed from the surface, as well as minimized the distance a leak could be from any point on the barrier to its closest monitoring port.

(a) $C_o=45,000$ ppm; $D=5.0e-6$ m²/s; $L_b=2$ feet; $t=2$ weeks

(b) $C_o=45,000$ ppm; $r_o=2$ inches; $L_b=2$ feet; $t=2$ weeks

(c) $C_o=45,000$ ppm; $D=5.0e-6$ m²/s; $L_b=2$ feet; $r_o=2$ inches

(d) $C_o=45,000$ ppm; $D=5.0e-6$ m²/s; $r_o=2$ inches; $t=2$ weeks

Figure E1. Predictions of tracer concentrations outside the barrier for various parameter combinations. C_o = source concentration; D =diffusivity of the tracer through the soil gas; L_b =thickness of the barrier; r_o =radius of the leak; t =elapsed time from the start of the leak.

Figure E2. Typical exterior port spacing for the test experiment.

9. REFERENCES

- Betsil, J. D., and R. D. Gruebel. 1995. "VAMOS, The Verification and Monitoring Options Study, Current Research Options for In-Situ Monitoring and Verification of Contaminant Remediation and Containment with in the Vadose Zone." Sandia National Laboratories, TTP#AL2-2-11-07.
- Falta, R., K. Pruess, S. Finsterle, and A. Barristelli. 1995. *T2VOC User's Guide*. Lawrence.LBL-36400. Berkeley, CA: Berkeley National Laboratory.
- Heiser, J. H. 1994. "Subsurface Barrier Verification Technologies." BNL-61127. Brookhaven National Laboratory.
- Lowry, W., S. Dalvit Dunn, C. Williams, and D. Ward. 1996. "Tracer Verification and Monitoring of Containment Systems." In *Nuclear and Hazardous Waste Management*, 1243-49. Vol. 2. Proceedings of the International Topical Meeting – Spectrum '96, August 18-23, Seattle Washington. La Grange Park, IL: American Nuclear Society.
- Ouenes, Ahmed. 1992. "Application of Simulated Annealing to Reservoir Characterization and Petrophysics Inverse Problems." Ph.D. Thesis, New Mexico Institute of Mining and Technology.
- Rumer, R., and J. Mitchell, ed. 1995. "Assessment of Barrier Containment Technologies – A Comprehensive Treatment for Environmental Remediation Applications." International Containment Technology Workshop, August 1995. National Technical Information Service Publication #PB96-180583.
- Wilson, R. D., and D. M. Mackay. 1993. "The Use of Sulphur Hexafluoride as a Conservative Tracer in Saturated Sandy Media." *Ground Water Journal* 31, no 5 (September-October):719-24.