

Technical Report No: ND08-02

AN INVESTIGATION INTO SUBSURFACE SAMPLING AND CHARACTERIZATION EFFICIENCY USING A HIGH RESOLUTION GIS BASED THREE DIMENSIONAL EARTH SYSTEM

by

Damion J. Knudsen Bernhardt Saini-Eidukat Department of Geosciences, North Dakota State University Fargo, North Dakota

February 2008

North Dakota Water Resources Research Institute North Dakota State University, Fargo, North Dakota

Technical Report No: ND08-02

AN INVESTIGATION INTO SUBSURFACE SAMPLING AND CHARACTERIZATION EFFICIENCY USING A HIGH RESOLUTION GIS BASED THREE DIMENSIONAL EARTH SYSTEM

by

Damion J. Knudsen¹

Bernhardt Saini-Eidukat² WRRI Graduate Research Fellow¹ and Associate Professor² Department of Geosciences North Dakota State University Fargo, ND 58105

February 2008

The work upon which this report is based was supported in part by federal funds provided by the United States of Department of Interior in the form of ND WRRI Graduate Research Fellowship for the graduate student through the North Dakota Water Resources Research Institute.

Contents of this report do not necessarily reflect the views and policies of the US Department of Interior, nor does mention of trade names or commercial products constitute their endorsement or recommendation for use by the US government.

Project Period: March 1, 2007 – December 31, 2007 Project Number: 2007ND148B

North Dakota Water Resources Research Institute Director: G. Padmanabhan North Dakota State University Fargo, North Dakota 58105 ii

TABLE OF CONTENTS

TABLE OF CONTENTSii	i
LIST OF TABLESiv	v
LIST OF FIGURESiv	v
LIST OF EQUATIONSiv	v
ABSTRACT	1
ACKNOWLEDGMENTS	2
BACKGROUND	3
DESCRIPTION OF THE STATE OR REGIONAL WATER PROBLEM	
INVESTIGATED	5
SCOPE AND OBJECTIVES	б
MATERIALS AND METHODS	6
RESULTS AND DISCUSSION	1
CONCLUSIONS	4
REFERENCES14	4

LIST OF TABLES

Table 1.	Simulation Data results		.12	2
1 4010 1.	Simulation Data results	•••••••••••••••••••••••••••••••••••••••	• • •	-

LIST OF FIGURES

Figure 1.	3-D Isosurface (3-D Contour) Source Zone Model	8
Figure 2.	Sample and Model Semi-Variogram	10
Figure 3.	NRMSE Plots	11
Figure 4.	Graph of Normalized Root Mean Square Error (NRMSE) vs.	
horizo	ontal and vertical sampling resolution	13
Figure 5.	Cost versus NRMSE	13

LIST OF EQUATIONS

Equation 1.	Anisotropy	
Equation 2.	LIF Costs Calculation	
Equation 3.	Sample Semi-Variogram	
Equation 4.	Model Semi-Variogram	
Equation 5.	RMSE	
Equation 6.	NRMSE Calculation	

ABSTRACT

The degree of homogeneity, dimensions, and anisotropy of a contaminant source zone (SZ) distribution gradient should allow one to roughly estimate the most cost effective three dimensional sampling resolution and method. We have quantified the effect that three dimensional systematic sampling density has on conceptual site model error. A high resolution Earth System Simulator (ESS) was applied to three investigative subsurface direct sensing case studies, plus a synthetic high resolution control site. The ESS has a resolution of 5ft in the horizontal and 0.05ft in the vertical. Site dimensions were 400ft x 300ft x 21ft with a total of 2,080,161 nodes. A square centered systematic sampling method was used in the sampling and characterization simulation effort. Accounting for high SZ heterogeneity, this research has shown that increasing vertical sampling resolution from 2ft to 0.1ft can decrease normalized model error on average 40% or more while reducing total characterization costs.

ACKNOWLEDGMENTS

Stipend support for the Research Fellow, Damion J. Knudsen, was provided by the North Dakota Water Resources Research Institute. Appreciations are conveyed to Leon Vetter and Kris Roberts of the North Dakota Department of Health for providing subsurface data sets.

BACKGROUND

Non Aqueous Phase Liquids (NAPL) such as benzene, toluene, ethyl-benzene, and xylene (BTEX) aromatic compounds are constituents of gasoline range organics (GRO) and diesel range organics (DRO). Benzene is the most biologically harmful of the BTEX compounds. For many years, groundwater remediation efforts have concentrated on the dissolved phase constituents instead of treating the source zone BTEX-containing NAPL.

Prior to the mid to late 1990's, the traditional site characterization (TSC) of shallow subsurface impacted sites was solely achieved by the taking of core samples with a hollow stem-auger rig or a direct push corer. Field personnel would log sample textures and color by hand on a low resolution interval of one foot or more. TSC can be considered to use traditional sampling methods (TSM). Regions in the core that appeared to have contaminant infiltration would be sent to a lab, or grab bag sampled with a field photo ionization detector (PID), or simply its texture would be logged with a description such as *tar like material* (TLM) or *oil like material* (OLM). This would generally lead to the assumption of a homogenous contaminant source zone or dissolved phase plume with the source zone simply floating on the water table or resting on an aquitard.

Currently intensive research is being carried out on direct sensing instruments (DSI). In the early to mid 1990's in conjunction with the Department of Defense (DoD), Dakota Technologies, Inc. developed the Site Characterization and Analysis Penetrometer System (SCAPS) which was a combination of the Cone Penetrometer Test (CPT), Membrane Interface Probe (MIP), and Laser Induced Fluorescence (LIF) (Bujewski and Rutherford, 1997a, b).

With the advent of DSI, the degree of source zone homogeneity has come into question (Crumbling et al., 2003). Source zone homogenous models may be an outcome of low resolution data collection. Alternating sand and clay lenses with a fluctuating water table would be expected to cause source zone heterogeneity given the differing hydraulic conductivities between sand and clay. This effect could be expected to cause over or under characterization of the source zone when using TSM at intervals greater than those of the thicknesses of the lenses described. DSI can collect on an average of one inch and provide a higher resolution log of the subsurface contaminant distribution than would TSM. A collection of directly sensed logs can then be set in 3-D space and a high resolution interpolation can be created showing in many cases a semi to fully heterogeneous distribution of the contaminant source zone. Crumbling et al. (2003) consider the use of direct sensing technology as a more efficient method supplementing TSM with regards to cost, time constraints, and effectiveness.

The SCAPS unit developed into the two major types of subsurface LIF devices used in subsurface characterization today. The first type uses an ultraviolet laser and goes by the name Ultra Violet Optical Screening Tool (UVOST) or Rapid Optical Screening Tool (ROST) (Bujewski and Rutherford, 1997b).

The second type of subsurface LIF device uses a green laser and is called the Tar Specific Green Optical Screening Tool (TarGOST) (Okin et al., 2006). This device was developed by Dakota Technologies, Inc. to specifically respond to high weight PAH containing NAPL. This includes Coal Tar from Former Manufactured Gas Plants (FMGP), creosote from wood preservation

facilities and other similar NAPL spills such as napthenic crude oil.

UVOST, ROST, and TarGOST are delivered by Geoprobe style direct push technology and can be hammered. SCAPS is delivered into the subsurface using CPT technology and is not hammered. This allows other technology that is sensitive to hammering to be used simultaneously. However, a shortcoming is that the delivery vehicle is very large compared to Geoprobe technology, which may even be wheeled by hand or by small skid steer vehicles.

LIF technology is considered a direct sensing direct push technology and is endorsed by the EPA's TRIAD approach. The TRIAD emphasizes that a greater number of lower cost, higher density samples such as directly sensed data, followed by lesser amounts of higher cost traditional sampling, is more effective in the characterization of contaminated sites (Crumbling et al., 2003).

During each LIF site characterization, laser light is sent down the rod string through fiber optics into the subsurface, and is projected onto successive geologic strata through an optically transparent sapphire window and collects between 4000 and 40,000 semi-qualitative and semiquantitative measurements, depending on the size of the site and the degree of characterization desired by the site investigator. LIF will only detect the source term or free phase aromatic constituents of the subsurface NAPL distribution. Fluorescence is a property of PAHs, which are common components of subsurface petroleum-based contamination. Excitation of the PAH with appropriate wavelengths of light stimulates the release of light of longer wavelengths. A portion of this light is collected through the same sapphire window. UVOST, ROST, or SCAPS excite at various ultra-violet excitation wavelengths including 266nm, 290nm, and 308 nm (depending on model) and collects at 340, 390, 440, and 490nm. This method is used mainly for detecting polycyclic aromatic hydrocarbons (PAH) in light non-aqueous phase liquid (LNAPL), that include various fuels, oils, and other light to medium viscosity petroleum products. TarGOST excites at 532 nm and collects at 532, 582, 632, and 682nm, and is used exclusively on former manufactured gas plant and creosote wood treatment sites (Grundl et al., 2003). Before each LIF direct push, a standard or reference emitter is placed in front of the laser's sapphire window. Results are presented as percent of this standard's fluorescence.

Applied Research Associates (ARA) produces a device called the Fuel Fluorescence Detector (FFD) (Haas, 1999). This device operates in a very similar manner to LIF devices, with the exception of emitting ultraviolet light at a wavelength of 254 nm for analyte excitation and detecting with dual PMTs tuned to different wavelengths for differentiation between LNAPL and DNAPL. LIF does collect on 4 channels so it may differentiate better than the FFD.

Dakota Technologies is also researching the use of a downhole halogen specific detector (XSD) or, more specifically, a halogen-containing hydrocarbon detector. This device also hypothetically can be set to record on a one inch interval.

Geoprobe developed the membrane interface probe (MIP) as a means to carry out continuous subsurface contaminant probing using the flame ionization detector (FID), photo ionization detector (PID) and electron capture detector (ECD) in a manner consistent with direct sensing methods where a measurement is logged every one centimeter or one inch.

A hand held version of the cone penetrometer test (CPT) was originally developed to determine ground stability for roads, bridges and related structures. Subsequently the CPT was moved to a

large direct push vehicle. This device provides data that correspond to sediment lithology and can be used to delineate sand and clay lenses and other subsurface material such as peat.

LIF, FFD, XSD, MIP and CPT are all considered subsurface direct sensing instruments and theoretically should be able to provide vertical logs in the one inch resolution range. However, these devices are specific to certain analytes, where one device in a certain situation may provide more reliable data compared to another. For example, LIF will not respond to BTEX fluorescence where FFD may, but 532 nm LIF will respond to coal tar and heavy weight aromatic fractions where FFD may not. Calibrating MIP may be easier than LIF and FFD, but it usually operates at a slower pace than LIF.

An added benefit of using DSI is that 3-D geostatistical models can be updated continuously in real time while in the field, versus TSM alone where sample analysis is of low resolution and can take days or even weeks to be processed (EPA, 2003). Thus by guiding sampling through model uncertainty, one would want to sample in a manner that would effectively and efficiently minimize model uncertainty with budget constraints a priority. One major goal of sample designs is to locate regions of high free phase contaminant concentrations, which are ultimately the source zone of dissolved phase ground water pollution.

There are three main subsets of sample placement design under which a sample plan can be executed. The first method is the "*Simple Random Sampling Method*." This method uses no normalized spacing or professional judgment to determine its regularity. This randomness can be achieved with a computer or by hand. The second method is "*Judgmental Sampling*" which is determined by a field specialist or site manager and is based on a gut feel or professional opinion of where the next sample should be taken. The third method is "*Systematic or Grid Sampling*" in which sampling is regularly spaced in either a hexagonal equidistant grid design or in a square or rectangular grid (EPA, 2003). Studies have shown that there is little difference in the prediction error between a hexagonal or square centered sampling grid (Webster and Oliver, 2001). For this reason, a square centered grid was used for the ESS in this study, simplifying the virtual sampling effort at the different northing and easting densities of 100ft, 50ft, and 25ft.

DESCRIPTION OF THE STATE OR REGIONAL WATER PROBLEM INVESTIGATED

Morton County Site (Site M), ND Diesel Fuel Spill

In 1984, North Dakota state regulators became aware of significant source zone (SZ) groundwater contamination at a site in Morton County, where diesel fuel was uncovered at a construction project. At this site, 1.5 to 3 million gallons of diesel fuel had been spilled over a period of 50 years (Hostettler and Kvenvolden, 2002). Many different remediation efforts have been attempted at the site, including air-sparging, soil-vapor extraction, pump-and-treat, and a collector trench. It has been estimated that as of 2006 between 0.5 to 1 million gallons have been recovered (Anonymous, 2006). In 2003 laser induced fluorescence (LIF) analysis discovered that a considerable amount of diesel fuel remains at the site.

Watford City (Site WF), ND Mixed Contaminant Spill

This site is unique in that it appears to contain different contaminants ranging from gasoline, used motor oil, 1,2-dichloroethane, a chlorinated dense non-aqueous phase liquid (DNAPL), and brine. The impacted area is proximal to a municipal well and initial site assessments began in

1991, when 9 underground storage tanks (USTs) were excavated and some of them broke open, spilling used motor oil and other hydrocarbons. Remediation efforts in the past have included partial excavation. A LIF analysis done in 2005 and 2006 and a subsequent core sample and lab analysis show that the groundwater is still impacted by hydrocarbon based contaminants.

Two other sites were used as controls for this research. **Site S**, a synthetic gradational setting and **Site WT**, a coal tar impacted site in Codington County, SD.

SCOPE AND OBJECTIVES

Every year vast sums of money are used in the remediation of contaminated sites. Many investigators of these sites currently use traditional sampling methods (TSM), such as hollow stem auger coring, hand held PID, and laboratory analysis, to determine the source and extent of subsurface contaminant SZ. These methods are very time consuming and create large amounts of waste. Budget, spatial, and time constraints limit the number of samples that can be analyzed from a site. High resolution subsurface direct sensing instruments (DSI) should help reduce these limitations. This research project developed and applied an Earth System Simulator (ESS) to investigate the benefits of merging TSM and DSI in site characterization and management of three dimensional subsurface analyte distributions.

The main objective of this research has been to:

- 1. Characterize contaminated sites for use in the ESS using "real world" high resolution subsurface data and modern geostatistical theory.
- 2. Simulate site investigations with the ESS.
- 3. Complete a statistical analysis of simulation outcomes.
- 4. Produce a work flow for future site investigations.

MATERIAL AND METHODS

The ESS is similar to the Stanford V Reservoir Dataset (SVRD) simulator in that a three dimensional virtual sampling and characterization effort can be carried out (Gratwick and Rosales, 2000). The difference is that the SVRD simulator used bilinear interpolation to calculate values along a borehole trace, because in some of the cases the boreholes deviated from vertical, or were simulated horizontal wells as is now common in the oil industry. For the ESS, all logs were considered vertical so that all virtual logs could be taken directly from the three dimensional grid without any interpolation.

Steps in producing the 3-D Earth System Simulator (ESS) and methods of statistical comparison

The first step in the production of an ESS is to produce a three dimensional volumetric data distribution from borehole data in the form of measurement vs. depth. In the case of LIF logs, the measurement is uncalibrated fluorescence versus depth (FVD). This can be converted to area versus depth (AVD). The AVD is the final data to be submitted to a log processing database such as that found in Rockworks 2006. Rockworks 2006 is based on a Delphi database using Microsoft Access.

Digital DSI logs were gathered in EXCEL and exported to a file to be used in CTECH EVS, a geostatistical three dimensional modeling program. Using CTECH EVS an interpolation was carried out using ordinary kriging with X nodes = 60, Y nodes = 80, and Z nodes = 410. All nodes had a 5ft resolution in the X and Y directions and a 0.05ft resolution in the Z direction. For this simulator the 3-D grid dimensions were 400ft x 300ft x 21ft.

A completely synthetic grid was produced by diffusing BIC blue ink through porous paper using a solvent of 70% EtOH and 30% H_2O . These pieces of paper were scanned and the same number of nodes as the interpolated "real world" grids were extracted through digitization. The scanned images were imported into ArcGIS to create a three dimensional gradational distribution. This formed a gradient which appeared similar to effects observed in natural subsurface diffusion. The three dimensional distribution was smoothed in the Z direction using CTECH EVS to form a more natural gradient.

Using Surfer 8.0 or ArcGIS, three dimensional grid nodes of all three sites plus the synthetic grid were georeferenced to a common location, the Morton County site coordinates. Virtual logs were sampled from the grids using ArcGIS at predetermined XY locations to represent a horizontal spacing of 25ft. Sampling from the ESS at a 25ft spacing allows nodes of the three dimensional grid to be used as logs. Using a Rockworks Command Language (RCL) script in Rockworks 2006, logs were downsampled from 0.05ft using a distance weighted algorithm to 0.1ft, 0.3ft, 0.5ft, 1ft, and 5ft. resolutions.

Rockworks Code:		
PROJECT: C:\filemaker		
DEFINE: PDATA_EXPORT	SINGLE_LOG	False
DEFINE: PDATA_EXPORT	LOG_NAME	
DEFINE: PDATA_EXPORT	TRACK	re
DEFINE: PDATA	RESAMPLE	True
DEFINE: PDATA	DEPTH_INTERVAL	0.1
DEFINE: PDATA	RESAMPLING_METHOD	2
DEFINE: PDATA_EXPORT	DECIMALS	9
DEFINE: PDATA_EXPORT	OUTPUT_TYPE	0
DEFINE: PDATA_EXPORT	REPORT_NAME	$C:\filemaker\25ft10.txt$
DEFINE: PDATA_EXPORT	DELIMITER	9
DEFINE: PDATA_EXPORT	INCLUDE_TITLES	True
DEFINE: PDATA_EXPORT	EDIT_FILE	False
EXECUTE: PDATA_EXPORT		

HALT:

The downsampled logs were imported into ArcGIS and were reduced to 50ft and 100ft horizontal spacing for all logs at 0.1ft, 0.3ft, 0.5ft, 1ft, and 5ft. resolutions. Files were formed from the 25ft, 50ft, and 100ft sampling efforts for reinput into CTECH EVS, and kriging interpolations were carried out with resolutions equal to the downsampled log resolution.

Each sampled log data set has individual anisotropy. In general, three dimensional spatial data sets have anisotropy that can be relative to both three dimensional sampling intervals and concentration trends. For this research a mono-anisotropic value was calculated by dividing the orthogonal horizontal resolution by the orthogonal vertical resolution.

$$Anisotropy = \frac{XY_{res}}{Z_{res}}$$
(Equation 1)

Equation 1 worked well for this research because of the virtual systematic grid centered sampling carried out. Figure 1 shows the affect of not accounting for anisotropy in the data set. In the real world, logged data spacing is not regular, and generally this is true in all three dimensions. In these cases, determining approximate anisotropy may require the assistance of cross validation and three dimensional semi-variogram analysis (Jones et al., 2003). This is the most time consuming procedure of geostatistics. Anisotropy had to be entered into the software algorithm for each interpolation.



Figure 1. View of a 3-D source zone model facing North. The affect of applying improper anisotropy to a geostatistical model is apparent in the bottom model. Smooth shaded isosurfaces have a blocky columnar appearance. The top model had a proper amount of anisotropy applied.

CTECH EVS was then used to upsample the low resolution 3-D grids using linear interpolation. The final upsampled vertical grid resolution was 0.05ft in the vertical, so the grids could be compared to the original grid of equal resolution. Grids were exported to an ASCII text format, opened in Surfer 8.0 and a statistical comparison using Root Mean Square Error (RMSE) was carried out.

RMSE and cost values were input into Surfer to produce surfaces for each of the different models. The Z resolution of the interpolated models was designated as the X axis, the XY resolution was designated as the Y axis and the RMSE and cost values were designated as the Z axis for the surface graph. From this information, five two-dimensional surface graphs were formed. The first four were the model RMSE graphs and the fifth was the cost graph. The average of the four model graphs was computed, and this value was used to form a sixth graph. Standard deviation (SD) was produced from the four graphs to form error surfaces by adding and subtracting the SD from the mean surface.

A cost analysis was carried out by calculating the costs of the simulated sampling methods and resolutions. The TSM simulation used direct push coring with volatile organic compound (VOC) analysis done offsite. The DSI simulation used LIF resolutions that are usually collected between 0.05ft and 0.2ft. For this research, LIF resolutions were extended to 0.5ft and TSM resolutions ranged from 0.5ft to 5ft in the vertical.

Equation 2 was used to estimate LIF costs:

Total Cost of LIF = $((t_p + t_{jp} + t_{dg}) \times B \times C) + K$ (Equation 2) where: Total Cost of LIF = $((t_p + t_{jp} + t_{dg}) \times B \times C) + K$ t_p = pushing time per borehole t_{jp} = time to join pipe per borehole t_{dg} = time to drive between bore locations and grout per borehole B = number of boreholes C = Cost per hour for LIF K = Calibration cost per site (5 TSM bores with analysis offsite)

There are many different interpolation algorithms at the disposal of scientists and engineers. Among the most popular is the geostatistical kriging algorithm, of which there are many variants. Generally, ordinary kriging is carried out on point or block data. A prerequisite to kriging is that a sample semi-variogram (SV) be produced to which a function will be fit.

Sample Semi variogram

$$\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} (z_i - z_{i+h})^2$$
 (Equation 3)

Spherical Model Semi variogram

$$\gamma(h) = c_0 \left[\frac{3h}{2a_0} - \frac{1}{2} \left(\frac{h}{a_0} \right) \right]^3$$
 (Equation 4)

Equation 3 represents half of the summed variances of all values at a certain distance (h) from data point (Z). This is why it is defined as a semi-variogram instead of a variogram. The variable (h) is considered to be the lag distance. The sample semivariogram will then have a function or

multiple functions fit to it. This is called the model semivariogram. This function will be used to predict unknown values at nodes throughout a 2-D or 3-D grid (Keckler, 1995).



Figure 2. Model and sample semi variogram

The model semi-variogram in Figure 2 has three main variables associated with it: range, sill, and nugget. The range is the point where there is no more correlation between the data values. The sill correlates to the point where the semi-variance no longer changes given the maximum range. The nugget affect would be considered the y intercept of the function of the model semivariogram. This is generally used in cases where a large amount of quantifiable noise exists. With CTECH EVS, the nugget value is zero. Using a nugget value other than zero will smooth the interpolation.

A related geostatistical prediction approach is sequential gaussian simulation which at times is a better predictor for certain highly heterogeneous subsurface distributions such as porosity and hydraulic conductivity modeling (Webster and Oliver, 2001). For this research, ordinary kriging was carried out with a spherical model (Equation 4) (Copsey, 2007). All geostatistical methods available give a standard deviation which can be used to further calculate confidence and uncertainty (Webster and Oliver, 2001).

$$I_{obs} = \begin{bmatrix} XYZ_{1,1} \\ XYZ_{1,2} \\ \vdots \\ XYZ_{1,n} \end{bmatrix} \text{ and } I_{est} = \begin{bmatrix} XYZ_{2,1} \\ XYZ_{2,2} \\ \vdots \\ XYZ_{2,n} \end{bmatrix}$$

$$RMSE(I_{obs}, I_{est}) = \sqrt{MSE(I_{obs}, I_{est})} = \sqrt{\frac{\sum_{i=1}^{n} (XYZ_{1,i} - XYZ_{2,i})^{2}}{n}}{n}} \quad \text{(Equation 5)}$$

$$n = 2080161$$

$$NRMSE = \frac{RMSE}{Max RMSE} \qquad \text{(Equation 6)}$$

In the calculations, *XYZ* is used to define the nodes in 3D space. I_{obs} represents the ESS 3-D grid, and I_{est} represents the geostatistically estimated grid. The common Root Mean Square Error (RMSE) (Equation 5) value was calculated to quantify model accuracy (Jones et al., 2003). RMSE is the square root of the average of the squared differences between the original grid nodes and the predicted grid nodes. Squaring converts any negative difference into a positive number. The method is similar to that of Jones et al. (2003) in that a normalized (NRMSE) value from zero to one was used, with one being the highest RMSE attainable for a given model set. NRMSE is calculated using Equation 6. The difference is that Jones et al. (2003) used cross validation to calculate NRMSE values. This research resampled from a known grid in attempts to recreate the value distribution of that grid by means of kriging, and the final values were compared to the original or observed grid distribution values.

RESULTS AND DISCUSSION

Figure 3, produced from data presented inTable 1, shows that decreasing the vertical sampling resolution on Site S from 0.05ft to 0.5ft has little effect on NRMSE values when there is high degree of homogeneity. However, on average Figures 4 and 5 show that decreasing vertical sampling resolution from 0.05ft to 0.5ft greatly increases NRMSE values. An expected observation is that higher resolution data produce less error when delineating in three dimensions, heterogeneous source zones.



Figure 3. 25ft horizontal grid model NRMSE plots showing effects of degree of homogeneity on RMSE values.

Table 1. Simulation Data rest	ults
-------------------------------	------

Mode	l Res.	Site M		Site WF		Site WT		Site S		n urd t	
x (vert. res.)	y (horiz. res.)	z (RMSE)	z (NMRSE)	NRMSE Mean of 4 models	NRMSE Standa Deviation of ² models						
0.05	25	5.41	0.19	0.24	0.13	3.80	0.19	1.74	0.20	0.18	0.03
0.1	25	5.75	0.20	0.80	0.42	5.69	0.29	1.78	0.21	0.28	0.10
0.3	25	7.51	0.26	1.27	0.67	9.05	0.46	1.85	0.21	0.40	0.21
0.5	25	9.73	0.34	1.49	0.78	11.04	0.56	2.12	0.25	0.48	0.24
1	25	13.33	0.46	1.64	0.86	13.77	0.69	3.62	0.42	0.61	0.21
2	25	16.63	0.58	1.71	0.90	15.98	0.80	5.55	0.64	0.73	0.15
5	25	28.72	1.00	1.83	0.96	19.90	1.00	8.48	0.98	0.99	0.02
0.05	50	14.31	0.50	0.76	0.40	8.45	0.42	3.31	0.38	0.43	0.05
0.1	50	14.37	0.50	0.90	0.47	9.09	0.46	3.36	0.39	0.45	0.05
0.3	50	14.70	0.51	1.26	0.66	11.02	0.55	3.40	0.39	0.53	0.11
0.5	50	15.11	0.53	1.43	0.75	12.45	0.63	3.57	0.41	0.58	0.14
1	50	16.73	0.58	1.64	0.86	14.47	0.73	4.51	0.52	0.67	0.15
2	50	18.46	0.64	1.73	0.91	16.28	0.82	5.99	0.69	0.77	0.12
5	50	28.00	0.98	1.83	0.96	18.76	0.94	8.57	0.99	0.97	0.02
0.05	100	21.64	0.75	1.71	0.90	12.80	0.64	6.26	0.73	0.76	0.11
0.1	100	21.41	0.75	1.73	0.91	12.91	0.65	6.30	0.73	0.76	0.11
0.3	100	20.77	0.72	1.78	0.93	14.12	0.71	6.29	0.73	0.77	0.11
0.5	100	20.66	0.72	1.91	1.00	14.45	0.73	6.31	0.73	0.79	0.14
1	100	20.99	0.73	1.74	0.91	15.91	0.80	6.51	0.75	0.80	0.08
2	100	21.06	0.73	1.81	0.95	16.66	0.84	6.98	0.81	0.83	0.09
5	100	23.79	0.83	1.86	0.97	18.66	0.94	8.63	1.00	0.94	0.08



Figure 4. Normalized Root Mean Square Error (NRMSE) vs. horizontal and vertical sampling resolution with estimated costs overlaid. This surface graph was produced from the average of the 84 ESS geostatistical models.



Figure 5. Sampling scenarios with collection resolutions given as XY and Z in feet.

CONCLUSION

When accounting for SZ heterogeneity, increasing vertical sampling resolution from average TSM resolutions of 2ft to TSM calibrated DSI resolutions of 0.1ft, decreases NRMSE on average 40% or more while simultaneously reducing costs.

This research provides evidence that subsurface direct sensing instruments can provide a more cost effective and accurate solution to the characterization of subsurface groundwater NAPL contaminant source zones when calibrated with minimal traditional sampling versus traditional sampling alone.

REFERENCES CITED

- Anonymous (2006) Groundwork for Mandan's Future. Mandan Remediation Trust Report to the Community. www.cityofmandan.com/ Accessed Feb. 22, 2008.
- Bujewski, G. and Rutherford, B., (1997a) Site Characterization and Analysis Penetrometer System (SCAPS) Laser-induced Fluorescence (LIF) Sensor and Support System. (S. Billets, PO.) EPA/600/R-97/019.
- Bujewski, G. and Rutherford, B., (1997b) Rapid Optical Screening Tool (TM) Laser-induced Fluorescence System for Screening of Petroleum Hydrocarbons in Subsurface Soils. (S. Billets, PO). EPA/600/R-97/020.

Copsey, R., (2007) CTECH EVS Manual.

Crumbling, D.M., Griffith, J., Powell, D.M., 2003. Improving decision quality: making the case for adopting next-generation site characterization practices. Remediation. pp. 92-97.

- Gratwick, D. and Rosales, D., (2000) Seismic Velocity and Attribute Study Based On Well Interpolated Data, Stanford Exploration Project, Report 105, pp. 157–202.
- Grundl T.J., Aldstadt, J.H. 3rd, Harb, J.G., St. Germain, R.W., and Schweitzer, R.C., (2003) Demonstration of a method for the direct determination of polycyclic aromatic hydrocarbons in submerged sediments. Environ Sci Technol. Mar 15;37(6):1189-97.
- Haas, John W., (1999). Use of a Spectrometer with the Fuel Fluorescence Detector. Applied Research Associates, Vertek. South Royalton, Vermont.

Hostettler, F. and Kvenvolden, K., 2002, Studies of contaminated ground water yield new insights into degradation of diesel fuel. Soundwaves, August 2002. http://soundwaves.usgs.gov /2002/08/research.html. Accessed November 16, 2006.

Jones, N.L., Davis, R.J. and Sabbah, W., (2003) A comparison of three-dimensional interpolation techniques for plume characterization, Ground water 41 (4), pp. 411-419.

Keckler, D. (1995) The Surfer Manual. Golden, CO.: Golden Software, Inc.

- Okin, M.B., Carroll, S.M., Fisher, W.R., and St. Germain, R.W., (2006) Case study: confirmation of TarGOST laser-induced fluorescence DNAPL delineation with soil boring data. Land Contamination & Reclamation 14 (2), pp. 502-507.
- U.S. EPA, (2003) The DNAPL Remediation Challenge: Is There a Case for Source Depletion?, EPA/6000/R-03/143, (December) Ada, OK 111 p.
- U.S. EPA, (2000) DQO Guidance for the Data Quality Objectives Process (G-4). EPA/600/R-96/055. August.
- U.S. EPA, (2002) Guidance on Choosing a Sampling Design for Environmental Data Collection (QA/G-5S). EPA/240/R-02/005. pp 10-20.
- Webster, R. and Oliver, M.A., (2001) Geostatistics for Environmental Scientists, John Wiley and Sons, pp. 184-185.