FINAL REPORT

Forecasting Effective Site Characterization and Early Remediation Performance

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14. ABSTRACT
The DIVER Project (Data Information Value to Evaluate Remediation) has developed technical guidance on the value of data in both the site characterization and remediation contexts based on detailed site data, empirical evidence gathered from some of the most respected and successful practitioners in the field, highly detailed virtual site investigations, and stochastic approaches to quantifying both the value of additional information and optimal remediation designs. The overall research objective of the DIVER project is to develop a framework and associated methodologies for the optimization of the site characterization process, such that the life cycle cost of any remedy is minimized while remaining protective of human health and the environment.

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This project originated from many lengthy discussions over the years with colleagues working on Dense Non-aqueous phase liquid (DNAPL) impacted sites and searching for methodologies and strategies to improve decision making at various stages of the life cycle of a contaminated site and who were interested in developing virtual tools for teaching purposes. In response to the Fiscal Year 2013 (fy2013) Core Statement of Needs (SONs), we submitted a proposal to address several of the objectives established under the SONs including;

- *Development of field measurements or methodologies that provide predictive capability of performance to reduce the uncertainty associated with long-term performance so that decisions can be made early in the remedial process to avoid years of suboptimal operation.*
- *Development of assessment procedures and methodologies that aid in the decision to discontinue operation of a technology and implement an alternative technology.*

Our project, titled "Forecasting Effective Site Characterization and Early Remediation Performance", ER- 2313, (named "DIVER" or Data Information Value to Evaluate Remediation for ease of reference) formulated and tested a methodology designed to provide enhanced tools for decision making during several transition stages in conducting site remediation. The technical approach relied on the use of computer simulations of hypothetical releases of a chlorinated solvent (trichloroethylene), virtual site investigations by experienced based teams of remediation practitioners to characterize the site, and assessment of the effectiveness of remedial plans created by the teams and applied to the hypothetical sites, using the Enhanced In-Situ Biodegradation (EISB) technology, with outcomes simulated using a numerical remediation model developed at Queen's University under the direction of Dr. Bernie Kueper. Value of information analyses (VOIA) were used to compare the experienced based teams' outcomes to those generated virtually using "perfect data". The value of data was also assessed by simulations of remediation outcomes using the Stochastic Cost Optimization Toolkit (SCOToolkit) code generated in Strategic Environmental Research and Development Program (SERDP) project ER – 1611 and ER-2310. This comparison provided the basis to select the appropriate site characterization strategies for generating the most accurate CSM, that is, the development of effective practice for key parameters within a CSM. The overarching goal of DIVER was confirming the utility of a methodology applicable as a training tool and as a site decision tool based on defining best practices for CSM development at sites impacted by DNAPLs.

We wish to acknowledge the many contributions to this Report from each of the co-PIs on the project, including Dr. Kueper, and Dr. Kevin Mumford from Queen's University and our colleagues at Geosyntec, including Dr. Silvia Mancini, Sean Bryck, Dr. Cathy Crea, James Rayner, and Dr. Dave Major, all of whom contributed many ideas and content summarized in this report. We also wish to acknowledge the critical support from Dr. Peter Kitanidis from Stanford University, and Dr. Jack Parker and Dr. Ungtae Kim who assisted in the application of the most recent versions of the SCOToolkit, developed in SERDP Project ER-2310, that provided the basis for assessing the statistical value of additional site characterization data applied to remedial designs proposed by design teams who conducted virtual site investigations of several hypothetical sites. We appreciated the opportunity to collaborate on these topics.

We also acknowledge the participation of staff from five excellent consulting firms who were willing to engage in this experiment to undertake virtual site investigations and implement a remedial design of one technology in a manner that simulated actual practice, albeit with constraints on budget and time. We know these teams engaged in this research project with enthusiasm and willingness to take the risk of failing to achieve the desired outcomes when competing against computer simulations with access to perfect data generated at a scale impossible to duplicate with standard site investigation techniques. The firms represented include the following: (Ramboll, Golder Associates, CDM Smith, Patrick Consulting, and Haley and Aldrich). We thank them for their contributions to the effort.

Finally, our thanks to Dr. Andre Leeson for her support and patience as we explored unknown territory in a new virtual world that may someday be viewed as the early stages of enhanced computer simulations for more accurate decision making. Our overall conclusion, however, is that human decision makers (DMs) will prevail for many decades before the machines take over implementing site remediation.

Mike Kavanaugh and Dave Reynolds
Geosyntec Consultants

ABSTRACT

Objective: The DIVER Project (Data Information Value to Evaluate Remediation) has developed technical guidance on the value of data in both the site characterization and remediation contexts based on detailed site data, empirical evidence gathered from some of the most respected and successful practitioners in the field, highly detailed virtual site investigations, and stochastic approaches to quantifying both the value of additional information and optimal remediation designs. The overall research objective of the DIVER project is to develop a framework and associated methodologies for the optimization of the site characterization process, such that the life cycle cost of any remedy is minimized while remaining protective of human health and the environment.

Technical Approach: The project developed detailed, large-scale data sets through simulation, which acted as "sites" under investigation and remediation. These "virtual" sites provided the basis for assessment of "Experienced Based (EB)" and "Decision Theoretic (DT)" approaches to remediation design. The "sites" were investigated (virtually) by several decision maker (DM) teams, comprised of some of the most experienced and senior practitioners in the industry. The DM teams developed site investigation plans, followed by investigation of the large-scale data sets to produce site investigation data. The DM teams then developed CSMs for each site with a focus on selected quantitative parameters and developed remediation plans based on their CSMs to achieve pre-defined performance objectives. The CSMs and remediation performance were assessed against "true" values (known from the simulations) and optimal remediation designs based on this "perfect data". Effective practice for selected CSM parameters was then developed with stochastic modeling used to determine the value of additional site characterization information in reducing uncertainty in the accuracy of the parameters. In the DT approach, the CSM parameters developed by the DM Teams were used in a stochastic framework, where the most likely remedial design was identified through the minimization of cost functions given probabilistic distributions of the input data. The final stage of the project tested the validity of the proposed effective practice on another virtual site based on an existing Department of Defense (DoD) site where remediation performance has been found to be sub -optimal.

Benefits: This project will have the immediate benefit of improving remediation outcomes across the DoD, by identifying the key parameters which, through reduction of uncertainty, can lead to more cos t-effective and efficient remediation of DNAPL impacted sites. The project has also developed highly beneficial effective practice based on scientific principles that determine the value of data and the value of current site investigation practices, which in turn can be used by the DoD to assess the cost effectiveness of proposals and work plans submitted by contractors for applicable groundwater contaminated sites.

EXECUTIVE SUMMARY

Problem Statement

This project, titled "Forecasting Effective Site Characterization and Early Remediation Performance", ER- 2313, (named "DIVER" or Data Information Value to Evaluate Remediation) formulated and tested a methodology designed to provide enhanced tools for decision making during several transition stages in conducting site remediation. The overarching goal of DIVER was confirming the utility of this methodology for suitability as a training tool and as a decision tool for remedial decisions at any stage of a site life cycle, based on defining effective practices for CSM development at sites impacted by Dense Non-Aqueous Phase Liquids (DNAPLs) and within the context of application of Value of Information concepts for improving the efficiency of site investigations and the accuracy of CSMs.

An optimal site investigation is one that minimizes costs while maximizing the reduction in uncertainty in the estimated values of key site characteristics used to define the nature and extent of the problem (i.e., contributing to a fit-for-purpose CSM). Classical decision analysis theory involves the use of Value of Information Analyses (VOIA) approaches, whereby the value of a piece or pieces of information are determined in the context of making a decision. This allows a practitioner to decide if or what new information is of most value, thereby providing a basis for decision making on undertaking further investigations. Unfortunately, the highly heterogeneous characteristics of the geology, geochemistry and microbiology at most contaminated groundwater sites have limited the widespread use of VOIA for optimization of remedies as noted by the recent survey of remediation practitioners (Wilson, 2017). Thus, current practice for remedial decision making continues to rely on expert judgment, with an increased emphasis on more comprehensive CSMs

Overall Project Approach

The technical approach adopted in DIVER utilized computer simulations of hypothetical releases of the most widely chlorinated solvent found at DoD sites, namely trichloroethene (TCE), to create virtual sites that could be investigated virtually by experienced practitioner teams, to characterize each site, and develop Conceptual Site Models (CSMs) for each virtual site. The computer simulations where then used to assess the effectiveness of remedial plans created by the teams and applied to the virtual sites, using the Enhanced In-Situ Biodegradation (EISB) technology, using a numerical remediation model developed at Queen's University under the direction of Dr. Bernie Kueper. Simulated performance outcomes were then compared to the experienced based teams' outcomes to those generated virtually using "perfect data" and best practice design procedures. The value of data was also assessed by simulations of remediation outcomes using the Stochastic Cost Optimization Toolkit (SCOToolkit) code generated in Strategic Environmental Research and Development Program (SERDP) project ER-1611 and ER-2310. EISB was chosen as the remedy for the site based on its documented suitability for remediating TCE releases, availability as a remedy in SCOToolkit, and Decision Maker (DM) Team design experience with this technology. The effective practice recommendations were based on results of the virtual site assessments by DM Teams, stochastic assessment of the "perfect" data sets, and on industry experience and team knowledge on best practices for CSM development at DNAPL impacted sites. The utility of these revised strategies was then assessed through application of effective practice by new experienced based teams for a new virtual site.

The overall technical approach in the DIVER project is illustrated in Figure ES-1.

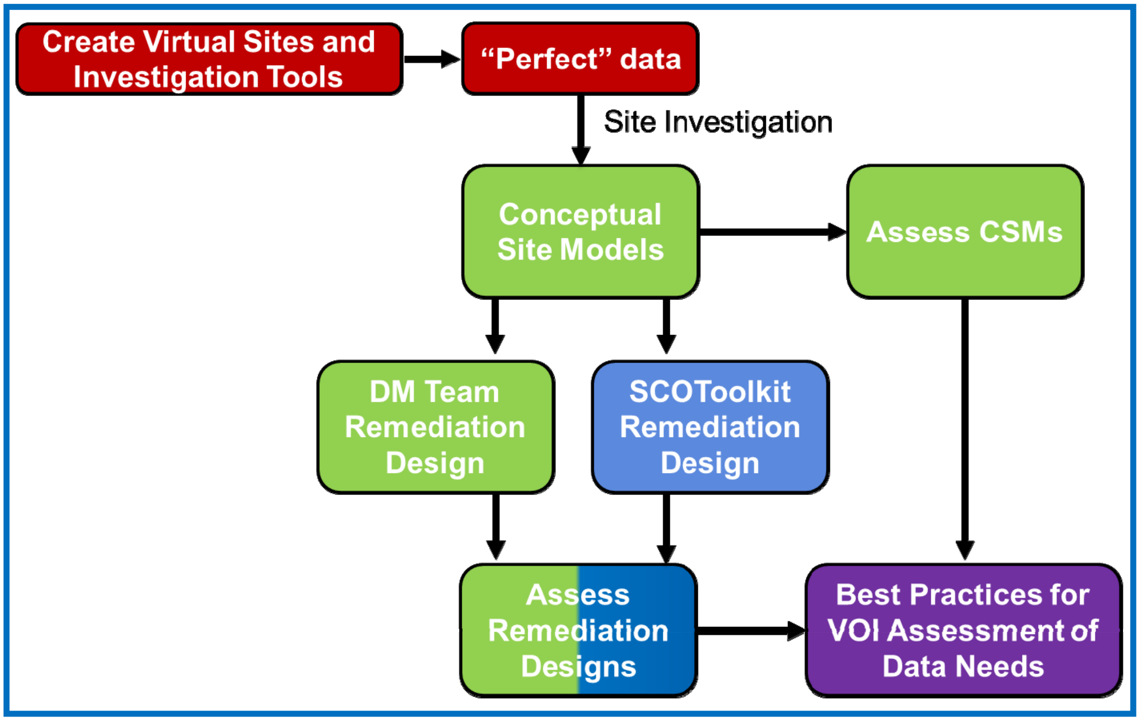

Figure ES -1: Conceptual Summary of Technical Approach in the DIVER project

Project Objectives

The specific objectives of the DIVER project were:

- Evaluate the use of various site investigation tools and approaches as chosen and applied by experienced practitioners in the industry to generate more accurate CSMs through the lens of Value of Information (VOI) considerations.
- Develop effective practices for characterization of complex sites (including DNAPL sites) that increase accuracy and decrease uncertainty in CSMs in scenarios common to challenging DoD sites.
- Quantify the value of additional information gathering for the estimate of some key parameters in CSMs.
- Compare and evaluate stochastic and deterministic approaches to remediation design based on a common CSM.
- Investigate the relationship between CSM deficiencies, remediation designs and remediation outcomes.

The project followed an adaptive strategy to the proposed technical approach which resulted in several distinct technical phases over the life of the project. These included the following:

1) Phase I - Project Infrastructure for Virtual Investigations
    a. Conceptual model creation for three hypothetical sites, translation to a numerical model, and creation of the foundational data for each virtual site (Virtual Site Datasets ("VSD"),
    b. Development of correlations for virtual investigation tools that could be used by DM Teams
    c. Selection of DM Teams and virtual interrogation of each site by the Experience Based (EB) approach,
2) Phase II - DM Teams CSM development, reporting and assessment (scoring) by DIVER Team
3) Phase III - Remedy design by DM Teams using an EB approach
    a. Numerical simulation, and assessment by comparison to optimal remedy design using perfect information by DIVER Team
4) Phase IV - Remedy design using Design Theoretic (DT) stochastic model by DIVER Team
    a. Model calibration, validation and assessment,
5) Phase V - Development of Effective Practices for improved decision making
    a. Assessment of utility of Effective Practices
    b. Applicability of VOI

Methods Summary - Phase I - Project Infrastructure for Virtual Site Investigations

The core of the DIVER project was a series of large-scale, high-resolution computer simulations of hypothetical DNAPL-impacted sites, using TCE as the representative DNAPL. The components of each hypothetical scenario in VSD1, VSD2 and VSD3 were based generally on the collective experience of the project team and were developed to represent different levels of complexity expressed through both the geological model and DNAPL distribution resulting from the hypothetical spill for each scenario. Following the development of VSDs 1 to 3, Phase I Environmental Site Assessment (ESA) reports were developed and provided to the DM teams.

Methods - Phase II - DM Teams CSM development, reporting and assessment (scoring) by DIVER Team

The EB virtual site investigation relied on the application of a series of virtual investigation tools by the DM teams to VSDs 1-3. Tools included were soil borings, conventional monitoring wells, CMT wells, membrane interface probe (MIP), hydraulic profiling tool (HPT), dye-enhanced laser-induced fluorescence (DyeLIF), slug tests, pumping test, hydrophobic dye test, various groundwater quality parameters, soil grain size distribution, and organic quality parameters for soil samples. Quantitative, qualitative and graphical parameters were used to evaluate the performance of the DM Teams' site investigation approaches extracted from reports documenting their CSMs. Costs for each DM Team's site investigation approach were estimated using documented unit costs of all components of the investigations including multiple virtual deployments.

Methods - Phase III - Experienced Based Remediation Design and Evaluation

DM teams designed their EISB remedies with the intent of meeting the functional Performance Objectives (POs) determined by the model simulations where the perfect information of each virtual site was known; these are referred to as the optimal remedies. These POs are defined as "technically achievable" within the timeframes that could be simulated and are not comparable to "absolute" objectives such as restoration goals (i.e., drinking water standards). The functional POs included performance parameters for the following: reduction in DNAPL mass, total VOC mass discharge and TCE concentrations at a location downgradient of edge of source footprint,

The total cost of remediation also included any costs associated with the optimizations or modifications to the initial remedy designs specified by requests from the DM teams. The total cost of remediation was calculated over the 5-year period of the EISB remedy in constant dollars.

Methods - Phase IV - Decision Theoretic Design and Evaluation

Remediation designs were optimized for VSD 1 and VSD 2 using SCOToolkit to assess the effects of increasing site characterization information on remediation strategy, success, and cost. The central component of SCOToolkit is a semi-analytical mathematical model used to simulate DNAPL source depletion and dissolved phase transport over time in response to natural and engineered conditions. The CSM data provided by the DM teams were used to calibrate the simulation model and to estimate parameter covariances and residual prediction error. Forward predictions of remediation performance and cost were performed for defined remediation strategies, operating rules, and remediation criteria. Stochastic design optimization was performed to determine values of remediation design variables that minimize the expected cost.

Methods - Phase V - Development of Effective Practices for improved decision making

DM Teams developed CSMs using virtual site investigative data and interpretation to determine specific qualitative and quantitative parameters. Some of those parameters, although commonly used, have limited effective practice guidance available and use is still evolving. The three CSM parameters that were amongst the least accurate across the DM Teams included a) Source zone footprint, b) DNAPL mass in source zone, and c) mass discharge/mass flux emanating from a source zone. Each of the above parameters was investigated by applying stochastic virtual sampling techniques to the perfect data from VSDs 1-3 with the goal of developing an effective practice for quantification as well as indications of the degree of uncertainty in the parameter estimate given a particular level of effort (e.g., how "close" can you expect to be to the actual DNAPL mass present after taking 100 "measurements").

Results - Phase II - CSM Scoring for DM Teams

Figure ES-2 presents the overall scoring for all DM Teams and VSDs for DNAPL mass and footprint (Figure ES-2a) and TCE plume mass and footprint (Figure ES-2b), with the true value at coordinate (1, 1). Estimates of DNAPL mass ranged from underestimates by a factor of 10 to overestimates by a factor of 5, and scores for footprint ranged from 0.12 to 0.87. Investigation strategies were more accurate for plumes than for DNAPL source zone parameters with dissolved TCE mass ranging from underestimates by a factor of 6 to overestimates by a factor of 2, while scores for the plume footprint ranged from 0.65 to 0.94.

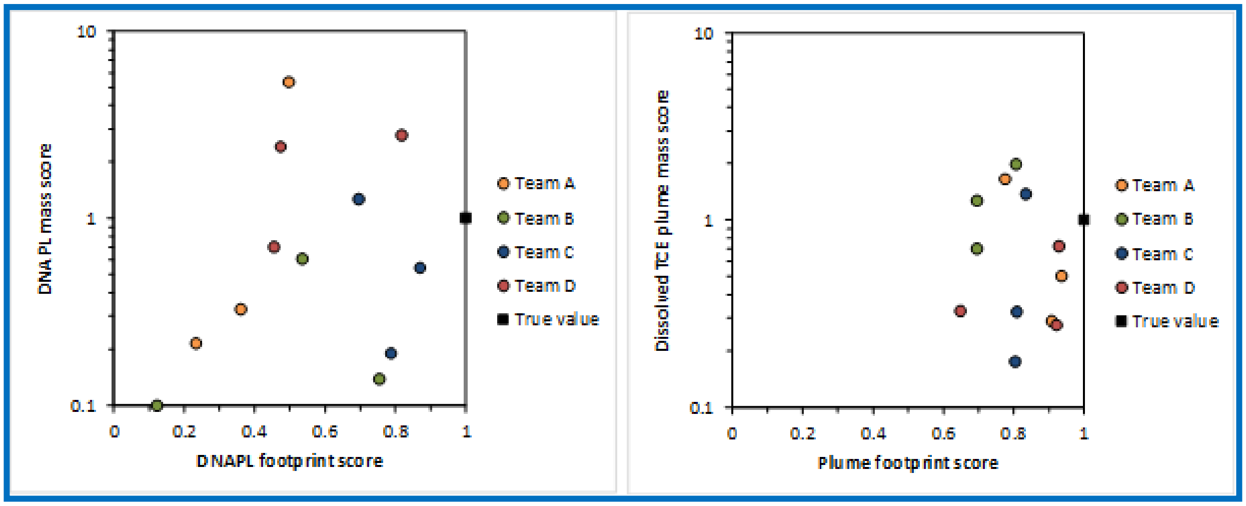

Figure ES -2: Scores for (a) DNAPL mass and DNAPL footprint, and (b) TCE plume mass and plume footprint for VSDs 1 to 3 based on the CSM reports from all DM Teams.

The cost of the virtual investigation conducted by each of the DM teams was tracked based on unit costs for investigation tool deployment, mobilization, and sample analyses and are shown in Figure ES-3.

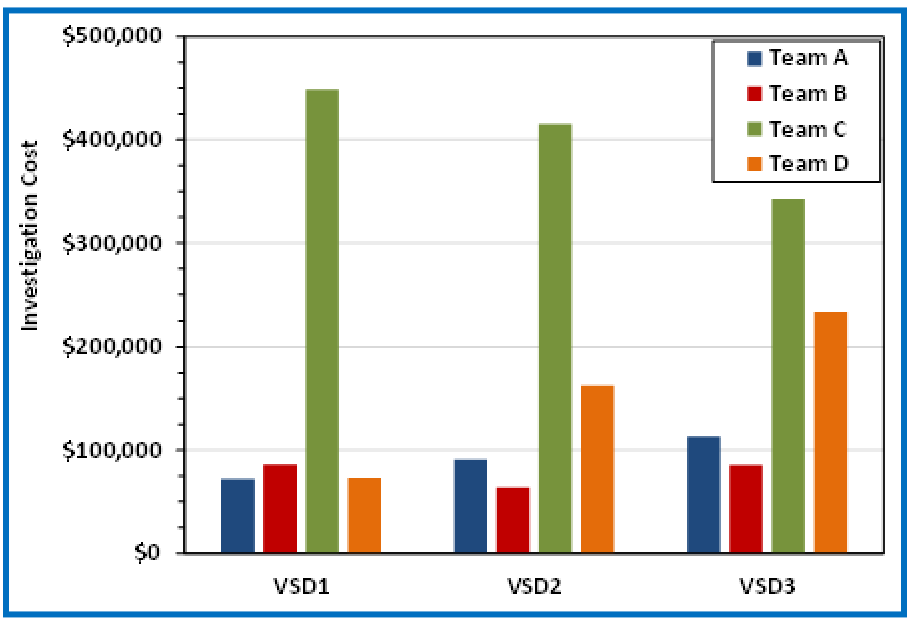

Figure ES-3: Investigation costs for each DM Team at VSDs 1 to 3

Of the 12 estimates of DNAPL footprint (DM teams A-D and VSDs 1-3) all three estimates by DM team C were in the top five most accurate, and all three estimates of plume footprint by DM team C were in the top seven most accurate. No other DM team showed that consistent accuracy over all three VSDs.

Results - Phase III - EB Design by DM Teams

The performance of DM team EISB remedies after 10 years for VSDs 1 to 3 was compared to the three POs identified by the DIVER Team. Only DM Team A achieved all VSD-specific POs primarily due to a very high factor of safety employed in remediation design (i.e., electron donor dose many hundreds of times larger than the stoichiometric dose) or through overdesign of the injection well system. Table ES-1 provides a summary of the performance of all DM teams for all VSDs including a comparison between the optimal remedy cost (based on using "perfect data") and the remedy costs resulting from DM teams designs and operations decisions.

Table ES-1: EISB remedy performance scores for VSD1, VSD2, and VSD3 evaluated 5 years following the conclusion of the EISB remedy. Green shading indicates a success at meeting the PO.

VSD1 Remedial Performance Objective	PO	Optimal	A	B	C	D
DNAPL Mass Reduction	30%	84%	64%	43%	41%	71%
Total Chlorinated VOC Dissolved Phase Mass Discharge Reduction	50%	75%	53%	-27%	25%	43%
Average Maximum TCE Groundwater Concentration Reduction	60%	62%	68%	2%	38%	37%
Total Cost of Remedy ($M)	--	1.75	3.36	1.29	1.34	2.38

VSD2 Remedial Performance Objective	PO	Optimal	A	B	C	D
DNAPL Mass Reduction	25%	58%	63%	36%	53%	73%
Total Chlorinated VOC Dissolved Phase Mass Discharge Reduction	50%	53%	88%	-38%	49%	73%
Average Maximum TCE Groundwater Concentration Reduction	50%	64%	91%	-8%	21%	12%
Total Cost of Remedy ($M)	--	1.49	6.34	0.81	2.25	2.48

VSD3 Remedial Performance Objective	PO	Optimal	A	B	C	D
DNAPL Mass Reduction	25%	48%	33%	16%	19%	68%
Total Chlorinated VOC Dissolved Phase Mass Discharge Reduction	50%	59%	83%	-38%	4%	-25%
Average Maximum TCE Groundwater Concentration Reduction	50%	64%	90%	9%	0%	55%
Total Cost of Remedy ($M)	--	2.64	5.07	0.49	1.33	3.62

The EISB remedies implemented by DM Teams B to D failed to achieve all three VSD-specific POs at VSDs 1, 2, or 3. Of the 36 scored remedy POs, only 10 (83%), 4 (33%), and 4 (33%) DM team remedies achieved the DNAPL mass reduction, total chlorinated VOC dissolved phase mass discharge reduction, and average maximum TCE groundwater concentration reduction POs, respectively.

Results - Phase IV - Decision Theoretic Design and Evaluation

The results of the DT evaluation using the SCO-Toolkit highlighted several challenges using this model. Even for a site with low complexity/heterogeneity such as VSD1, this approach to model parameterization resulted in a poor match to observed data. Flow and transport modeling based on DM Teams CSMs predicted very different plume dimensions that reported. The uncalibrated flow and transport model (using priors estimated from access to perfect information) generated a plume that was a better match for observed data but still contained a degree of error. Identification of this inconsistency using simple analytical flow and transport modeling to check and/or refine parameter estimates against observed plume data would have resulted in improvements to the CSM before proceeding to design a remedy.

Model calibration to groundwater concentration data (to create the posteriors) altered the estimates of key flow and transport parameters. For example, use of a deterministic simulation using SCOToolkit resulted in incorrectly choosing MNA when active intervention was required.

The differences between the 3-D process-based numerical model used to generate the VSDs and the analytical averaged model used within SCOToolkit presented insurmountable obstacles to accurate decision outcomes regarding optimization of remedies. Field-scale variability in permeability, DNAPL saturation, and sorption, for example, present challenges that an analytical model struggles to overcome with the prior estimates (i.e., before calibration). For the sites in this work, the stochastic approach also struggled to find remedies to meet POs (achieved POs in 52% of realizations) even when given an accurate CSM based on access to perfect information. SCOToolkit is a powerful tool for optimization of remedy design at sites with long temporal datasets for many observation points. It is desirable for linear regression to have at least 5 times the number of calibration data points as calibration parameters. Given that SCOToolkit has up to 17 calibration parameters a minimum of 85 calibration points would be required (Parker et al., 2018). A numerical model that can account for spatial variability of key parameters is preferred if the level of site characterization can support developing such a model.

Results - Phase V - Developing Effective Practice

The DIVER VSDs provide a platform for stochastic assessment of each of the key CSM parameters without the high costs of actual field investigation. Each of these parameters was virtually investigated on VSDs 1-3 with the goal of developing an effective practice for quantification as well as indications of the degree of uncertainty in the parameter estimate given a particular level of effort (e.g., how "close" can you expect to be to the actual DNAPL mass present after taking 100 "measurements"). Figure ES-4 presents a comparison of DM teams for DNAPL source mass estimates in terms of the expectations based on using effective practice. The confidence intervals are based on a random selection of several borehole locations used to calculate the DNAPL Mass. None of the DM Teams used effective practice in calculating their estimates of DNAPL mass for VSD 1. In 3 of 4 cases, had the DM teams been using effective practice for calculating DNAPL mass, the estimate would have had a higher likelihood (>99%) of a more accurate estimate.

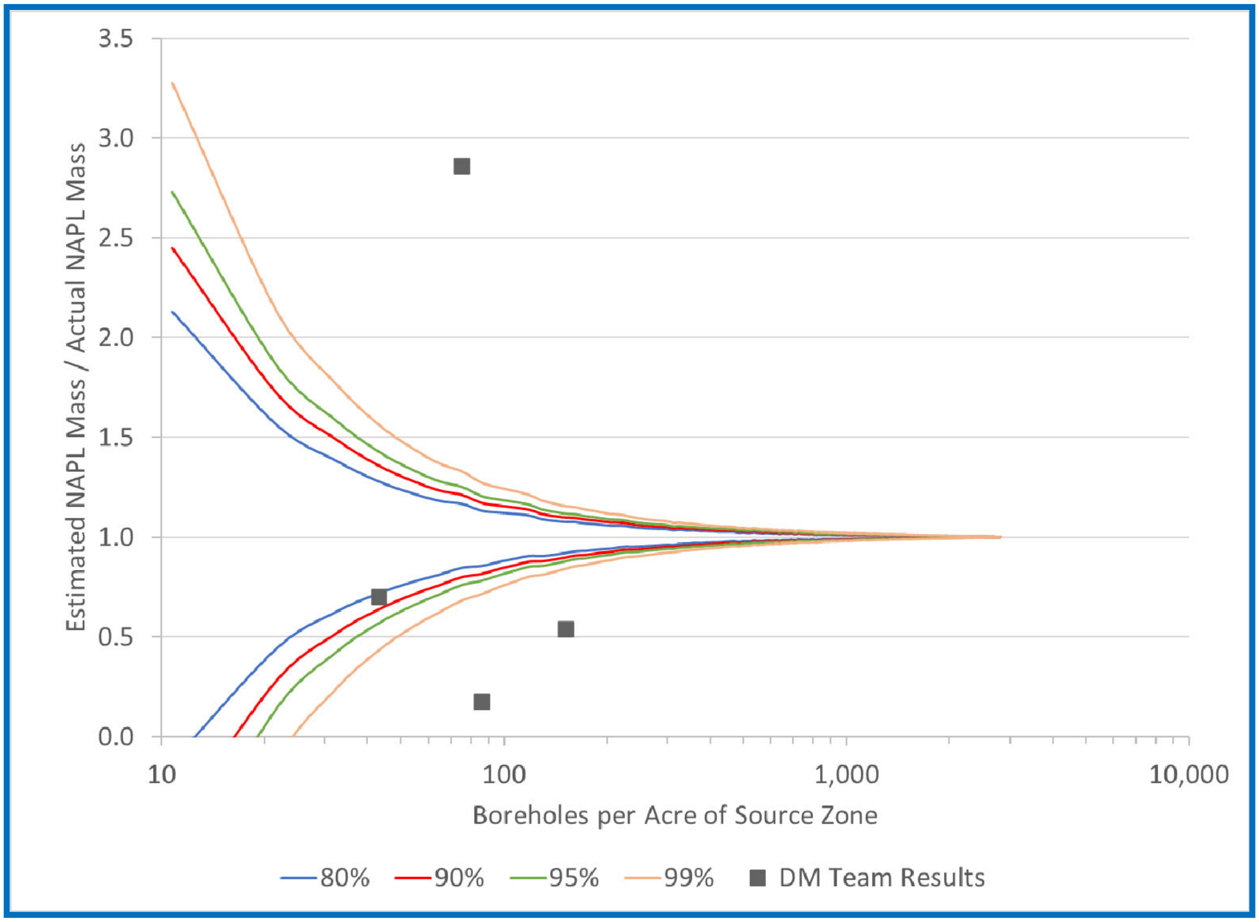

Figure ES - 4: DM Team DNAPL mass predictions for VSD 1 compared to the expectations using effective practice

The Effective Practice approaches developed during the project were tested by having the DM Teams develop CSMs for a new VSD 4 in a manner analogous to that used for VSDs 1–3. To increase the sample size, six additional DM Teams were selected for the verification process. A total of eight CSMs were submitted, and the results were assessed to determine if using effective practice led to improved parameters and lower costs.

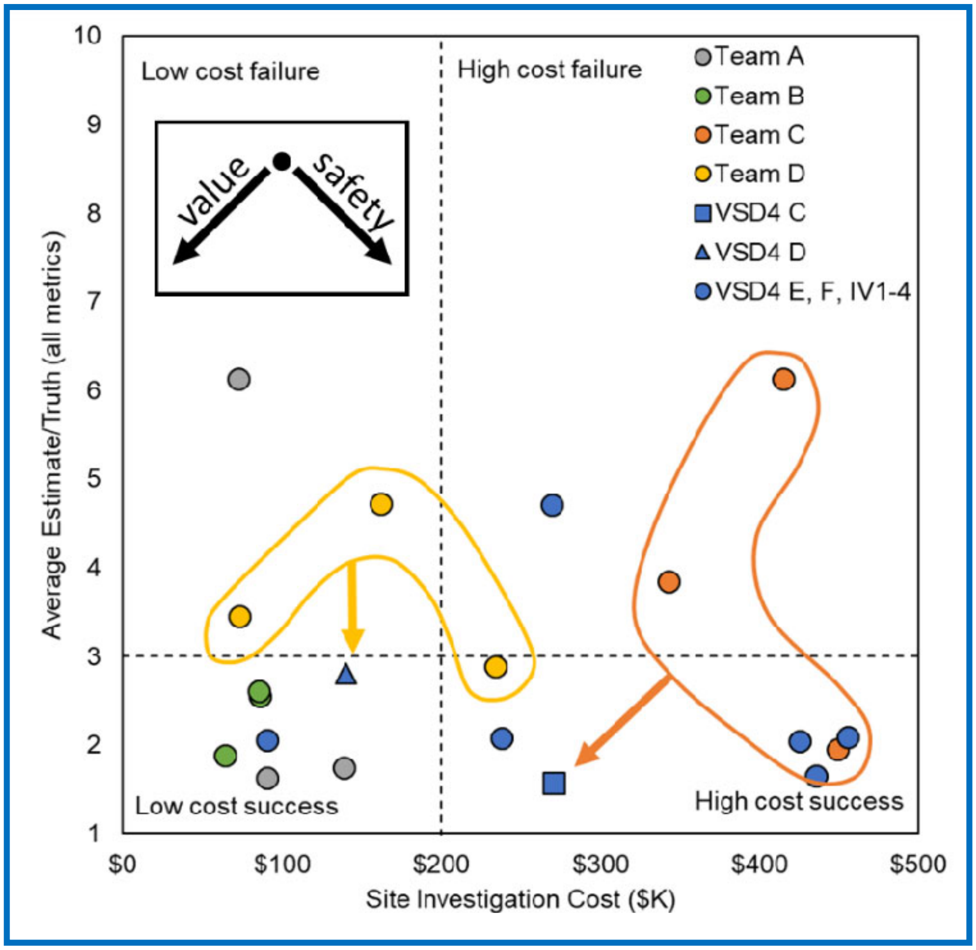

Figure ES - 5: Overall improvement under the "quadrants" approach

The differences in the overall accuracy and cost of the CSMs developed under effective practice are shown in Figure ES-5. Higher values on the vertical axis indicate an overall worse score on the CSM parameters. Combining the overall average parameter score with the total cost creates quadrants that define success and failure, and high and low cost on a relative basis. Using effective practice generally resulted in a translation down (greater accuracy) and to the left (less cost), particularly for teams that demonstrated lower accuracy in their VSD 1-3 CSMs. Deviations from this observation were due to interpretation errors made in following the effective practice guidance document by the new teams of DMs.

<u>Results - Phase V- Exploring Relationship between Site Investigation and Remedy Outcomes</u>

It is reasonable to assume that accuracy in site investigations should correlate to improved remediation success and lower remediation cost. A more accurate CSM should lead to better remedial decisions, less uncertainty in remediation design and reduction in both the life cycle cost and the likelihood of failure.

Figure ES – 6 compares site investigation costs and remediation costs across all VSDs and DM Teams and identifies individual data pairs based on the success or failure of the remediation design. Team B consistently spent the least for site investigation and remediation but in all cases, failed to achieve the POs. Team A on the other hand spent similar amounts as Team B on site investigation, significantly more on remediation, and achieved success meeting all POs for each VSD. Team C consistently spent the most for site investigation and significantly less than Team A on remediation yet achieved success in only 1 PO in two of the three VSDs.

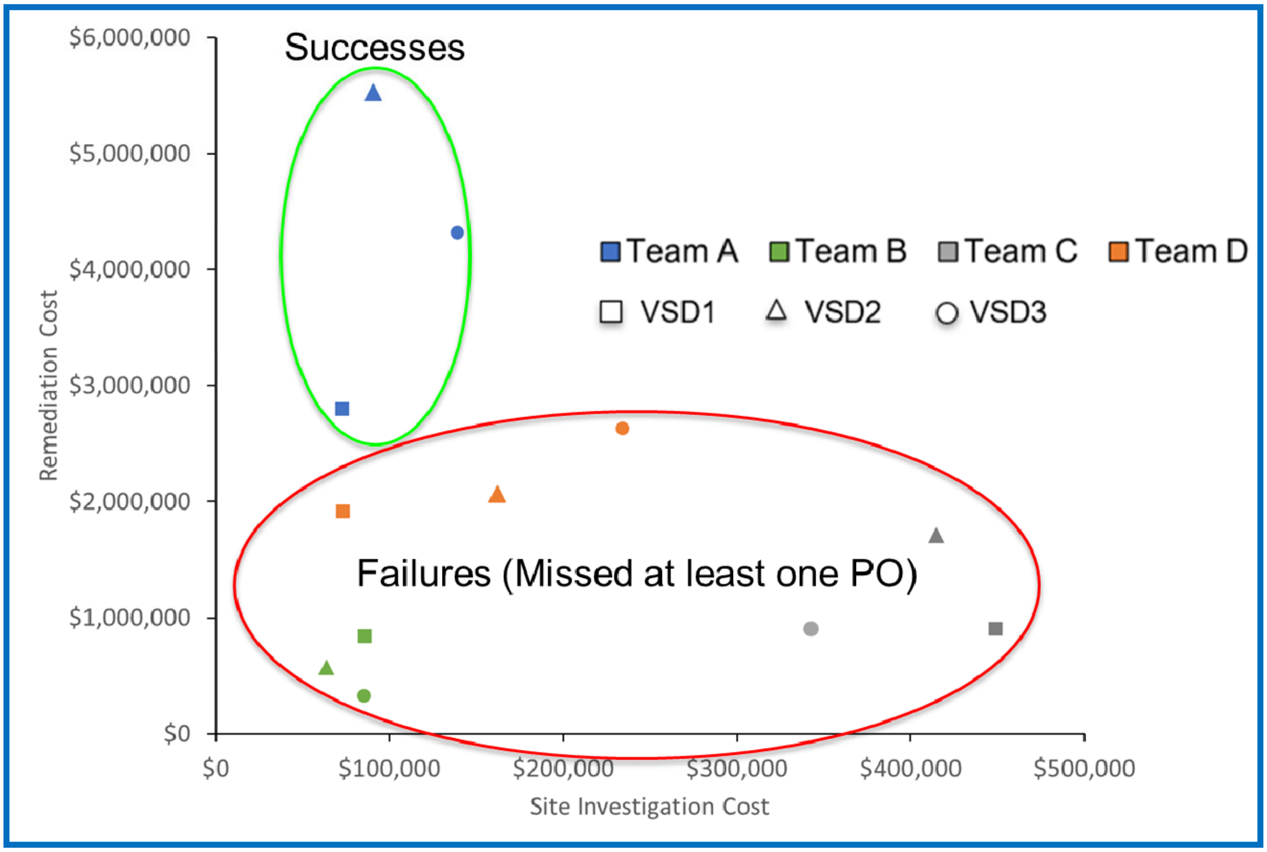

Figure ES – 6: Site investigation cost vs. remediation cost correlated to remediation success and failure

We evaluated each DM Team remedy in terms of its reason for failure, its overdesign to achieve success in some scenarios, and the benefit that could have been achieved through use of the effective practice derived for the key parameters (DNAPL Mass, Source Zone footprint, Source Mass flux/discharge). The primary reasons for remedy success were the use of either an overdesign of number of injection wells or the use of a very high safety factor for electron donor added, where the safety factor is defined as the lactate mass added by the DM team compared to the stoichiometric TCE DNAPL mass estimated by the DM teams in their CSM. Team A safety factors ranged up to 370, compared to industry experience of a factor below 50 for successful EISB remedies. Excessive electron donor dosing results in a more expensive remedy. In general, design failures resulted from several problems including a) insufficient electron donor, b) inaccurate source footprint, c) underestimate of source zone mass, d) missing a second source zone, e) inadequate number of injection wells.

For each of the DM Team's remediation designs and performance, five possible endpoints can be identified and are illustrated in Figure ES-7.

1) Success at reasonable cost (0 of 12 designs)
2) Success at excessive cost (3 of 12 designs)

3) Failure based on bad interpretation of good data (4 of 12 designs)
4) Failure due to poor CSM (5 of 12 designs)
5) Design failure (0 of 12 designs)

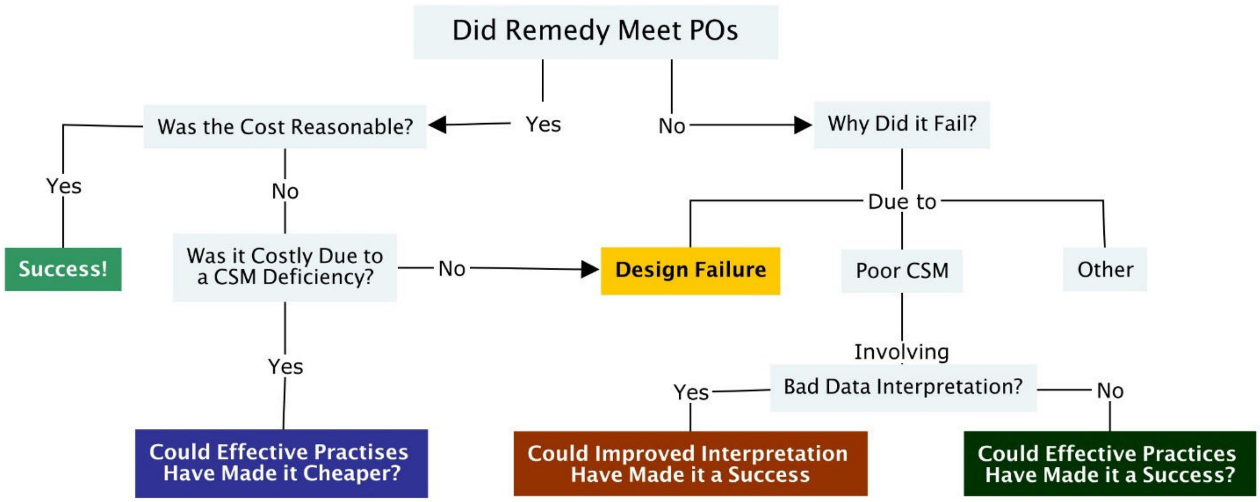

Figure ES - 7: Flowchart illustrating assessment process for DM Team remedies

To assess the benefit that could have been achieved through use of the effective practice derived for the key parameters (DNAPL Mass, Source Zone footprint, Source Mass flux) in terms of successful outcomes, we undertook an evaluation of some DM teams' strategies and outcomes and then assessed whether the effective practice approach developed in the DIVER project for source zone footprint could achieve cost reduction while still meeting the POs and to link conclusively the excessive cost to the errors in one or more of the key CSM parameters.

Each of the remedies proposed by Team A was examined in detail as examples of the "Could effective practices have made it cheaper?" endpoint given that POs were met in all cases. Table ES – 3 summarizes the cost and achievement of each of the remedies compared to the optimal (achieves the three POs at lowest cost) design based on access to "perfect information".

Table ES -3: Comparison of Team A remedies to optimal remedies

VSD	Team	Cost	DNAPL Mass Reduction	Total VOC Dissolved Phase Mass Discharge Reduction	Average Maximum TCE Groundwater Concentration Reduction
VSD 1	Team A	$3.36M	64%	53%	68%
	Optimal	$1.75M	84%	75%	62%
VSD 2	Team A	$6.34M	63%	88%	91%
	Optimal	$1.49M	58%	53%	64%
VSD 3	Team A	$5.07M	33%	83%	90%
	Optimal	$2.64M	48%	59%	64%

Each of the three "success at excessive cost" end points for DM Team A for all VSDs was analyzed in detail by revising the CSMs based on use of effective practice to estimate the CSM source footprint and

DNAPL mass parameters. The remedy designs were modified by adding additional injection wells to newly "discovered" areas of the source zone and scaling the lactate mass to the new DNAPL mass estimate. In all cases POs were achieved at lower remedy costs, (Table ES - 4) demonstrating positive return on the additional investigative costs.

Table ES - 4: Remediation return on investment of site investigation costs

VSD	Team A Designed Remedy Cost	Additional Investigation Cost Using Effective Practice	Revised Remedy Cost Considering Effective Practice Information	Remedy Cost Savings	Return on Site Investigation Investment
1	$3.36M	$0.45M	$2.31M	$1.05M	1.3x
2	$6.34M	$0.20M	$2.53M	$3.81M	18.0x
3	$5.07M	$0.25M	$3.46M	$1.61M	5.4x

Summary of Findings

Phase II – DM Teams CSM development, reporting and assessment (scoring) by DIVER Team

1. The original four DM Teams engaged in the DIVER project used a wide variety of site investigation tools and approaches to gather data for the generation of their CSMs. The DM Teams tended to follow similar approaches and use similar tools (within each team) across the three VSDs. Even when presented with alternate approaches for estimating a parameter of a CSM (effective practice) the DM Teams did not uniformly adopt the practice, but rather attempted to incorporate some aspects of effective practice into their existing approaches.

2. Most (92%) of the twelve quantitative CSM metrics were within a factor of 10 and 64% were within a factor of 3 of the true values, and both over- and underestimates of most metrics were reported.

3. Estimates of plume footprint were often more accurate than estimates of DNAPL footprint, and a higher accuracy footprint did not necessarily result in a higher accuracy estimate of mass for either the plume or DNAPL source, confirming that both the investigation strategy and the approach used to interpret the data are important in developing an accurate CSM.

4. None of the site investigation approaches resulted in a high accuracy for all CSM metrics, and the development of best practices will likely require the incorporation of elements from multiple approaches used by the DM teams as well as the results of the stochastic analyses presented in this report.

5. The most common error, leading to inaccurate delineation of source zone distribution and the subsequent inaccurate estimate of source mass, was the use of qualitative tools in a quantitative manner, e.g., attempting to correlate MIP readings to dissolved concentrations, as an indicator of the presence of NAPL, or to estimate CVOC soil concentrations. The use of MIP to delineate plumes, however, was appropriately done by the DM Teams.

6. Other analysis errors included extrapolating DNAPL saturations (pooled versus residual) over large soil volumes based on borehole log notations.

7. Most of the DM Teams (except for DM Team C) did not collect what experience and effective practice indicates would be enough data to develop sufficiently accurate interpretations and estimations of key CSM parameters.

8. No evidence was found that the DM Teams used the concepts of Value of Information in planning their investigation approaches.

9. The wide-ranging approaches (and relatively mixed outcomes) taken by the DM Teams to developing estimates for key parameters of the CSMs indicate there is no widely accepted standardized approach or effective practice in the industry for several key parameters needed for development of an accurate CSM.

Phase III - Remedy design by DM Teams using an EB approach

1. The exploration of the correlations and relationships between CSM costs/accuracy and remediation costs/success (in the context of life cycle costs) demonstrated there was no relationship across Teams and VSDs, and any general conclusions are limited by large factors of safety applied by some Teams to the EISB remediation design (that overcame errors in CSM parameters) as well fundamental errors arrived at through application of investigation or analysis approaches that are not considered effective practice leading to inaccurate CSMs.

2. The most critical finding in terms of source zone footprint is that using effective practice provides a primary line of evidence-based estimate at reasonable cost which was superior (in terms of cost and/or accuracy) to the estimates from the DM Teams.

3. Of the 36 scored remedy performance objectives across VSDs 1 to 3, only 10 (83%), 4 (33%), and 4 (33%) DM team EISB remedies achieved the DNAPL mass reduction, total chlorinated VOC dissolved phase mass discharge reduction, and average maximum TCE groundwater concentration reduction POs, respectively.

4. For the EISB remedy implemented in this project, poor estimates of DNAPL mass and source zone footprint were directly linked to failure to meet POs following remedy implementation. Other CSM deficiencies such as inaccurate values of groundwater velocity, plume age, and source zone mass discharge were also linked to some failures of the DM team remedy.

Phase IV - Remedy design using DT stochastic model by DIVER Teams

1. During model calibration with SCOToolkit, significant changes from priors to posteriors were observed for many parameters (Section 5.3.2), indicating the inadequate nature of the priors, that is, inaccurate estimates of key CSM parameters. In addition, the parameter changes during calibration were, in most cases, still not enough to allow SCOToolkit to find a realistic optimized remedial design.

2. Improved descriptions of the distributions of inherently variable or uncertain parameters could have been obtained through integration of modelling approaches with CSM development, a path that would have required additional resources to support the Teams' efforts. Working under a fixed price contract may have limited the options for application of even simple modeling tools.

Conclusions

1. **The DIVER Project successfully created a virtual infrastructure that provided a digital environment capable of virtual investigations of hypothetical but realistic geological and contaminant distribution models.**

2. **The mixed outcomes by experienced practitioners of creating accurate CSMs for key parameters influencing design of in-situ technologies such as EISB reflected subsurface heterogeneity, insufficient density of subsurface testing, and some poor data interpretation.**

3. **Value of Information analyses showed that application of the effective practices developed in part from virtual interrogation of "perfect data" created for the project resulted in significant improvements in CSM accuracy for the parameter, DNAPL source mass, DNAPL footprint and source mass discharge.**

4. **Application of the SCO Toolkit proved problematic due to inherent limitations of using analytical models to simulate complex subsurface environments.**

   The stochastic approach using the SCOToolkit struggled to find remedies to meet POs (achieved POs in 52% of realizations) even when given an accurate CSM based on access to "perfect information". While parameter variability is considered by SCOToolkit, the spatial distribution of variable parameters, that likely contributed to the differences between the SCOToolkit and DIVER Team optimal solutions, is not. SCOToolkit is a powerful tool for optimization of remedy design at sites with long temporal datasets for many observation points. It is desirable for linear regression to have at least 5 times the number of calibration data points as calibration parameters. Given that SCOToolkit has up to 17 calibration parameters a minimum of 85 calibration points would be required (Parker et al., 2018). Furthermore, the usefulness of stochastic approaches cannot be expected to overcome inadequate or poor site characterization which usually results in inaccurate estimates of key CSM parameters and selection of inappropriate remedial actions.

5. **A small data set was the main constraint on developing the types of correlations that would be the fundamental basis of a general methodology for applying VOIA to remedial decision making.**

   While the DIVER project generated a very large amount of data considered as "perfect information" for four DNAPL release sites (i.e., four VSDs), the variability in the virtual investigation results did not provide sufficiently robust correlations between the level of data acquisition and the performance outcome of applying EISB to the problem. The VSD data sets, however, have significant value for generation of a larger set of correlations through use as a training tool, as presented in the related TEMPO project (ER-201566).

6. **For DNAPL impacted sites, applying effective practice for estimating DNAPL mass, source zone footprint, and mass flux from source areas will reduce life cycle costs and increase the probability of meeting POs and decrease the probability of failure of a remedy**.

   The primary error made by most DM teams was an inaccurate estimate of these three parameters, leading to either unsuccessful implementation of the EISB remedy, or an overly costly remedy with excessive amounts of electron donor (i.e., an excessive safety factor in design) as well as unnecessary injection wells. The effective practice method proposed here should lead to reduced life cycle costs at DNAPL sites.

7. **The assumption that a higher investment in site investigations would result in lower remediation costs proved unfounded.**

   It is generally perceived intuitively that more data will lead to a better outcome for remedial decisions. DIVER has shown clearly that more data will only lead to this outcome if the right tools are applied, and the data are properly evaluated with a focus on those parameters in a CSM that have the largest impact on remedial outcomes.

8. **Remedial decisions to address groundwater contamination fall in the category of "noisy" problems.**

   We found surprisingly little agreement between the various expert teams investigating four different "case studies", namely the four VSDs that formed the basis of the virtual investigations and the subsequent performance of the EISB technology. While the DM teams made some reasonable estimates of CSM parameters, only one of the DM teams succeeded in meeting all remediation POs in all three of the VSDs. This result is due in part to the heterogeneous nature of subsurface environments, and the non-random distribution of system properties. The same experts with similar levels of experience all arrived at very different outcomes analyzing the same problem, a characteristic of "noisy" decision problems (Kahneman et al., 2020), analogous to medical diagnoses. This clearly highlights the difficulties in developing correlations for algorithms that can be generalized using a small data set.

9. **VOIA has not been widely used by remediation practitioners for a variety of reasons. However, VOIA is a very powerful conceptual framework for decision making, even though the underlying statistical principles may be well beyond most practitioners.**

   In an ideal hypothetical future, it may be possible to predict more precisely the exact value of any additional site characterization data on the final outcome of any remedial pathway in a complex decision tree model identifying the alternative combinations of technologies. This would require accurate models at an appropriate scale of the underlying geology and hydrogeology, the rate of all biogeochemical processes controlling the fate of the chemicals of concern, distribution and speciation of those same chemicals over long temporal scales, and the rates of transformations for all applicable physical, chemical or microbially-mediated processes in the subsurface. This scenario is beyond current technical capabilities and requires such a massive amount of data that the likelihood of success is low. Alternatively, artificial intelligence and machine learning using large data sets of performance data for remedial technologies applied at many thousands of sites with similar chemicals could provide algorithms that would allow for computer simulations to make the VOIA component of decision tree models a common tool for remedial decision making. We consider the DIVER project as a very early-stage entry towards a more accurate basis for applying VOIA to the overall remedial decision framework.

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List of Acronyms and Symbols

A	Cross-sectional area
$A_{correct}$	Area of overlap between the estimate and the true
AFB	Air Force Base
$A_{incorrect}$	Area estimated that does not overlap with the true
ARAR	Applicable relevant or appropriate requirements
ASTM	American Society for Testing of Materials
A_{ta}	Area of false
A_{tp}	Area of true
cDCE	cis-Dichloroethene
CERCLA	Comprehensive Environmental Response, Compensation and Liability Act
CFB	Canadian Forces Base
CMT	Continuous multichannel tubing
CSM	Conceptual site model
C_w	Contaminant concentration
CVOC	Chlorinated volatile organic compound
DEP	Department of Environment Protection
Dhb	Dehalobacter
Dhc	Dehalococcoides
DIVER	Data information value to evaluate remediation
DM	Decision maker
DNAPL	Dense Non-aqueous phase liquid
DO	Dissolved oxygen
DOC	dissolved organic carbon
DoD	Department of Defense
DPT	Direct push technology
DQO	Data quality objective
DT	Decision theoretic
DyeLIF	Dye-enhanced laser-induced fluorescence
EB	Experience based
EC	Electrical conductivity
ECD	Electron capture detector
EISB	Enhanced in-situ bioremediation
ENV	Expected net value
ESA	Environmental site assessment
ESTCP	Environmental security technology certification program
ETH	Ethene
EV	Expected value
EVI	Expected value of information
f_{oc}	Fraction organic carbon
ft	feet
ft/yr	feet per year
gpm	gallons per minute

List of Acronyms and Symbols (cont'd)

g/L	gram per liter
g/yr	gram per year
GIGO	garbage in garbage out
FS	Feasibility study
HPT	Hydraulic profiling tool
ITRC	Interstate technology and regulatory Council
k	Intrinsic permeability
kg	kilogram
kg/m^3	kilogram per cubic meter
kg/day	kilogram per day
kg/L	kilogram per liter
kg/yr	kilogram per year
L	liter
L_{sz}	Length of true DNAPL footprint
m	meters
MC	Monte Carlo
MCL	Maximum contaminant level
Md	Mass discharge
m^2	meter square
m^2/s	meter squared per second
m/day	meter per day
mg/kg	milligram per kilogram
mg/L	milligram per liter
mL/g	milliliter per gram
mol/L	mole per liter
MIP	Membrane interface probe
MNA	Monitored natural attenuation
mV	millivolt
NAS	Naval air station
NCP	National contingency plan
NFA	No further action
nmol/L	nanomoles per litre
NPL	National priorities list
NR	not reported
NRC	National Research Council
ORP	Oxidation reduction potential
OSWER	Office of solid waste and emergency response
OU	Operable unit
Pa	pascal
PDF	probability density function form
PFAS	per- and polyfluoroalkyl substances
PFM	Passive flux meter
pH	Potential of hydrogen

List of Acronyms and Symbols (cont'd)

PID	Photoionization detector
PO	Performance objective
QA/QC	quality assurance and quality control
RAO	Remedial action objective
RE	Relative emittance
R_e	DM Team estimate
RI	Remedial investigation
ROD	Record of Decision
Rt	True value
SCOToolkit	Stochastic Cost Optimization Toolkit
$Score_c$	Score for graphical metric
SERDP	Strategic environmental science and technology program
SlnC	Natural log standard deviation of concentrations
S_{nw}	Non-wetting phase saturation
SON	Statement of need
SVOC	Semi-volatile organic compound
TCE	Trichloroethene
TEMPO	Training for environmental monitoring performance optimization
TI	Technical impracticability
TOC	Total organic carbon
UCL	Upper confidence limit
µg/L	microgram per liter
US EPA	United States Environment Protection Agency
UUUE	Unlimited use and unrestricted exposure
USCS	Unified Soil Classification System
VC	Vinyl chloride
VI	chromium
VOC	Volatile organic compound
VOI	Value of information
VOIA	Value of information analysis
VPI	Value with perfect information
VSD	Virtual site data
W_{sz}	Width of true DNAPL footprint
β	Indicator of pooled or residual DNAPL

1 INTRODUCTION

1.1 Nature of the Problem

Over the past four decades since the passage of the Comprehensive Environmental Response, Compensation and Liability Act (CERCLA) in 1980 (42 U.S.C. §9601 et seq. (1980) , the so-called "Superfund" statute, thousands of sites with contaminated soil and groundwater have progressed through a process of discovery, preliminary assessment, prioritization, characterization, risk analysis, selection of remedial technologies, and implementation of remedies designed to achieve site specific remedial action objectives (RAOs). The Superfund process is described in the National Contingency Plan (NCP) (EPA, 1990) updated by the United States Environment Protection Agency (US EPA) to establish a consistent methodology for addressing the management of sites from identification to closure for sites included on the National Priorities List (NPL). This methodology, with some modifications, has generally been adopted by state environmental agencies to address contaminated sites not included under the NPL sites managed within the Superfund Program (see e.g., New Jersey DEP, 2019).

While approximately 440 sites have been delisted from the NPL (www.epa.gov/superfund/deleted-national-priorities-list-npl-sites-state), and many non-Superfund sites have achieved some form of closure, with or without institutional controls, a substantial number of sites remain under active remediation and costs associated with those remaining sites may be large (NRC, 2013). In the portfolio of sites managed by the Department of Defense (DoD), despite ambitious goals to achieve "remedy complete" at 95% of the more than 39,000 sites (DoD, 2018), the remaining sites will demand continuing significant investment to achieve site closure.

In addition, the majority of NPL sites with significant groundwater contamination have not yet reached the general goal of restoration, defined as unlimited use and unrestricted exposure (UUUE) as required under CERCLA. EPA recently indicated that up to 17 of the NPL sites had achieved restoration and such successes are expected in the future as well (EPA, 2018). However, for the sites that have not yet been restored and contamination persists at levels that exceed applicable, relevant or appropriate requirements, (ARARs), specified for the contaminated medium of interest (e.g., soil, groundwater, surface water) the sites are subject to five-year reviews to determine whether the existing remedy is still protective of human health and the environment (OSWER No. 9355.7-03B-P). Although the pace of site discovery and listing of sites on the NPL has decreased since the early stages of Superfund, new sites are still being added and other sites are being identified, in some cases due to the discovery of new chemicals of concern, such as per- and polyfluoroalkyl substances (PFAS). A study completed for the National Research Council (NRC, 2013) indicated that there may be more than 120,000 sites in the U.S. where groundwater cleanup objectives have not yet been achieved. That report further indicated that a substantial portion of those groundwater contaminated sites may not achieve restoration goals in a reasonable time frame, a topic further recently assessed by the Interstate Technology and Regulatory Council (ITRC) (ITRC, 2017).

During the life cycle of a contaminated site, remedial decisions must be made based on limited data and information, given that costs of subsurface investigations are high. Thus, decision makers (DMs) are faced with a tradeoff decision between the extent of investigations and the level of accuracy desired for effective remedial decision making. This is a classic challenge of decision-making under uncertainty, a topic that has a long history and which still demands the attention of scientists, engineers and policy analysts on the optimum methods to use to reach decisions (NRC, 2009; Morgan and Henrion, 2007; Kahneman et al, 2016).

In the context of site remediation, decision making under uncertainty arises at key phases in the life cycle of a site, from initial discovery of the problem to achievement of closure. Data quality objectives (DQO) (EPA, 2006) can provide a road map for the characterization phase. EPA Guidance states,

> "*Use of the DQO Process leads to efficient and effective expenditure of resources; consensus on the type, quality, and quantity of data needed to meet the project goal; and the full documentation of actions taken during the development of the project.*"

Typical decisions in all phases of the life cycle of a site (e.g., preliminary investigations, detailed site characterization in a Remedial Investigation (RI), creating a conceptual site model (CSM), assessing the need for modifications to an existing remedy, establishing a performance and compliance monitoring program, supporting or confirming a closure recommendation) will include; a) sampling density i.e., the location and number of soil borings and monitoring wells, b) depth of these investigations, c) site physical, chemical and microbial characteristics, d) selection of the appropriate investigative tools, e) chemical analytes and quality objectives (e.g., detection limits, level of accuracy required, and f) frequency of sampling. A decision is then made whether the data are sufficient to address the specified data quality objectives associated with the particular phase of the site life cycle.

Once implemented, following completion of the feasibility study (FS), selection of a remedy, and remedial design phase, remedial technologies incorporated into the Record of Decision (ROD) are subjected to performance monitoring to determine time frames likely required to meet site RAOs. If achievement of these objectives appears uncertain or not achievable in a "reasonable time frame", a decision then must be made to determine whether the remedial strategy in the ROD requires modifications to improve the likelihood of achieving the agreed upon RAOs or whether the site is a candidate for waivers of achieving the ARARs, such as technical impracticability (TI) waivers (EPA, 1993). At the state level, other alternative strategies have also been considered in the context of technical limitations on achieving restoration goals (e.g., Deeb, R. et al, ESTCP, 2011).

At some point in the site life cycle, usually after one to two decades of operation of the remedy, and assuming that restoration of the groundwater has not yet been achieved, the remedy has been subjected to optimization of operations, and if restoration appears unlikely in a reasonable time frame, the site is a candidate for a transition assessment to determine the optimum long term management strategy (see for example, EPA, 2011; NRC, 2013). This strategy could include selection of additional remedial technologies, increased reliance on natural attenuation processes, and a long-term monitoring program to ensure continued elimination of human health or environmental exposures (NRC, 2013). All of these decisions may require additional site characterization efforts consistent with the increasing use of adaptive management strategies in addressing cleanup of the more complex contaminated sites (ITRC, 2017; EPA, 2018; EPA, 2020).

1.2 Decision Making Under Uncertainty

Decision making under uncertainty characterizes the human condition. All decisions, from trivial to historical must confront an uncertain future and the limitations of having imperfect or incomplete data characterizing the problem of interest. All such decisions thus pose a risk of failure and balancing the risks of the decision against alternative options captures the challenges in various fields such as human health risk assessment (NRC, 2009), public policy (Morgan and Henrion, 1990), medical decisions (Yokota, et al, 2004), financial investment decisions (Bernstein, 1996), and environmental decision making in general (NRC 2013b). In the context of engineering decisions such as the design of an in-situ remediation system designed to capture or remove subsurface contamination in groundwater, the risks of system failure due to uncertainty in site characterization can be addressed by applying site specific "safety factors" (see e.g., James & Gorelick, 1999). Depending upon the consequences of system failure, and the degree of uncertainty inherent to the site in question, such safety factors may lead to increased life cycle costs compared to less conservative design choices.

Conceptually, the decision-making process under uncertainty can run the gamut from relying exclusively on intuition based on experience to the use of highly data rich analyses using the most recent numerical models and high-powered computers. In "Blink", Malcolm Gladwell (Gladwell, 2005) relates the story of a war game simulation in the middle east between an experienced military veteran leading one team and the second team equipped with the full simulation computer tools of the Marine Corps. Relying on years of experience dealing with the chaos of war, the veteran's team used unconventional tactics and easily defeated the Marines relying on the use of computer simulations.

Experienced based decisions, however, may not always lead to an optimum outcome because of known human behavior dealing with various cognitive biases (Kahneman, Slovic, Tversky, 1982; Kahneman, 2011). Examples include over reliance on small data sets, improper rules of thumb, confirmation biases, and improper reliance on initial anchoring assumptions (anchoring bias). In addition, the nature of the problem may also present a high degree of uncertainty which can lead to excessive "noise" in the predicted outcome (see Kahneman, et al, 2020), that is, a higher degree of variability in predictions than would be expected based on the nature of the problem. Examples of "noisy" decisions identified by Kahneman and his colleagues include judicial sentencing decisions, medical diagnoses, personnel decisions, forensic science and forecasting. As we will see in the results of this project, environmental remediation decisions also exhibit characteristics of a "noisy" decision problem.

In the remediation context, the analyst is faced with several factors that increase the level of uncertainty for remedial decisions. Geologic properties such as hydraulic conductivity vary over several orders of magnitude at most sites over relatively small spatial dimensions. Multiple chemicals may be present in different phases or in the case of ionic constituents in various valence states. The geochemistry can be very complex and varies spatially and temporally. Finally, microbial population densities and species distribution can vary over short distances. In the context of engineering decisions at contaminated sites, a recent survey (Wilson, 2017) of decision tools used by generally experienced practitioners highlighted the dominance of intuition, rules of thumb, and expert opinions compared to the use of decision analysis tools and stochastic models, with experienced based methods used at least twice as often as more analytical tools.

Remediation professionals have evolved numerous strategies to reduce these inherent uncertainties in characterizing sites, creating more accurate CSMs and designing more cost-effective remedial systems. These have included emphasis on more effective sampling strategies such as the Triad approach (Crumbling, et al, 2001), the use of strategic sampling methods with the use of more diagnostic tools (EPA, 2010; EPA, 2018; ITRC, 2003) and more widespread use of high resolution characterization tools (ITRC, 2019; **https://clu-in.org/characterization/technologies/hrsc**). Improving the accuracy of a CSM demands investment in site characterization, but the balance between costs of the additional data and likely benefits in improved performance of a technology remains a site-specific challenge for practitioners. Impediments to finding the balance include resistance to spend money on more data and appropriately defining and limiting acceptable scopes of work under standard contracting approaches.

There is relatively little guidance on effective practice in relating site characterization decisions to the ultimate impact on the life cycle costs of the engineering design choices for the combination of remedial technologies selected or modifications of those technologies after performance assessment has been completed. These decisions represent an opportunity to evaluate the value of the information that can be obtained from improved or expanded site characterization. For example, some geostatistical analyses of data needs at Dense Non-aqueous phase liquid (DNAPL) sites suggest a high density of sampling of up to 8% of a transect area, to estimate accurately the mass flux of a contaminant at a point downgradient of a source area (Li and Abriola, 2007). The cost of such high-density sampling may not be justified if the data do not result in a comparable reduction in life cycle costs.

1.3 Value of Information Challenge

Selection of appropriate remedial options at groundwater contaminated sites to meet regulatory requirements in some time frame requires a balancing of many factors, as outlined primarily in the NCP. Each of these and other decision points in the site life cycle represents an opportunity to assess the value of information obtained. The decisions to undertake additional investigations could be subjected to an assessment of the benefits of the investment designed, generally, to reduce the degree of uncertainty in the multiple attributes included in a conceptual site model (CSM) leading to a more cost-effective remedy selection and design.

The subject of value of information analysis (VOIA) in the context of groundwater remediation has been explored by several research teams in the late 1980s and beyond. Examples include works by Allan Freeze and associates (Massman & Freeze, 1987; Freeze, et al, 1990; Massman, et al, 1991; Freeze, et al, 1992; Freeze & Gorelick, 1999) who applied VOIA concepts to groundwater remediation and decision analysis applied to several hydrogeologic problems. James and Gorelick (1994) used VOIA approaches on assessing the value of monitoring data to optimize a pump and treat system. More recent work by Parker, Kim, Kitanidis and others (Kitanidis, 1996; Parker, et al, 2008; Parker, et al, 2010; Park & Parker, 2005; Lee, et al, 2012), has applied VOIA analysis to optimization of groundwater remediation using a range of in-situ remedial technologies other than pump and treat. Norberg and Rosen (2006) presented a model for estimating the cost effectiveness and the optimal number of samples for characterization of soil in the remediation phase of a contaminated land project. Back et al (2007) summarizes the application of VOIA concepts to site characterization under various scenarios.

Successful application of the VOIA methodology rests on the reliability of several models of decisions that must be made. For groundwater remediation, sub-models needed for the VOIA analysis include: a) a geologic model of the subsurface, b) a model to predict the outcome of each remedial action under consideration, c) a cost benefit economic model, and d) an optimization model. The net benefit of the investments to obtain additional information, such as additional site characterization data, must be compared to the financial impact on the life cycle costs of the remedy, incorporating appropriate financial penalties should the remedy fail to meet cleanup targets (see Freeze & Gorelick, 1999 and other references discussed in Chapter 3).

Unfortunately, the highly heterogeneous characteristics of the geology, geochemistry and microbiology at most contaminated groundwater sites have limited the widespread use of VOIA for optimization of remedies as noted by the recent survey of remediation practitioners (Wilson, 2017). The degree of uncertainty usually encountered in key site attributes, such as the location and magnitude of the source(s) of the contamination, the presence of preferential pathways, and back diffusion phenomena, affecting fate and transport of contaminants in the subsurface limits the applicability of the sub-models needed to complete a theoretical based decision. Thus, current practice for remedial decision making continues to rely on expert judgment, with an increased emphasis on more accurate CSMs (see e.g., USEPA, 2011; Sutherson, et al, 2016; USEPA, 2017; New Jersey DEP, 2019).

Given expected high future costs associated with remediation of potentially a large number of sites with groundwater contamination where restoration in a reasonable time frame may be impractical (ITRC, 2017; NRC, 2013), better tools are needed to enhance successful outcomes compared to outcomes based primarily on expert human judgment for decision making under the degree of uncertainty encountered at most sites impacted by releases of hazardous chemicals and waste, particularly chlorinated solvents that represent the most widely found chemicals at Superfund sites (EPA, 2020).

1.4 Project Description

In the Fiscal Year 2013 (fy2013) Core Statement of Needs (SONs), the Strategic Environmental Research and Development Program (SERDP) of the DoD solicited proposals for applied research to address the need for improved assessment and optimization of remedial technologies designed to mitigate impacts of releases of chlorinated solvents to groundwater. Specific objectives of that solicitation, which were developed at the 2011 SERDP and Environmental security technology certification program (ESTCP) Workshop on Investment Strategies to Optimize Research and Demonstration Impacts in Support of DoD Restoration Goals include:

- Determination of which parameters or processes may be measured to quickly determine the feasibility of a treatment approach.

- Development of field measurements or methodologies that provide predictive capability of performance to reduce the uncertainty associated with long-term performance so that decisions can be made early in the remedial process to avoid years of suboptimal operation.
- Development of field measurements or methodologies that provide data to optimize treatment if current operations are not expected to meet performance objectives (POs).
- Development of assessment procedures and methodologies that aid in the decision to discontinue operation of a technology and implement an alternative technology.

In response to this solicitation, Geosyntec Consultants, Inc (Geosyntec), in collaboration with researchers from Queen's University, Kingston, Ontario, and from Stanford University, Stanford, California hypothesized that decision making in the context of uncertainty at contaminated groundwater sites could be significantly improved through development and testing of a methodology to enhance decision making at any phase in the life cycle of a site including the appropriate level of effort needed to create an accurate CSM. Accurate CSMs are the precursor to more cost-effective decisions affecting the life cycle costs of a site. While there are numerous guidance documents available defining what a CSM is and what information should be included (EPA, 2011; USCOE, 2012; ASTM,2014; NJDEP, 2019)), relatively little guidance is available to determine what level of investment will provide the greatest benefits for achieving more accurate CSMs, and accordingly, potentially more effective remedies at lower cost to the potentially responsible parties, or to society as a whole, addressing many orphan sites with a more cost effective strategy.

Our project, titled "Forecasting Effective Site Characterization and Early Remediation Performance", ER-2313, formulates and tests a methodology designed to provide inputs to decision making during several transition stages in conducting site investigation and remediation. The development of this methodology relies on a technical approach utilizing the following components: a) the use of computer simulations of hypothetical releases of a chlorinated solvent (trichloroethylene), b) virtual site investigations by experienced based teams of remediation practitioners to characterize the site and develop a CSM, and c) assessment of the effectiveness of remedial plans created by the teams and applied to the hypothetical sites, using Enhanced In-Situ Biodegradation (EISB) technology, and d) comparison of the team plans with predicted outcomes simulated using a numerical remediation model developed at Queen's University.

For ease of discussion, we have named the project "DIVER" or Data Information Value to Evaluate Remediation. The concept of "virtual site investigation" is premised on the generation of perfectly characterized sites through state-of-the-art simulation, and subsequent interrogation of the data via site investigation schemes proposed by experienced teams of remediation practitioners. VOIA are used to compare the experienced based teams' outcomes (CSM parameters described in Section 4.5) to those generated virtually using "perfect data". The value of data was also assessed by simulations of remediation outcomes using the Stochastic Cost Optimization Toolkit (SCOToolkit) code generated in SERDP projects ER-1611 and ER-2310.

The utility of these revised strategies was then evaluated (Section 6.2) through application of effective practice by new experienced based teams for a new virtual site. The effective practice document, included in Appendix A of this Report, contained recommendations based in part on the results of the virtual site assessments, and in part, based on industry experience and team knowledge on best practices for CSM development at DNAPL impacted sites.

1.5 Project Implementation

Project implementation progressed through five phases. In Phase I, project infrastructure was established including selection of the Design Teams (DMs), development of the virtual site investigation tools, creating the virtual sites with hypothetical spill scenarios, and developing secure computer interfaces to maintain separation between the simulated data and the data collected from virtual interrogation by the DMs. Phase II consisted of virtual site characterization efforts by the Decision theoretic (DTs), and generation of the "perfect" data sets for comparison to the CSMs prepared by the DMs. Phase III included the generation of remediation plans for the application of the EISB technology, modeling of the DM remediation plans, and comparison of the outcomes to simulated remediation based on use of the "perfect" data. Phase IV incorporated completion of a practitioner's guide, determination of the effectiveness of the revised site characterization strategies, and assessment of the value of data through use of the analytical model from the SCOToolkit. In Phase V, the results of the previous phases were integrated to provide proposed improved site characterization methodologies. Additional details on the individual phases are provided in later sections of this report.

2 OBJECTIVES

The SERDP SON for FY13 solicited proposals for applied research related to improved assessment and optimization of remediation technologies for treatment of chlorinated solvent-contaminated groundwater including how to determine (in a cost-effective manner) the performance limitations of a remedial approach. The overall research objective of the DIVER project is to develop a framework and associated methodologies for the optimization of the site characterization process, such that the life cycle cost of any remedy is minimized while remaining protective of human health and the environment.

The specific objectives of the DIVER project were to:

1) Evaluate the use of various site investigation tools and approaches as chosen and applied by experienced practitioners in the industry to generate more accurate CSMs through the lens of Value of information (VOI) considerations.
2) Develop effective practices for characterization of complex sites (including DNAPL sites) that increase accuracy and decrease uncertainty in CSMs in scenarios common to challenging DoD sites.
3) Quantify the value of additional information gathering for the estimate of some key parameters (source footprint and mass, source discharge, biodegradation rate) in CSMs.
4) Compare and evaluate stochastic and deterministic approaches to remediation design based on a common CSM.
5) Investigate the relationship between CSM deficiencies, remediation designs and remediation outcomes.
6) Assess remedial design optimization based on life cycle costs under conditions of inaccurate CSMs using a value of information approach.

The outcomes of the DIVER project will enable practitioners to make better decisions in site investigation and remediation design based on a better understanding of the value of information.

3 DECISION MAKING AND VALUE OF INFORMATION IN THE ENVIRONMENTAL CONTEXT

Site investigation and remediation design are processes where decisions are made (often the choosing between different alternatives) under conditions of uncertainty. Compared to more traditional science and engineering fields, contaminant hydrogeology investigation and design contains uncertainty in the system properties and conditions as well as uncertainty in the very geometry of the system under investigation. The decision analysis approach commonly used in engineering is based on an economic analysis of possible alternatives and considers the costs and benefits of each alternative but also the associated risks (Raiffa and Schlaifer 1959). Decision analysis has also been widely used in health care under conditions of uncertainty (Briggs et al. 2006). The considered risks within the decision analysis approach often reflect or contain elements of uncertainty and in the context of contaminant hydrogeology these uncertainties, and the risks associated with them are quite high.

Reducing uncertainty and the associated risks is often undertaken by the process of site investigation. Contaminated site investigations can, however, incur significant costs, and the benefits gained in terms of reduction of uncertainty are often difficult to quantify. An optimal site investigation is one that minimizes costs while maximizing the reduction in uncertainty in the estimated values of key site characteristics used to define the nature and extent of the problem (i.e., contributing to a fit-for-purpose CSM). Classical decision analysis theory involves the use of VOIA approaches, whereby the value of a piece or pieces of information are determined in the context of making a decision.

3.1 Value of Information and Decision-Making Basics

The fundamental principle of VOIA is to compare the benefit/cost at the present state of knowledge (current level of uncertainty) with the benefit/cost that is expected after an investigation has been performed (future level of uncertainty). As a simple binary decision example of VOIA, take a potentially contaminated site undergoing assessment for remediation ("yes" remediate or "no" leave as is). The expected value (EV) of the remediation project can be estimated from the benefits (B), the costs (C) and the risks (R):

$$EEEE = BB - CC - RR \qquad \textbf{[3-1]}$$

For most contaminated sites the failure costs (as opposed to capital costs) are often the most important risk consideration, which agrees with experience from other economic decision analysis models (Norman, 2004). The failure cost can be interpreted as the consequences if the decision is made not to remediate when the site is in fact contaminated. Such consequences can be long-term human health risks and environmental risks, as well as additional and unexpected remediation costs in the future, if the contamination is detected at a later stage.

In the simplest form of VOIA, some objective function is calculated for: (a) the present situation with no additional information supplied (prior analysis), and (b) the situation that is expected when sample information (data) becomes available (preposterior analysis). It is important to note that preposterior analysis is not performed with the actual additional site data but rather under the assumption of what the actual additional data will provide and the resultant expectation of the reduction of uncertainty.

The difference in total expected benefit (between prior and preposterior) is called the expected value of information (EVI), often considered as the worth of the collected data. "Ideal" data collection occurs at the maximum of the expected net value (ENV) which is the difference between the EVI and the cost of the collection of the data. It should be noted that preposterior analysis does not provide an update as to the decision, but only on the value of information. An update on the actual decision is performed with a posterior analysis after the data has been collected (Figure 3-1).

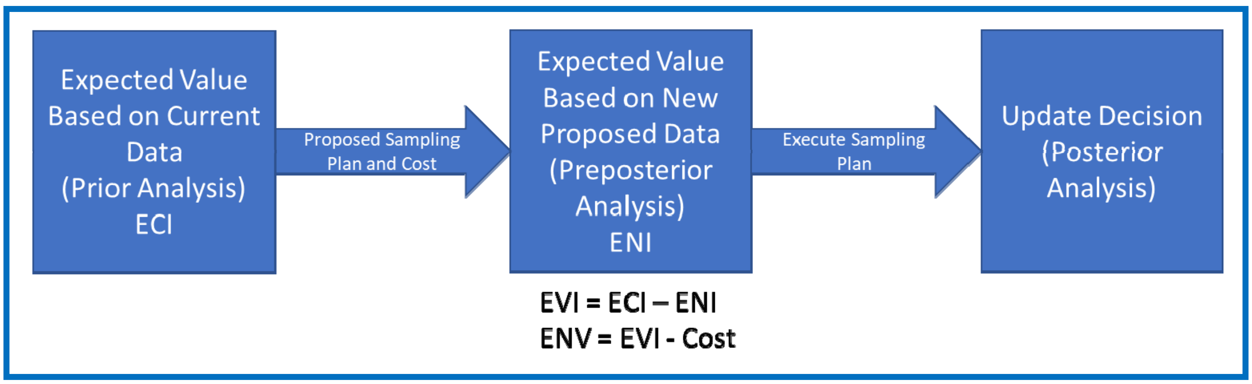


Figure 3-1: VOIA concepts

An upper bound will always exist on EVI, based on the EV of the objective function with perfect information. The upper bound to the possible worth of any proposed data collection is the difference between the EV with perfect information and the EV with current information (prior analysis). Understanding or deriving the EV with perfect information is challenging in most realistic scenarios, however the DIVER project provides a unique opportunity for exploring the concepts of EV with perfect information because within the framework of the virtual sites all information is known, and thus EVs with perfect information can be estimated.

To further illustrate the basic application of VOIA, consider three different scenarios (Figure 3-2) for the simple remediate/leave binary example (Back et al, 2007).

First, a situation where the cost of an incorrect decision (failure cost) is very low, i.e., close to the remediation cost (region A in Figure 3-2). The ratio of failure cost to remediation cost is therefore close to 1. This means that there is no significant difference in total expected cost if remediation is performed or not, therefore, there is no incentive to reduce the uncertainty. Consequently, the most cost-efficient strategy is to take only a few samples or even no samples at all because EVI is low (Figure 3-2).

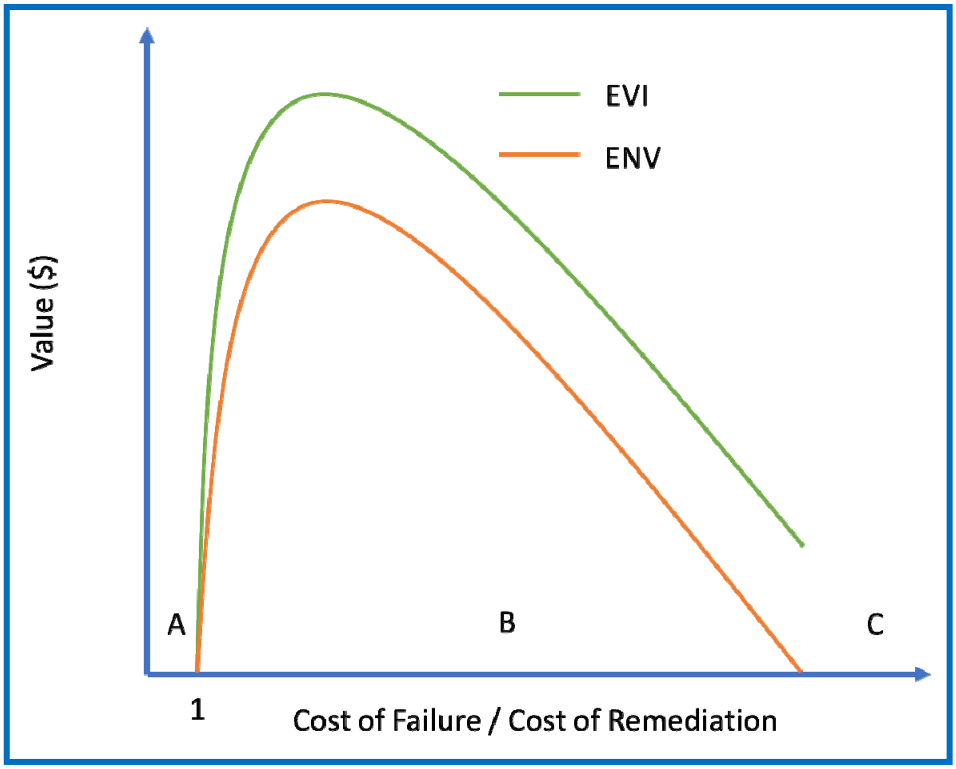


Figure 3-2: The expected net value concept

Secondly, imagine that the failure cost is higher than the remediation cost (region B in Figure 3-2). The wrong decision will now result in significantly higher cost than if the correct decision was made. Therefore, reduction of uncertainty by sampling is worthwhile. The sampling program is regarded as cost-efficient when ENV > 0, i.e., the value of sampling is higher than the cost of sampling. The optimal number of samples is found where ENV is the highest. This is the typical situation faced at contaminated sites.

In the third case the failure cost is orders of magnitude larger than the remediation cost (region C in Figure 3-2). The uncertainty must therefore be significantly reduced because making the wrong decision would result in large consequences. However, realizing a large reduction in uncertainty often requires extensive sampling at significant cost. In some cases, the sampling cost is so high that it cannot be compensated for by the reduced uncertainty (i.e., sampling cost for reducing the difference between the failure cost and the remediation cost by an order of magnitude is on the order of the remediation cost and ENV <0). Therefore, it is likely a better decision to remediate immediately, without spending money on a costly sampling program.

At first impression, this third case may seem unrealistic, but a car-owner comes to a similar conclusion every day when he arrives at home in the evening and locks the car. An alternative approach would be to leave the car unlocked and spend the night investigating if there are any thieves around. The high cost of investigation (lost sleep) and the limited data acquired for that cost (can't check every person) is unlikely to reduce the difference between prior and preposterior analyses and combined with the potentially high failure cost (lost car), the car-owner makes the more cost-efficient decision to lock the car instead. The same principle often applies to contaminated land if the consequence of leaving contamination in place is sufficiently high.

3.2 Using VOIA in the Context of Environmental Decision Making

The general concepts behind the use of VOIA in the context of environmental problems has been developed since the 1950s (Raiffa and Schlaifer 1959). Freeze et al (1990) developed a framework for the applications of decision analysis to engineering design for problems where hydrogeological analysis plays an important role. Freeze et al (1990) derived the objective function for a given alternative (e.g., different remedial approach) as:

$$\theta_j = \sum_{t=0}^{T} \frac{1}{(1+i)^t} \left[B_j(t) - C_j(t) + E_j(t) - R_j(t) \right] \quad \textbf{[3-2]}$$

Where θ_j is the objective function for alternative "j", Bj(t) are the actual benefits of alternative "j" in year "t" [$], Cj(t) are the costs of alternative "j" in year "t" [$], Rj(t) are the risks of failure of alternative "j" in year "t" [$], Vj(t) are the probabilistic benefits of alternative "j" in year "t" [$], "I" is the discount rate [-], and T is the time horizon [years]. The risks Rj(t) are defined as the expected costs associated with the probability of failure of alternative "j" in year "t".

An increase in the EV of the objective function is realized through a decrease in the risk term, and a decrease in the risk term is realized through a decrease in the probability of failure, and a decrease in the probability of failure often requires the acquisition of additional information at some cost. The key to the use of VOIA lies in accurate determination of the probability function which defines Rj(t) (and to a lesser extent Vj(t)) and linking the cost and reduction of uncertainty to the probability function which defines $R_j(t)$. The difficulties in the use of VOIA however, also lie in the probability functions, as approaches for defining the functions or the probability distributions are poorly understood and may be highly dependent on the variabilities of important parameters in hydrogeological analysis. For example, there is little in the literature on the likely distribution of source zone mass at a site (to allow for the accurate creation of a probability distribution) and the distribution itself is likely highly dependent on geology, release strength and duration, and time since release.

3.2.1 A Simple Example

Freeze et al (1992) provide an example of VOIA based on a new landfill scenario. The decision to be made is whether to install a liner in the landfill. There is an impermeable clay layer known to be present at the site that is sufficient to protect the underlying groundwater from the landfill leachate. The uncertainty revolves around the potential existence of a hole or window in the clay layer. If a window exists, then leachate reaches the underlying groundwater, and a failure state exists. It is easy to see that the prior probability of failure is 0.5 (the window either exists or it doesn't). A drilling program will either confirm the presence of a window, in which case the probability of failure becomes 1 and the liner will be the preferred design, or else it will not encounter a window, and the probability of failure will be reduced to some new value less than 0.5 based on the new drilling information. To utilize VOIA, a well-founded relationship between the number of drill holes and the reduction in the probability of failure is required. With such a relationship, various preposterior calculations can be performed, to determine the maximum ENV for this problem. Such a relationship for the drilling example does exist based on search theory, where the probability of encountering a circular target of some diameter with a given drill spacing can be calculated and used in the preposterior analyses.

There are common situations in environmental site investigation and remediation where no clear relationship exists (unlike as in the previous example) to define the probability distributions, e.g., a relationship between the number of soil samples taken and the uncertainty in the estimation of DNAPL mass (for example for use in estimating oxidant or electron dose calculations). The DIVER project aims to develop relationships, based on the virtual site data (VSD), and the ability to access perfect information, that can be used within a decision analysis approach to make the method more "reachable" for industry practitioners for a variety of decisions. As an example, imagine a scenario where thermal remediation is being considered for a DNAPL source. A unit cost can be calculated for treatment of the source zone. If a probability relationship between the cost of additional sampling and the uncertainty in the volume estimate could be derived, then it would allow for optimization of the remedial design within some acceptable level of uncertainty.

3.2.2 A More Complex Example

The use of VOIA becomes more complex when the decision is not binary, or the collected data is not translatable to a deterministic probability distribution representation, or the overall process requires stochastic approaches for the performance of prior or preposterior analyses. Take for example a decision-making scenario that relies on an estimate of groundwater velocity and direction (e.g., will contaminants migrating in groundwater reach a receptor?). Groundwater velocity and direction are a function of the geology and stratigraphy, the hydraulic conductivity, the hydraulic gradient, and the porosity of the porous medium. Hydraulic conductivity is spatially variable, and spatially correlated, and is thus often represented by a distribution that can be defined by a mean, a variance, and a correlation length.

Without perfect information, the exact hydraulic conductivity at a location is not known, and thus a stochastic approach to the determination of the probability distribution is required, when multiple realizations of a hydraulic conductivity field that obeys the distribution statistics are generated and used to predict failure/no failure (reach/not reach the receptor). The probability of failure is then determined based on the percentage of realizations (as compared to the total number of realizations) that "failed".

For the scenario described above, prior estimates are generated based on the known data, which would include, for example, some subjective estimates of the mean, variance, and correlation lengths for hydraulic conductivity. The value of data question in this case concerns the worth of additional measurements of hydraulic conductivity within the flow region. Pre-posterior estimates (estimates assuming additional information as defined in Section 3.1) are calculated through a stochastic approach to defining the probability distribution, under some assumptions of the effect of additional measurements on the estimates of the mean, variance, and correlation length. A more detailed explanation of this situation and an example of this is provided in (Freeze et al., 1992). The level of knowledge and effort required to undertake full VOI analyses is relatively high compared to the level required for standard site investigation and remediation design, particularly considering that hydraulic conductivity is only one of many parameters that will affect the decision. This could be one of the reasons why VOI approaches have not been widely adopted within the environmental remediation industry.

3.2.3 How is DIVER Using VOIA?

Understanding and using appropriate relationships (e.g., relationship between number of soil samples and source zone mass estimates) in the derivation of the probability distributions within VOIA is a key to successful outcomes. Many relationships already exist for site investigation and remediation (e.g., sample spacing to limit missed "hot-spot" size), and others can be derived under highly simplifying assumptions (e.g., homogeneous geology, homogeneous sources, exponential source decay, first-order degradation reactions). The DIVER project, through its generation of physically based, highly detailed virtual sites allows for the development of new and powerful relationships for derivation of probability distributions. Stochastic sampling of the data will allow for the development of relationships for uncertainty in, for example, DNAPL mass versus number of samples. The use of these relationships to determine the value of information for various questions (decisions) will be explored through investigating their effects on the remediation designs of the various DM Teams.

The DIVER project created the unique situation to evaluate objective functions for decisions at contaminated sites with perfect information. The most straightforward application can be illustrated by considering an objective function for the design, implementation, and monitoring of a remedy at a site. This objective function can be simplified to a "cost-only" function:

$$\sigma\sigma = \sum_{tt=00}^{TT} \frac{11}{(11+ii)^{tt}} [-CC(tt)] \qquad \textbf{[3-3]}$$

Where the "benefits" are not included (as remediation is required) and it is assumed that only a single remedial approach is considered (to eliminate multiple options), and risk of failure (incorrect decision) is not considered. The value of the objective function under perfect information (VPI) is essentially the optimized remediation cost (with access to all information). The value of the objective function under current information (VCI) is the remediation cost of a single design. EVPI is thus VPI – VCI which provides the upper bound to the possible value of any additional information. The DIVER project allows the assessment of ENV (VCI – Value of Objective Function with New Information (VNI) – Cost of additional information) of various levels of new information (based on the previously developed probability distribution relationships) that could have been used to improve the "design" of a remedy. This allows a practitioner to decide if or what new information is of most value providing a basis for decision making on undertaking further investigations.

4 METHODOLOGY, APPROACH AND METHODS

While there has been a strong focus on developing new site diagnostic tools and approaches to characterizing the strength of source zones (e.g., architecture, total mass, mass discharge) and plume behavior (e.g., preferential flow paths, vertical concentration distribution, mass flux) [ITRC, 2010; Abriola et al, 2013; Sale and Newell, 2011], only recently have generic tools been developed to assist site managers, regulators, engineers and remediation scientists to determine how to combine existing and new approaches to arrive at a level of site characterization suitable for an intended purpose such as remediation (ITRC, 2011). Cost-effective site characterization is important when determining the feasibility of treatment approaches, to assess process performance during operation, and to reduce the uncertainty of long-term performance through support for optimization strategies.

Site characterization is a process of reducing uncertainty, with the eventual aim of the development of an accurate conceptual site model (CSM) that is appropriate for the remedial objectives of the site; referred to here as "fit for purpose". The economic cost of a "fit for purpose" CSM is highly variable and dependent on many factors, and little in the way of formal guidance exists on the balancing of the production of data from intensive and costly site characterization activities, the associated cost of the activities, and the ultimate benefit to achieving remedial goals more cost effectively. A similar lack of guidance exists for understanding which elements of site characterization translate to the highest value data for remediation planning, as well as in understanding which parameters are the most critical in assessing operational performance and in the prediction of long-term effectiveness (or early prediction of likelihood of not meeting goals, e.g., MCLs) of the applied remedy. In general, there is a growing shortfall: without better integration of information both within and between site characterization and remediation, an increasing wealth of information is left unused, and the benefits of specific information (value of information) are poorly understood.

The DIVER Project aimed to develop technical guidance on the value of data in both the site characterization and remediation contexts based on detailed VSD, empirical evidence gathered from some of the most respected and successful practitioners in the field, highly detailed virtual site investigations, and stochastic approaches to quantifying the value of additional information. The concept of "virtual site investigation" is premised on the generation of perfectly characterized sites through state-of-the-art simulation, and subsequent interrogation of the data via site investigation schemes proposed by experience practitioners.

There are fundamentally two conceptual and methodological frameworks to evaluate the value of information: DT and experienced based (EB). EB approaches rely on the experience of practitioners to evaluate data (through both empirical and modelling approaches). DT approaches rely on modelling, stochastic simulation, and probabilities to make decisions on the value of additional data. Many similarities exist between the two frameworks because they both try to address the same issue, but there are important differences in the emphasis. At a conceptual level, both approaches recognize that the value of a particular piece of information (or data) is simply the difference between the expected cost when a decision is taken without the benefit of this information and the expected cost when the decision uses this information. The EB approach considers the available evidence through the experience of the practitioners, and their intuition into the problem based on prior exposure to similar scenarios. The DT approach considers available evidence, but it heavily stresses the integration of this evidence, expressed in probabilistic terms, into a decision-making problem under uncertainty.

The challenge with using the EB approach in the classical sense in developing a framework for this project is that it requires long time spans to collect and properly evaluate evidence. The DIVER project overcomes this limitation, through the instant availability of data sets for any testing that may be envisioned by the practitioner. The DT approach also has limitations, in that it is much harder to adjust to the conditions in environmental remediation, does not allow the intuition of the DM to come into play, and is based on a rigid set of rules that may not consider all aspects of the problem under consideration. The DT approach is not well utilized in the remediation field, potentially due to its perceived complexity and the lack of guidance and tools that are accessible to the average practitioner. The DIVER project aims to use both DT and EB approaches based on identical "perfect" data sets, to evaluate head-to-head the benefits and limitations of both processes (Figure 4-1).

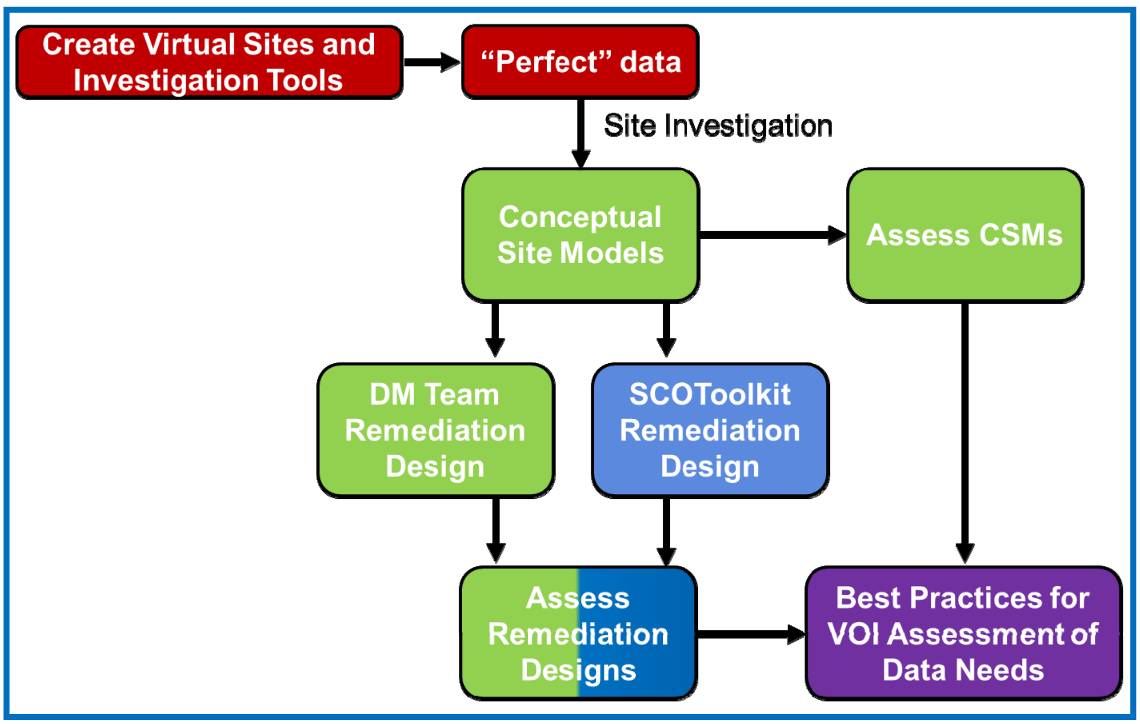


Figure 4-1: Methodology of DIVER project

The foundation of the DIVER Project is the creation of highly detailed virtual sites (perfect data) through state-of-the-art numerical simulation. These VSD are then investigated via the EB approach (by DM Teams) to develop conceptual site models as a basis for design of a remediation system. The conceptual site models are then used (under both the EB and DT frameworks) as the basis for remediation design to meet certain POs. SCOtoolkit (Parker et al, 2018) was used to undertake the DT approach. Assessment steps along the project timeline will generate comparisons of the performance of EB vs. DT for remediation as well as the level of uncertainty in the CSMs based on the specific investigation methods used by the teams investigating the VSDs. The following sections provide details on each of the different steps of the DIVER project.

4.1 Overall Technical Approach Summary

The project comprised seven distinct technical tasks, which can be broadly grouped into:

- Conceptual model creation for each site, translation to a numerical model, and creation of the data for each site (VSD creation),
- Selection of DM Teams and investigation of each site by the EB approach,
- CSM development and assessment,
- Remedy design by the EB approach, numerical simulation, and assessment,
- Remedy design by the DT approach, execution, and assessment,
- Optimal remedy design using perfect information,
- Stochastic analyses to develop framework and associated methodologies for reducing uncertainty in site investigation, and
- Validation of outcomes.

Broadly, the project developed detailed large-scale data sets through numerical simulation, which acted as "sites" under investigation and remediation. Figure 4-2 provides a conceptual schematic of the technical approach followed to develop CSMs for each site. In the EB assessment, the virtual sites were investigated (virtually) by four (4) DM teams (resulting in a total of 12 CSMs), comprising some of the most experienced and senior practitioners in the industry. The approach is like that adopted by Lowry et al. (2008) in a study looking at the calibration requirements of complex flow models. The DM teams developed site investigation plans, which were "implemented" by interrogating the large-scale data sets and producing site investigation data. The DM teams developed CSMs for each site (Section 5.1), and remediation plans to achieve pre-defined goals and endpoints. The CSMs and remediation performance were assessed against true values and performance objectives, and the worth of each investigation approach used (mass flux measurements, high-resolution tools, etc.) evaluated in terms of the benefit.

The DM Teams then used their CSMs to design EISB remedies for each site. EISB was chosen as it is an adaptable remediation technology widely used for the contaminants at the sites and is one of the remedies incorporated into SCOToolkit. The teams were provided with a set of remediation performance objectives that needed to be met within a given timeframe. The remedial designs were then modeled (DM Teams were allowed a single update to their design based on interim results provided during the remediation) and performance against the objectives evaluated.

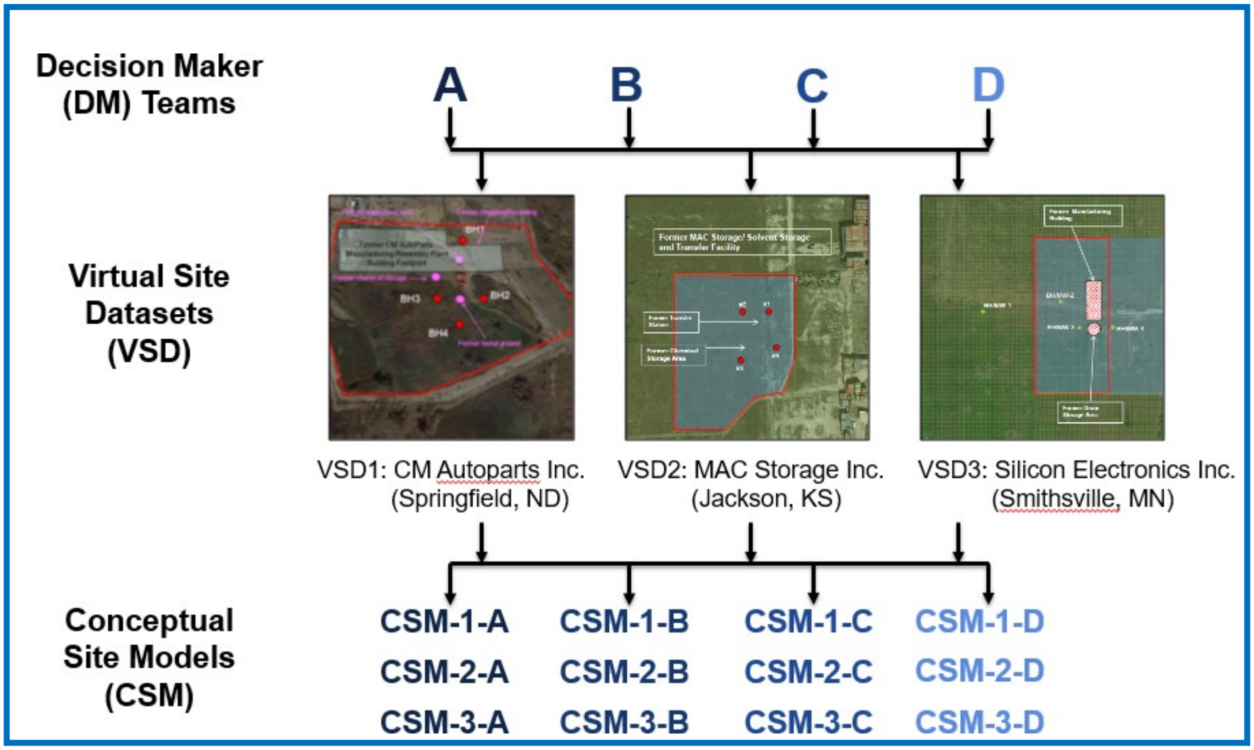


Figure 4-2:Technical approach for the experience-based assessment

In parallel with the DM Teams remedy modeling, a stochastic modeling program was run (DT approach) based on the CSMs developed by the DM Teams to compare the performance of a stochastic design approach to the EB approach. The central component of the DT approach is a semi-analytical mathematical flow and transport model (SCOToolkit) to simulate DNAPL source depletion and dissolved phase transport of a target chlorinated hydrocarbon (TCE) over time in response to natural and engineered conditions. The flow and transport model is coupled with cost functions for enhanced bioremediation. In the inverse modeling mode, historical site data (the site investigation data from the DM teams) were used to calibrate the flow and transport model and to estimate parameter covariances and residual prediction error. Forward predictions of remediation performance and cost were performed for defined remediation strategies, operating rules and remediation criteria. A Monte Carlo (MC) method was used to quantify uncertainty in performance and cost considering uncertainty in model parameters, measurements employed for real-time decisions, and cost function variables. Design optimization is performed to determine values of design variables that minimize the expected net present value (average over MC realizations). Additional technical details for SCOToolkit can be found in Parker et al (2018).

The entirety of the data collected to this point of the project (including access to perfect information) was then used to explore potential relationships between investigation approaches and uncertainty in parameters produced and evaluated as part of the CSMs (e.g., source mass and discharge, source size, plume size, plume mass, groundwater flow direction). The analyses included production of probability relationships that could be used within a VOI framework (such as expected uncertainty in DNAPL mass estimates based on number of soil samples) as well as development of a practitioner's guide (Appendix A) outlining effective practice for different aspects of site investigation (e.g., estimation of DNAPL mass, source zone footprint and mass flux).

The final stage of the project involved the testing of the developed practitioner's guides through application to a fourth VSD, patterned on an existing DoD site. The DM teams (original and six new teams engaged for this stage) were tasked with developing CSMs for the new site analogous to the procedure used for the first three sites. A number of the teams were provided with the practitioner's guides, and some were not. A comparison of results both with and without the guides formed a foundation for validation of the guides themselves and the overall framework developed within the project.

Detailed descriptions of each technical task are provided in the following sections.

4.2 Creation of Virtual Sites and Datasets

4.2.1 Overview

The core of the DIVER project was a series of large-scale, high-resolution computer simulations of hypothetical DNAPL-impacted sites, using trichloroethylene (TCE) as the representative DNAPL. These simulations were referred to as "virtual sites" and the collection of parameters that characterized each of these simulations, including input parameters such as permeability and output parameters such as DNAPL saturation and dissolved TCE concentrations, were designated as a 'virtual site data set' (VSD) (Table 4-1). The components of each hypothetical scenario in VSD1, VSD2 and VSD3 were based generally on the collective experience of the project team and were developed to represent different levels of complexity expressed through both the geological model and DNAPL distribution resulting from the hypothetical spill for each scenario. VSD4 was developed based on a particular DoD site and was used specifically to test and improve the application of effective practice guidance (see Section 4.8 for further discussion of VSD4). Access to information from VSDs 1 to 4 was restricted to a small subset of the project team to preserve confidentiality and prevent bias during virtual investigations (see Section 5.1.1 for further discussion of VSD investigation) by the DM Teams. Because the details of VSDs 1 to 4 could not be shared internally or externally during the project, a fifth VSD (VSD0) was created for initial comparison to tools used in the DT approach (Section 4.3.1). VSD0 was not investigated by the DM teams, and information (input and output) from VSD0 was shared by project team members across tasks to align the methodology.

Table 4-1: Purpose of each VSD and associated level of complexity

Virtual data set	Purpose	Complexity*
VSD0	Comparison between project tasks	Low
VSD1	DM team investigation and remediation	Low
VSD2	DM team investigation and remediation	Medium
VSD3	DM team investigation and remediation	High
VSD4	Validation of DIVER approach	Medium

* Complexity refers to the geologic heterogeneity, source zone topology, and final DNAPL distribution. Additional details can be found in Section 4.3.

Each VSD contained values of hydrogeological, chemical, and biogeochemical parameters, as described in the following sections, and summarized in Table 4-2, to allow for comprehensive investigation and to replicate a real site to the extent possible.

Table 4-2: Hydrogeological, chemical and biogeochemical parameters for VSDs 1 to 4

Parameters		
Fraction of organic carbon	Manganese	Dissolved hydrogen
Hydraulic head	Calcium	Dissolved methane
Groundwater velocity	Magnesium	Nitrate
DNAPL saturation	Sodium	Nitrite
Dissolved TCE	Potassium	Ammonia
Dissolved cDCE	Bicarbonate	Geobacter
Dissolved chloride	Carbonate	Dhc
Sorbed TCE	ORP	Dhb
Sorbed cDCE	Dissolved oxygen	vcra
Intrinsic permeability	Dissolved iron	Sulfate

4.2.2 Multiphase Flow and Reactive Transport Modelling

VSDs 0 to 4 were created using the numerical model DNAPL3D-RX, developed since 1990 and refined under ESTCP project ER-0424. DNAPL3D-RX is a three-dimensional, multiphase flow and reactive transport model capable of simulating DNAPL migration (release and redistribution) and reactive solute transport in heterogeneous porous media (Kueper and Frind, 1991a,b; Gerhard and Kueper, 2003; Grant and Gerhard, 2007; West and Kueper, 2012). Multiphase flow (groundwater and DNAPL) and solute transport are simulated by coupling the model based on Kueper and Frind (1991a,b) with RT3D (Clement, 1997; Clement et al., 1998) using a split-operator approach (Grant and Gerhard, 2007).

The multiphase flow equations for groundwater and DNAPL (wetting and non-wetting fluids, respectively) were solved using a fully-implicit finite difference method and a Newton-Raphson approach to solve non-linearities that arise from the relationships between capillary pressure, relative permeability and saturation (Kueper and Frind, 1991a,b). The Newton-Raphson solution was implemented using a SPARSKIT-ITSOL full orthogonalization method preconditioned iterative solver (Saad, 1994). Reactive solute transport equations, which account for advection, dispersion, sorption, dissolution and reaction, were solved using a third-order total variation diminishing solver to minimize the effects of numerical dispersion and artificial oscillation (Zheng and Wang, 1999). The reactive transport of two species (TCE and cis-Dichloroethene [cDCE]) was simulated during the development of VSDs 0 to 4, with first-order decay of TCE to cDCE. First-order decay was used here to shorten simulation times during the long dissolution of the DNAPL sources. A more comprehensive reaction model was used for the simulation of remediation using EISB strategies proposed by the DM Teams later in the project (Section 4.6.2). This comprehensive reaction model simulated seven chemical species and three microbiological species, using dual-Monod kinetics and accounting for competitive inhibition. A complete list of governing equations is presented in Appendix B.

4.2.3 Geology and Stratigraphy

Each of the VSD 0 to 4 domains were created as heterogeneous permeability domains consisting of unconsolidated porous media (clays, silts, sands and gravels) with spatially correlated random values of intrinsic permeability (k). These permeability fields were generated using the FGEN 9.1 algorithm (Robin et al., 1991) based on the mean and variance values listed in Table 4.2. Intrinsic permeability was assumed to follow a log-normal distribution, and values of the variance of $\ln(k)$ and correlation lengths were based on reported values from Canadian Forces Base (CFB) Borden aquifer (Sudicky, 1986; Woodbury and Sudicky, 1991; Turcke and Kueper, 1996; Allen-King et al., 2006), an unconfined aquifer in North Bay, Ontario, Canada (Sudicky et al., 2010), the Würmian Rhine glaciofluvial sand and gravel aquifer in Southwest Germany (Maji, 2005), and the Columbus Air Force Base (AFB) aquifer in Mississippi (Rehfeldt et al., 1992). Larger variance and larger correlations lengths signified more complex VSDs. Additional heterogeneity in the form of distinct silt and clay layers, as well as vertical trends in the mean intrinsic permeability, were implemented in specific VSDs to increase the level of complexity and create distinct aquifer units.

Table 4-3: Summary of heterogeneous permeability and organic carbon distributions

VSD	Mean k[a] (m^2)	Varianc e $\ln(k)$	Mean f_{oc}	Variance $\ln(f_{oc})$[b]	Correlation Length[c] (m)		Coherency Level
					Horizontal	Vertical[d]	
VSD0	9.8×10^{-13}	0.96	0.0030	0.35	5.0	0.5	0.608
VSD1	9.5×10^{-13}	1.31	0.0029	0.24	5.0	0.5	0.430
VSD2	3.0×10^{-12}	4.05	0.0030	0.28	5.0	0.5	0.304
VSD3	1.1×10^{-12}	4.10	0.0032	0.33	7.0	0.5	0.287
VSD4	8.7×10^{-13}	1.69	0.0030	0.27	5.0	0.5	0.351

[a] Calculated as a geometric mean for the values assigned to each VSD.
[b] Allen-King et al. (2006).
[c] Correlation lengths were applied equally for k and f_{oc} and were set to be horizontally isotropic.

The fraction of organic carbon (f_{oc}) was also treated as a spatially correlated random value to contribute to the heterogeneity of each VSD. These values were also generated using the FGEN 9.1 algorithm, and were set to be linearly, positively cross-correlated to the intrinsic permeability values. The coherency level (Table 4-3) describes the slope of the linear relationship between the cross-correlated $\ln(k)$ and $\ln(f_{oc})$ values.

4.2.4 Model Domains, Parameters and Boundary Conditions

For VSD1-4, the FGEN algorithm was used to generate k and f_{oc} values over a model volume that was 312-500 m in lateral extent and 23-30 meters (m) in vertical extent, depending on the VSD (Table 4-4). Domain sizes were chosen such that any dissolved phase plume would be fully contained within the domain at the time where site investigation was performed by the DM Teams. This volume was substantially larger than the domains simulated using DNAPL3D-RX (larger than the DNAPL source zone and the plume in each VSD) and was created to allow virtual investigations by the DM teams away from the DNAPL source zone and plume. Values of *k* and f_{oc} were assigned at a node spacing of 1.2 m horizontally and 0.15 m vertically (the model grid spacing).

Table 4-4: Physical dimensions of domains

VSD	VSD dimensions			Simulation domain dimensions		
	Length (m)	Width (m)	Depth (m)	Length (m)	Width (m)	Depth (m)
VSD0	126	76	10	126	76	10
VSD1	500	500	30	126	76	8
VSD2	500	500	30	140	84	10
VSD3	384	500	23	138	89	15

For simulation of the DNAPL release, migration and dissolution, and subsequent reactive transport of the VOC plume in each VSD, a simulation domain was defined within each VSD volume (Figure 4-3). This simulation domain was smaller than the VSD volume in lateral and vertical extent (Table 4-4). Node spacing used in the finite difference solution applied within the simulation domain was also 1.2 m horizontally and 0.15 m vertically. This low node spacing, particularly in the vertical direction, was selected to allow virtual investigations capable of representing high-resolution site investigation tools, such as membrane interface probes (MIP) and dye-enhanced laser-induced fluorescence (DyeLIF), applied in the field (Section 4.4.2). Boundary conditions with respect to groundwater flow were set to constant hydraulic head at the upgradient and downgradient boundaries, and no flow at all other boundaries. Boundary conditions with respect to DNAPL migration were set to constant DNAPL saturation at release nodes located on the top boundary and were no flow at all other boundaries. The release nodes were also set to no flow for both groundwater and DNAPL (in all VSDs) once the release period ended. Boundary conditions with respect to solute transport were set to zero concentration gradient at the lateral (cross-gradient) and vertical (top and bottom) boundaries, and free exit at the upgradient and downgradient boundaries. Care was taken to ensure that the VOC plume created by DNAPL dissolution did not contact the lateral (cross-gradient) boundaries. A series of preliminary simulations were conducted, and those in which the plume contacted the lateral boundaries were rejected (not used to create the VSDs) in favor of simulations in a larger domain. Input parameters for each VSD simulation are listed in Table 4-5.

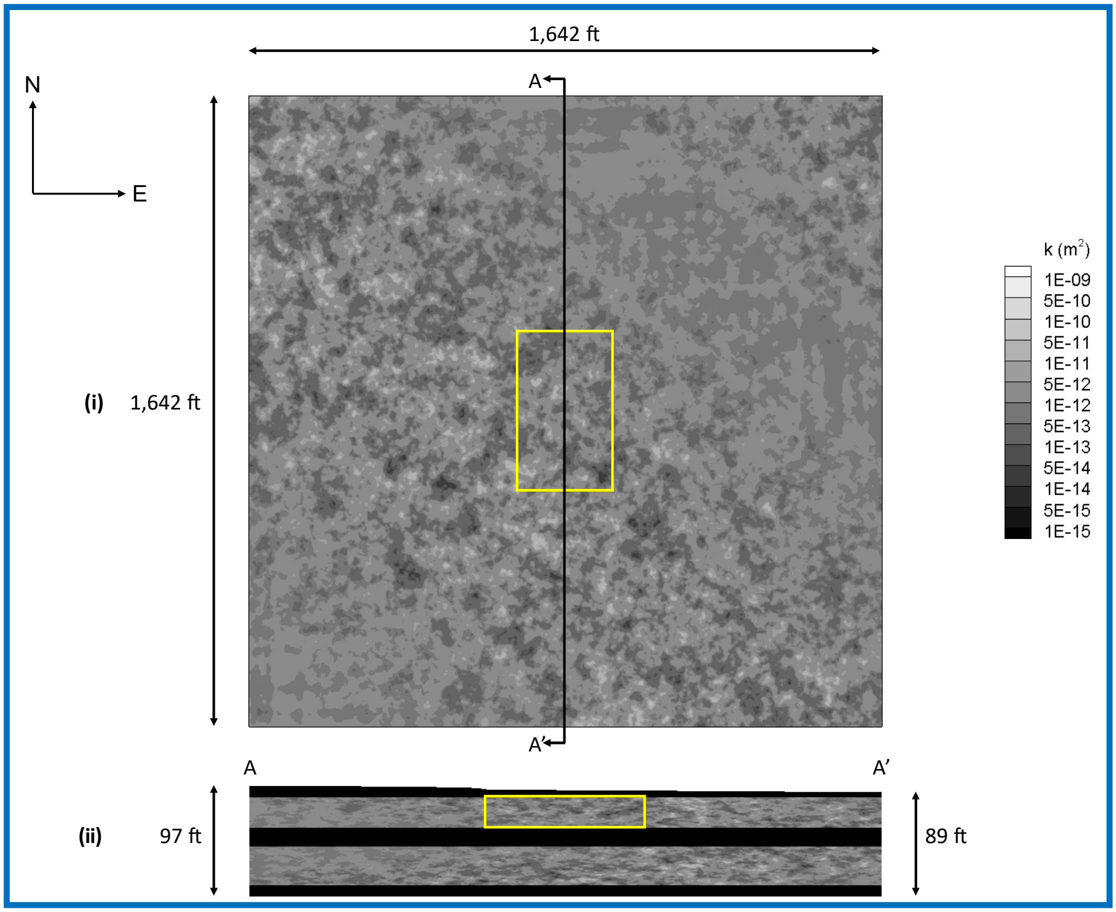


Figure 4-3: (i) Plan view and (ii) vertical cross section (A-A') of VSD1 showing the heterogeneous distribution of intrinsic permeability (greyscale), silt and clay layers between aquifer units (black), and the location of the simulation domain (outlined by a dashed box)

4.2.5 DNAPL release, migration and dissolution

TCE DNAPL was released in each of the simulations at the top of the upper-most aquifer layer. The release continued for 3.4 to 5.3 months and was then allowed to migrate (and redistribute) throughout the simulation domain for an additional 4.5 to 9.7 years, depending on the VSD (Table 4-6). Release sizes and pressures are analogous to slow to medium strength sources (as opposed to a catastrophic tank failure) and allow for the hydrogeology to control the DNAPL infiltration rate. The redistribution time was chosen to ensure that the DNAPL migration had essentially ceased (based on plateaued nodal occupancy) and varied between VSDs due to different geology and release volumes.

Table 4-5: Additional model parameters

Parameter	VSD0	VSD1	VSD2	VSD3
Water density (kg/m^3)	999.1			
TCE density (kg/m^3)[a]	1,460			
Water dynamic viscosity (Pa·s)	0.00139			
TCE dynamic viscosity (Pa·s)[a]	0.00057			
TCE-water interfacial tension (N/m)	0.025			
Soil matrix compressibility (Pa^{-1})[b]	1.0×10^{-8}			
Water fluid compressibility (Pa^{-1})[b]	4.4×10^{-10}			
TCE Soil organic carbon-water partitioning coefficient (mL/g)[a]	126			
cDCE Soil organic carbon-water partitioning coefficient (mL/g)[a]	86			
Porosity (-)	0.3			
Longitudinal dispersivity (m)	0.01			
Lateral dispersivity (m)	0.001			
Vertical dispersivity (m)	0.0001			
Tortuosity (-)[b]	0.7			
TCE first-order degradation rate constant (yr^{-1}) [c]	0.14			
TCE solubility (mg/L)[a]	1,100			
TCE free-water diffusion coefficient (m^2/s)[d]	9.1×10^{-10}			
cDCE free-water diffusion coefficient (m^2/s)[d]	1.13×10^{-9}			
Hydraulic gradient (-)	0.005	0.005	0.001	0.002
Number of nodes	443,205	350,595	548,730	851,000

[a] Pankow and Cherry (1996); [b]Freeze and Cherry (1979); [c]Assumed; [d]TRRP (2005)

Table 4-6: DNAPL release details

VSD	DNAPL volume released (US gallons)	DNAPL mass released (kg)	Release duration (months)	Redistribution duration (years)	Plume generation time (years)
VSD0	2,001	11,058	3.4	4.7	30.0
VSD1	1,998	11,044	4.1	4.7	20.0
VSD2	2,871	15,865	2.5	4.8	8.3
VSD3	4,001	22,113	3.5	9.7	14.5

Following redistribution, TCE dissolution was simulated for a period of 8.3 to 30 years (Table 4-6), assuming local equilibrium dissolution conditions (aqueous concentrations equal to the solubility of TCE) at DNAPL-occupied nodes. Simulation continued until the plume reached the end of the domain. The groundwater flow field was continually updated based on increases in aqueous phase relative permeability at DNAPL-occupied nodes due to DNAPL dissolution. Degradation of TCE to cDCE, according to first-order kinetics, was also simulated during plume generation to generate dissolved TCE and cDCE plumes. These plumes spanned the length of each simulation domain by the end of the plume generation period.

4.2.6 Biogeochemical Parameters

To reduce the time required for simulations, given the large size and high resolution of the domains, simulations used a first-order reaction rate expression for the biodegradation of TCE. This approach does not account for changes in the concentrations of other biogeochemical parameters that are commonly used to infer processes that are occurring at a site and, therefore, are measured as part of site investigations. Therefore, to efficiently account for these changes (and the use of a first-order reaction rate) a series of correlations were developed to estimate values of these biogeochemical parameters based on the simulated concentrations of TCE and cDCE at the time each VSD was investigated. The approach used for each correlation is described below, and examples are shown in Figure 4-4.

Oxidation reduction potential (ORP): A uniformly distributed random value with a mean of 200 millivolt (mV) was assigned to all nodes with a cDCE concentration less than a prescribed threshold concentration. A lower ORP was assigned to the remaining nodes based on the ratio of TCE and cDCE concentrations.

Dissolved oxygen (DO): A uniformly distributed random value with a mean of 0.2 milligram per liter (mg/L) was assigned to all nodes with an ORP less than 0.0 mV. A uniformly distributed random value with a mean of 3.0 mg/L was assigned to the remaining nodes.

Dissolved sulfate: A value of non-detect was assigned to all nodes with an ORP less than -210 mV. A uniformly distributed random value with a mean of 90 mg/L was assigned to all nodes with an ORP greater than -50 mV. A second-order empirical relationship between ORP and sulfate was used to assign values to nodes with -210 mV < ORP < -50 mV.

Dissolved hydrogen: A value of non-detect was assigned to all nodes with an ORP greater than 0.0 mV. A second-order empirical relationship (based on the experience of the DIVER team) between ORP and dissolved hydrogen was used to assign values to all other nodes, to a maximum value of 40 nanomoles per litre (nmol/L).

Dissolved methane: A value of non-detect was assigned to all nodes with an ORP greater than - 175 mV. A higher value was assigned to remaining nodes based on the dissolved hydrogen concentration, to a maximum value of 20 mg/L.

Dechlorinator species: Based on the DIVER teams experience, a uniformly distributed random value between 3 and 5 was assigned to the log(concentration) of the total dechlorinators at each node. The ratio of geobacter to Dehalococcoides (Dhc) and Dehalobacter (Dhb) was then assigned based on the concentration of TCE, with greater concentrations of geobacter for higher concentrations of TCE. The fraction of Dhb in other dechlorinators (not geobacter) was then assigned as a uniformly distributed random value with a mean of 0.2. vcrA was set to non-detect at all nodes.

Dissolved nitrate: A value of non-detect was assigned to all nodes with a TCE concentration greater than 5 microgram per liter (µg/L). A uniformly distributed random value with a mean of 0.3 mg/L was assigned to all remaining nodes.

Dissolved nitrite: A value equal to the concentration of nitrate multiplied by a uniformly distributed random value between 0.05 and 0.15 was assigned to all nodes.

Dissolved ammonia: A value equal to the concentration of nitrate multiplied by a uniformly distributed random value between 0.08 and 0.12 was assigned to all nodes.

Dissolved chloride: The chloride concentration at each node was increased above its background value (discussed below) by one mole per liter (mol/L) for every mol/L of cDCE present at that node.

In addition to the parameters listed above, background concentrations of major anions and cations were assigned to all locations in the VSD, generally based on their hypothetical geographical locations (North Dakota, Kansas, Minnesota or California; see Section 4.3). The mean values for each ion and each VSD are listed in Table 4-7, and values were assigned as a normally distributed random value.

Table 4-7: Background inorganic concentrations for VSD 1 - 3

Ion	Mean ion concentration (mg/L)		
	VSD1[a]	VSD2[b]	VSD3[c]
Iron	0.17	0.16	0.21
Manganese	0.31	0.09	0.15
Calcium	109	90	90
Magnesium	44	20	25
Sodium	250	60	6
Potassium	17	3	2
Bicarbonate	1060	305	273
Carbonate	3	5	3
Chloride	50	60	20

[a] Major ion concentrations based on North Dakota State Water Commission (2012)
[b] Major ion concentrations based on Jian et al. (2004)
[c] Major ion concentrations based on Minnesota Pollution Control Agency (1998)

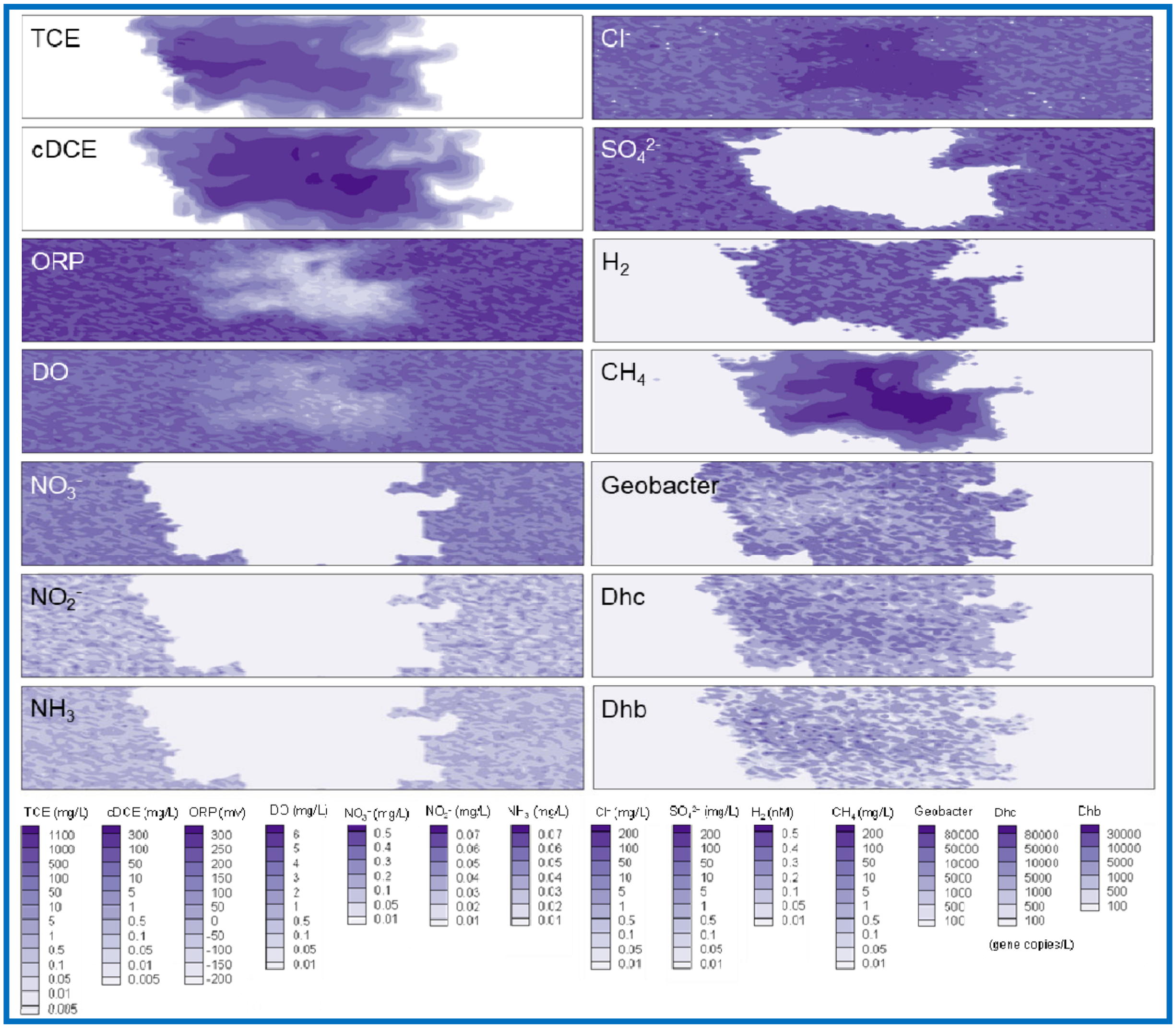


Figure 4-4: Vertical cross-section through the centerline of the TCE plume in VSD1 showing (a) dissolved TCE concentrations and (b) dissolved cDCE concentrations, along with the values of the biogeochemical parameters established using correlations to the TCE or cDCE concentrations for (c) oxidation reduction potential, (d) dissolved oxygen, (e) dissolved sulfate, (f) dissolved hydrogen, (g) dissolved methane, (h) Geobacter, (i) Dhc, (j) Dhb, (k) dissolved nitrate, (l) dissolved nitrite, (m) dissolved ammonia mg/L, NH3, and (n) dissolved chloride (mg/L Cl).

4.2.7 VSD Data Arrays

Output from the FGEN algorithm and the DNAPL3D-RX simulations was used to create a four-dimensional data array for each of VSDs 0 to 4 to store the values of the hydrogeological, chemical or biogeochemical parameters at each node location (northing, easting and elevation). The values of these parameters were those at the end of the plume generation time (one time point) and were used as input for the virtual site investigation tools (see Section 4.4). That is, virtual investigations by the DM teams were assumed to occur over a short enough time period that these parameter values did not change between investigation mobilizations.

In total, values for 30 parameters were stored for each node in each of VSDs 1 to 4 (Table 4-2), which resulted in approximately 10-25 million data values for each simulation domain, and approximately 0.4-1 billion data values for each larger VSD volume. Fewer values were stored for VSD0 because none of the correlated biogeochemical parameters were used in those simulations.

4.3 Descriptions of Virtual Site Datasets (VSDs)

4.3.1 VSD0: Methodology Verification

VSD0 was designed to act as a dataset that could be shared within the DIVER project team without jeopardizing the confidentiality of VSDs 1 to 4, which were investigated by the DM teams. Specifically, VSD0 allowed comparisons between results from simulations using DNAPL3D-RX and those using the SCOToolkit analytical model. However, results were also used to share information concerning the project approach outside of the project team (e.g., at early SERDP meetings). The simulation domain for VSD0 was chosen to be similar to VSD1, with respect to the distribution of intrinsic permeability (Table 4-3), size of the domain (Table 4-4) and volume of DNAPL released (Table 4-6). A smaller variance of $\ln(k)$ was chosen to promote a less complex DNAPL distribution, and the final DNAPL release realization was selected from multiple preliminary realizations to fit this objective. As described in Section 4.2.4, no larger VSD volume outside of the simulation domain (outside of the immediate vicinity of the DNAPL source zone and plume) was simulated and no biogeochemical parameter values were assigned for VSD0 because it was not designed to be investigated by the DM teams. Example cross-sections showing the distribution of intrinsic permeability, DNAPL and dissolved TCE concentrations are shown in Figure 4-5.

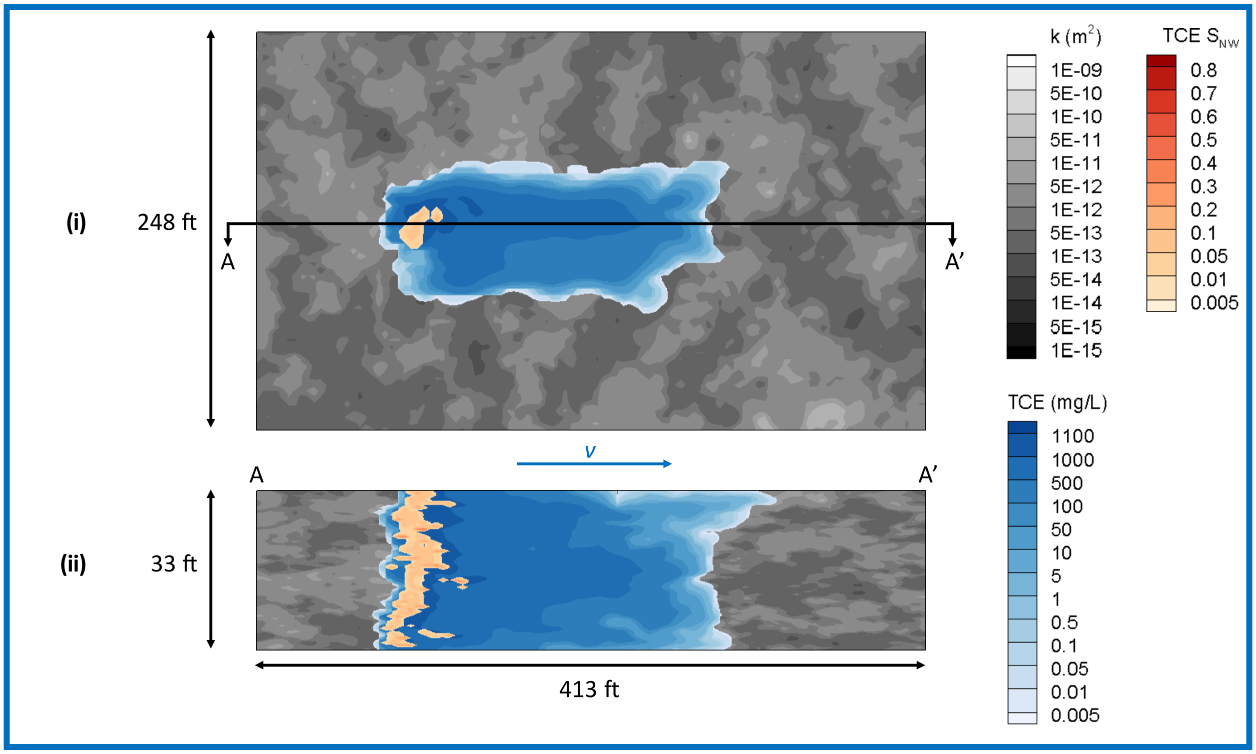


Figure 4-5: (i) Plan view and (ii) vertical cross section (A-A') along the plume centerline showing the intrinsic permeability, concentration of dissolved TCE and TCE DNAPL saturation for VSD0 at the end of the plume generation time. Direction of groundwater flow (*v*) is shown using the blue arrow symbol.

4.3.2 VSD1: CM Autoparts

VSD1 was designed to be a fictional site located in Springfield, North Dakota. The Site narrative had it operating as a manufacturer of automobile parts from 1964 to 2006. Primary operations at the Site included: i) Manufacture of brake pads and shoes (1964-1980); ii) Assembly of brake calipers (1980-2006); iii) bulk storage of various production chemical products; iv) finished product warehousing; and v) shipping and receiving. The manufacturing plant was shut down in 2006 and the narrative indicated numerous potential release sites (such as a former drum burial ground).

In addition to the intrinsic permeability distribution defined by the parameters listed in Table 4-1, a 5 m-thick homogeneous clay layer was created within the domain to separate VSD1 into upper and lower aquifer units, which were approximately 8 m and 10 m thick, respectively. An undulating homogeneous clay layer ranging from 1.2 to 3.7 m thick was also created above the upper aquifer to create confined conditions, and a 3 m-thick homogeneous clay layer was created below the lower aquifer. The VSD1 simulation domain was located in the upper aquifer unit, and constant hydraulic head boundary conditions were set to create groundwater flow from North to South. A TCE DNAPL release occurred at a single location (former drum burial ground). Example cross-sections showing the distribution of intrinsic permeability, DNAPL and dissolved TCE concentrations are shown in Figure 4-6.

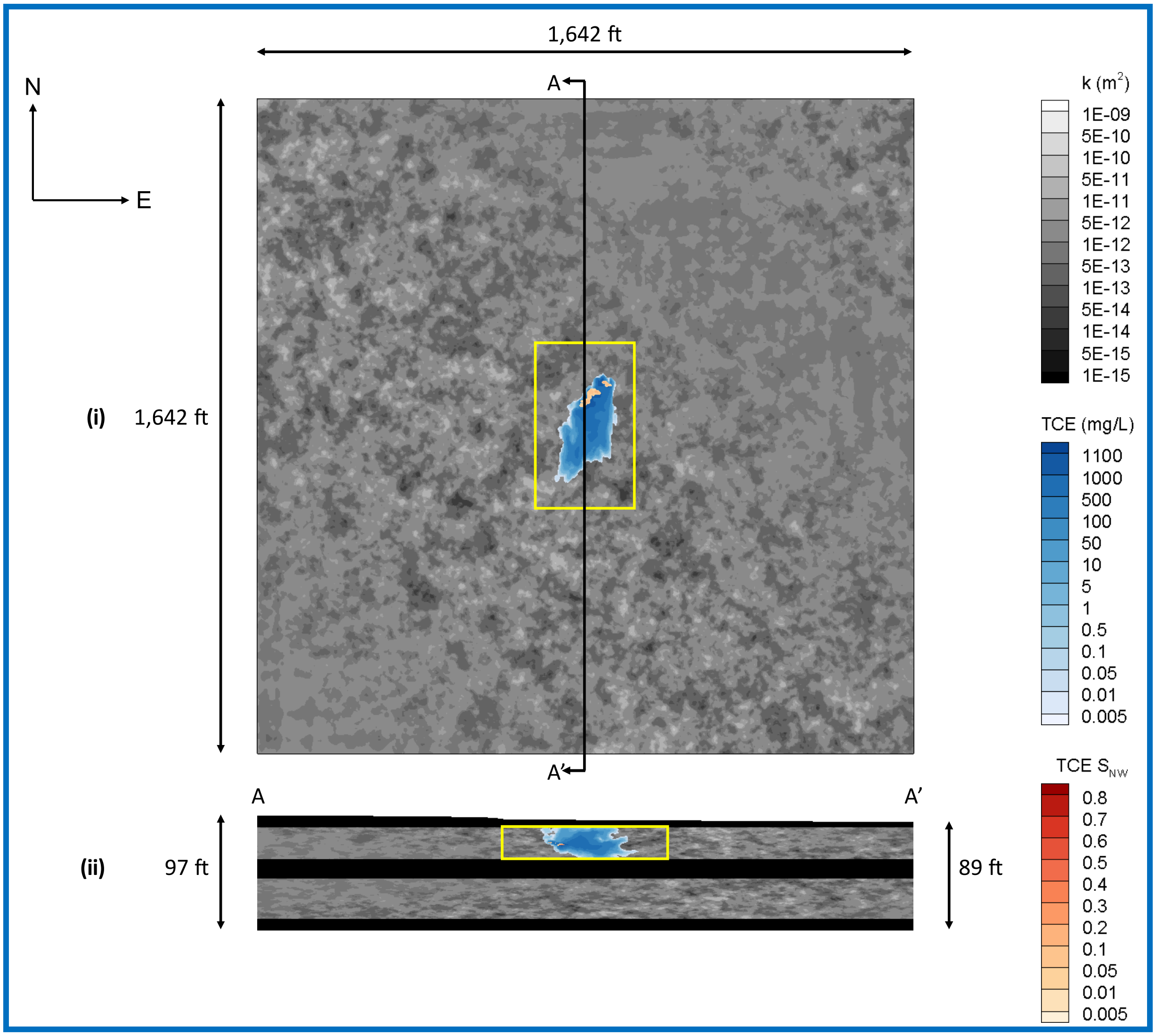


Figure 4-6: (a) Plan view and (b) vertical cross section (A-A') along the plume centerline showing the intrinsic permeability, concentration of dissolved TCE and TCE DNAPL saturation for VSD1 at the end of the plume generation time. The simulation domain is shown outlined by a dashed yellow line. Direction of groundwater flow was from North to South.

4.3.3 VSD2: MAC Storage

VSD2 was designed to be a fictional site located in Jackson, Kansas. The Site narrative had it operating as a solvent storage and transfer facility from 1990 to 2010. During its operation, the Site contained one office building, a covered transfer station situated in the eastern portion of the property attached to the office building, and a storage facility consisting of five 10,000 gallon above ground storage tanks at the southern side of the Site. An underground line connected the storage facility to the transfer station. Primary operations at the Site included the storage of trichloroethene (TCE) and transfer of TCE to small volume totes and containers for sale to local facilities.

A 1 m-thick homogeneous clay layer was created at the top of the model and a 3 m-thick homogeneous clay layer was created at the bottom of the lower aquifer, in addition to the intrinsic permeability distribution defined by the parameters listed in Table 4-3. A silt and clay layer ranging from approximately 5 to 8 m thick was also created within the domain to separate VSD2 into upper and lower aquifer units, each approximately 10 m thick. However, unlike in VSD1, that silt and clay layer was modified in three ways to increase the complexity of the site: (i) it sloped downward in the downgradient direction at an angle of 0.11° (approximate slope of 1/500), (ii) the top surface was undulating (using a sinusoidal function with an amplitude of 0.15 m, a period of 0.07 and a vertical shift of 2.775 + 0.0015x) and (iii) a stream meander feature (filled with higher-permeability sands) was included in the middle of the top of the layer, oriented in the downgradient direction. As a final modification, the upper aquifer unit was created to be a coarsening-downward unit by applying a linear gradient to the intrinsic permeability distribution output by the FGEN algorithm, where the intrinsic permeability of the deepest nodes in the upper aquifer were increased by a factor of 100, and the shallowest nodes were not modified. The VSD2 simulation domain was located in the upper aquifer unit, and constant hydraulic head boundary conditions were set to create groundwater flow from South to North. A TCE DNAPL release occurred at two locations (near the former chemical storage area and former transfer station), adding additional complexity to VSD2. Representative cross-sections showing the distribution of intrinsic permeability, DNAPL and dissolved TCE concentrations are shown in Figure 4-7.

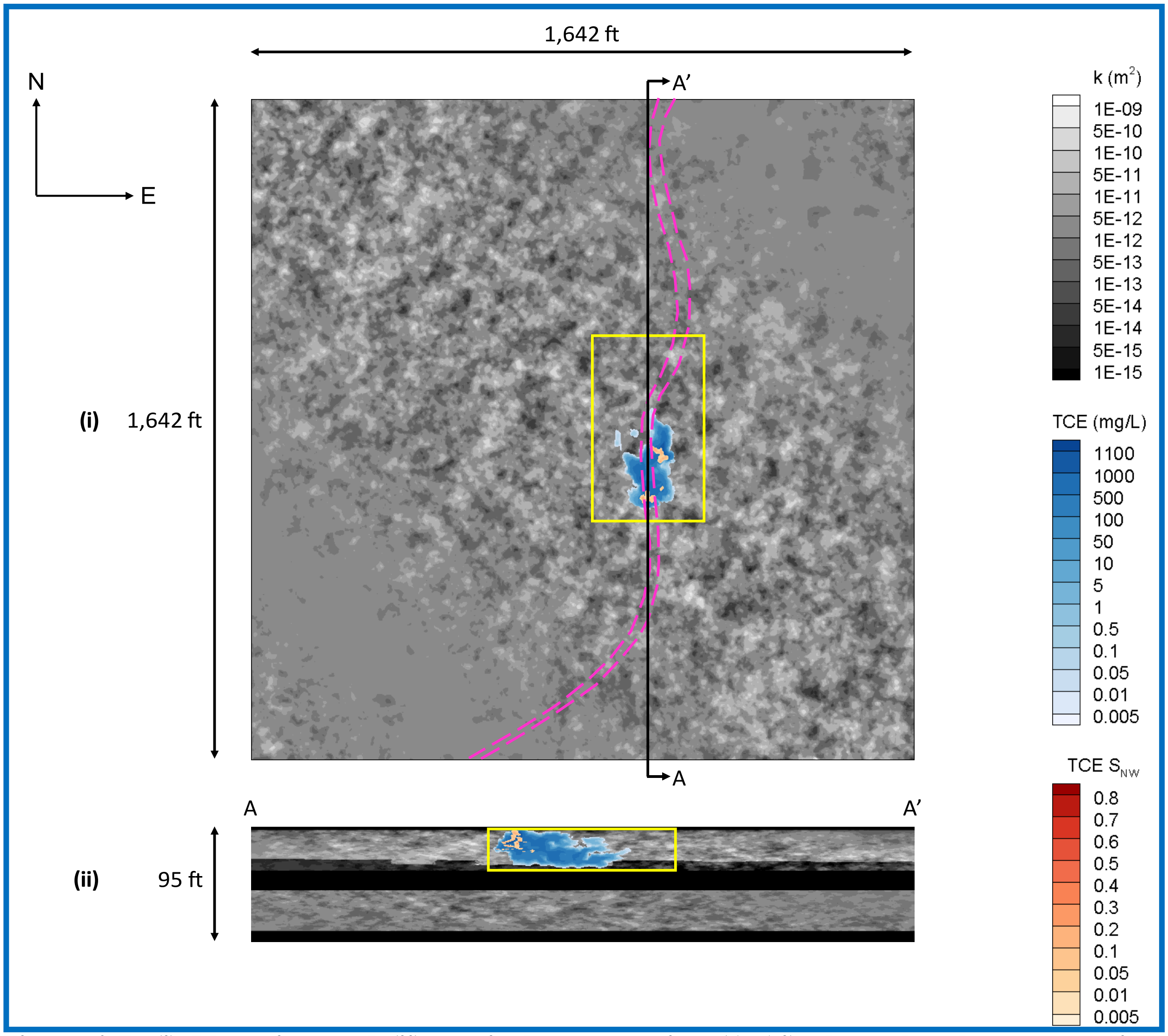


Figure 4-7: (i) Plan view and (ii) vertical cross section (A-A') along the plume centerline showing the intrinsic permeability, concentration of dissolved TCE concentrations and TCE DNAPL saturation for VSD2 at the end of the plume generation time. The simulation domain is shown outlined by a dashed yellow line. The plan view location of the stream meander feature is shown outlined by a dashed pink line. Direction of groundwater flow was from South to North.

4.3.4 VSD3: Silicon Electronics

VSD3 was a fictional site located in Smithsville, Minnesota. The Site narrative had it operating as an electronics manufacturing facility, providing manufacture of silicon semiconducting wafers from 1995 to 2007, when the company went out of business. A covered drum storage area was located directly to the south of the manufacturing facility during the time it was in operation. Drums were removed when the facility was shut down in 2007. Primary operations at the Site included the production of silicon semiconducting wafers. The production process included cleaning the wafers with a vapor degreaser unit using TCE. TCE was used inside the building for the cleaning process and was stored in the storage facility located south of the building.

A clay layer ranging from 1.0 to 3.1 m thick was created at the top of the geology model and an approximately 5.0 to 6.5 m-thick silt and clay layer was created at the bottom of the model, in addition to the intrinsic permeability distribution defined by the parameters listed in Table 4-3. For VSD3, the lowest silt and clay layer had an undulating surface. Instead of a continuous silt and clay layer near the vertical center of the model, three discontinuous undulating clay lenses were created. Two sloping discontinuous clay lenses were located near the former manufacturing building and former drum storage area, and one discontinuous clay lens was located further downgradient. Both lenses sloped downward toward the middle of the site, one sloping downward from North to South at 1.04° and the other downward from South to North at 0.88°. Therefore, unlike VSD1 and VSD2, VSD3 consisted of only one aquifer unit, and DNAPL migrated below the discontinuous clay lenses. The close spacing of the clay lenses resulted in DNAPL accumulation above and below these lenses, and location of the 'window' between the lenses was an important component of the site investigation by the DM teams as small-scale features such as this are challenging to identify and delineate during site investigation. The VSD3 simulation domain was located between the shallowest and deepest clay layers, and constant hydraulic head boundary conditions were set to create groundwater flow from East to West. A TCE DNAPL release occurred at a single location near the southwest corner of the former manufacturing building. Representative cross-sections showing the distribution of intrinsic permeability, DNAPL and dissolved TCE are shown in Figure 4-8.

4.3.5 VSD4: Flights R-US

VSD4 was designed to be a fictional site located in Ocean Township, New Jersey. The site history was set to include operation as an airport between 1951 and 1999 with solvents use and storage in different parts of the facility

The geology of VSD4 was generally based on Zone D of Naval air station (NAS) North Island Site 9, Operable Unit (OU) 20. This specific geological zone was comprised of a fine to medium/fine to coarse sand (with traces of mica and shell fragments and silty sands, clayey sands approximately 0.5 to 4 ft thick and clay/clayey silt lenses approximately 0.5 to 1 ft thick) and was located at an approximate depth interval of 60 to 80 ft below ground surface. This aquifer unit overlaid a (estimated) laterally extensive clay/clayey silt/sandy clay, which was located at approximately 80 ft below ground surface. Zone D was selected from three other reported geological zones (A, B and C) because it contained the most unidirectional plume with respect to hydraulic gradient (conditions that were the most compatible with respect to the modeling capabilities of DNAPL3D-RX).

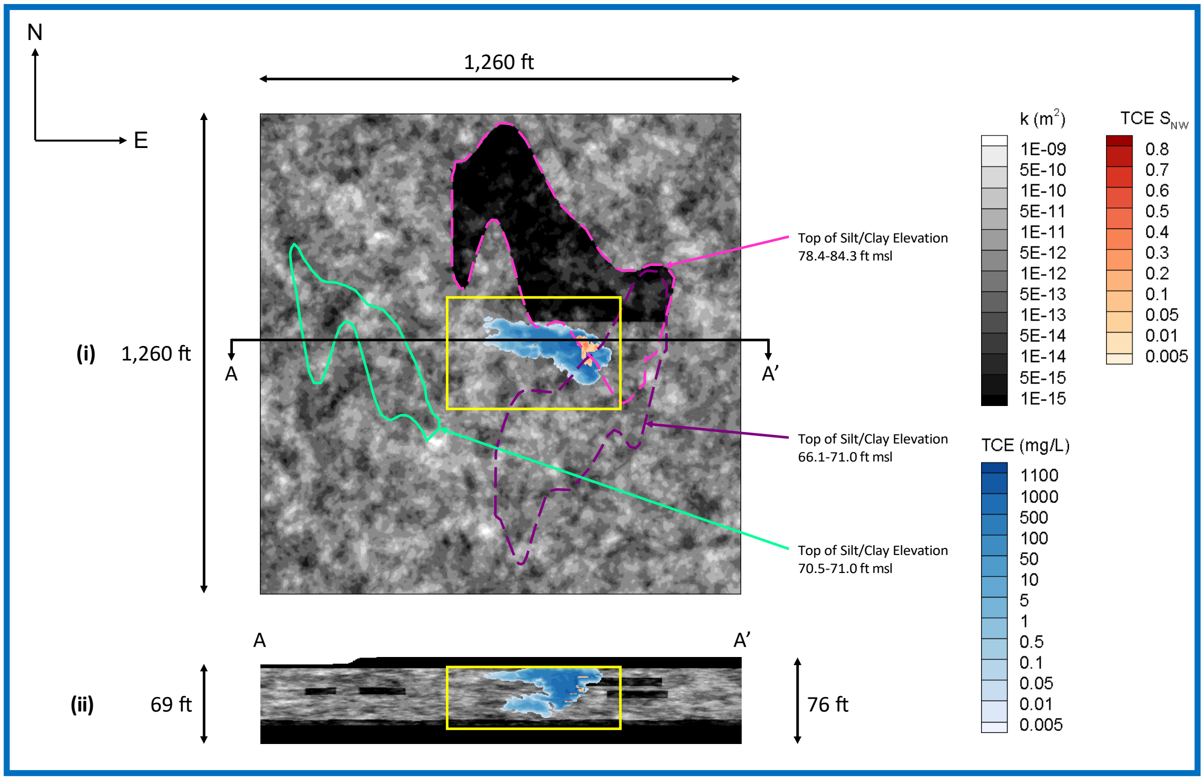


Figure 4-8: (i) Plan view and (ii) vertical cross section (A-A') along the plume centerline showing the intrinsic permeability, concentration of dissolved TCE and DNAPL saturation for VSD3 at the end of the plume generation time. The simulation domain is shown outlined by a dashed yellow line. The silt and clay lenses are shown in plan view outlined by a dotted green, pink, and dark purple lines. Direction of groundwater flow was from East to West.

Additional details for VSD4 are not provided as part of this report due to its use in Training for environmental monitoring performance optimization (TEMPO) (ESTCP ER19-5075). VSD4 forms the basis for the evaluation portion of TEMPO and as such the authors feel that revealing the "answers" to the CSM parameters would invalidate that highly useful portion of ER19-5075.

4.3.6 Phase I Environmental Site Assessment Documentation

Following the development of VSDs 1 to 3, Phase I Environmental Site Assessment (ESA) reports were developed and provided to the DM teams. No Phase I ESA report was developed for VSD0 because of its intended use as an internal verification dataset. The Phase I ESA reports contained site history and preliminary site investigation information, deemed by the project team to be representative of a TCE DNAPL-impacted site. Each Phase I ESA report included documentation of borehole logs, water levels and sampling results for eight borings (1 deep and 1 shallow at 4 locations) completed with monitoring wells. The associated data were generated using the same virtual investigation tools used by the DM teams (Section 4.4.2). The Phase I ESA reports for VSD1-3 are included in Appendix C.

4.4 Translating Model Data to Investigation Data

4.4.1 Overview

The EB virtual site investigation relied on the application of a series of virtual investigation tools by the DM teams to VSD1-3. These virtual investigation tools were designed to mimic site investigation tools currently available to practitioners by transforming hydrogeological, chemical and biogeochemical parameter values stored in the VSD data arrays (Table 4-2) to measurements and formats typically obtained in field investigations. For example, hydraulic conductivity values were converted to soil classifications and displayed as a borehole log and dissolved TCE concentrations were averaged over a specified screened interval and reported as a concentration in a groundwater sample. The virtual investigation tools that were available to the DM teams are listed in Table 4-8, and the approach used to transform parameter values from the VSD data arrays is described below. Here, investigation tool refers broadly to any installation, measurement, sampling or analysis. Example reports are provided in Appendix D.

4.4.2 Investigation Tools

Soil borings: Intrinsic permeability values between 1.02×10^{-15} meters squared (m^2) and 1.02×10^{-9} m^2 were divided into 13 categories, corresponding to the Unified Soil Classification System (USCS) definitions of low-to-medium plasticity clay through well-graded gravel. For soil borings at a requested location and depth interval, soil classification symbols and descriptions were assigned along the depth of a borehole log at a vertical spacing of 0.15 m, according to the intrinsic permeability in the VSD array at those locations. Handheld Photoionization detector (PID) screening response was assigned at a vertical resolution of 0.15 m. The response was based on a maximum response of 4,000 ppm(v), with a response proportional to the ratio of the dissolved TCE concentration to its solubility up to 3,000 ppm(v) for very low DNAPL saturation; proportional to the DNAPL saturation for 3,000-4,000 ppm(v) for low DNAPL saturation; and 4,000 ppm(v) for medium-to-high DNAPL saturation. Visual NAPL observations were based on DNAPL saturations, with extremely low showing no observation; very low showing ‘staining’; low showing ‘residual NAPL’ and medium-to-high showing ‘Pooled NAPL.’

Monitoring well and CMT well: Water levels were calculated based on the average hydraulic head over the specified screened interval.

Membrane Interface probe (MIP): PID and Electron capture detector (ECD) responses were calculated using correlations to the sum of the TCE and cDCE soil (total) concentrations based on those reported by Adamson et al. (2014), with maximum responses of 30 V for PID and 14 V for ECD. Electrical conductivity (EC) was calculated based on the intrinsic permeability using the correlation reported by Cheng (2012). PID, ECD and EC responses were based on values in the VSD data arrays spaced every 0.30 m (every other model node) and smoothed between points using polynomial functions to mimic the scalloped pattern typical of MIP responses.

Hydraulic profiling tool (HPT): The HPT response was included along with all requested MIP installations. Estimated hydraulic conductivity was based on the intrinsic permeability, water density and water viscosity, and was reported every 0.15 m. No error associated with the HPT response was included in the reported values.

Table 4-8: Site investigation tools available to the DM Teams

Investigation Tool	Reported Information
Installation	
Soil boring	Soil classification, handheld PID, visual NAPL observations
Monitoring well	Well construction detail, water level
Continuous multichannel tubing (CMT) well	Well construction detail, water levels in each channel
Membrane interface probe (MIP)	ECD, PID and EC response
Hydraulic profiling tool (HPT)	Estimated hydraulic conductivity (included with MIP)
DyeLIF	Relative emittance response
Measurement	
Slug test	Change in water level over time
Pumping test	Change in water level over time
Multiparameter meter	pH, EC, DO, ORP in groundwater
Sampling	
Groundwater	Depends on analysis requested
Soil	Depends on analysis requested
Hydrophobic dye test	NAPL indication (negative, weak positive, positive)
Groundwater analysis	
Volatile organic compounds (VOCs)	77 compounds (see Appendix D)
Semi-volatile organic compounds (SVOCs)	91 compounds (see Appendix D)
Metals	Arsenic, barium, cadmium, calcium, chromium (VI), chromium (total), iron, lead, magnesium, manganese, potassium, selenium, silver, sodium, strontium, zinc
Inorganics	Bicarbonate alkalinity, carbonate alkalinity, nitrate, nitrite, sulfate, chloride, specific conductance, total dissolved solids
Dissolved gases	Acetylene, methane, ethane, ethane, propane, propene, propyne, n-butane, oxygen, hydrogen
Gene-trac	Dhc, Dhb and vcra
Organic carbon	TOC, DOC
Soil analysis	
Volatile organic compounds (VOCs)	77 compounds (see Appendix D)
Semi-volatile organic compounds (SVOCs)	91 compounds (see Appendix D)
Metals	Arsenic, barium, cadmium, calcium, chromium (VI), chromium (total), iron, lead, magnesium, manganese, potassium, selenium, silver, sodium, strontium, zinc
Grain size distribution	Grain size distribution curve, bulk density
Organic carbon	TOC, f_{oc}

PID: photoionization detector, ECD: electron capture detector, EC: electrical conductivity, DO: dissolved oxygen, ORP: oxidation reduction potential, TOC: total organic carbon, DOC: dissolved organic carbon, f_{oc}: fraction of organic carbon.

Dye-enhanced laser-induced fluorescence: DyeLIF response, reported as a relative emittance (RE), was based on DNAPL saturations from the VSD data array at a vertical resolution of 0.15 m (every model node). Based in part on conversations with Dakota Technologies, locations with low DNAPL saturation were assigned a RE as a normally distributed random number with a mean of 1%, and locations with higher DNAPL saturation were assigned a RE as a normally distributed random number with a mean that was proportional to the DNAPL saturation. All RE values were constrained to be 0.5% < RE < 100%.

Slug test: Slug test response was based on the arithmetic mean of the intrinsic permeability values from the VSD data array at the locations over the specified screened internal. Decreases in water level over time were calculated using the approach of Hvorslev (1951).

Pumping test: Pumping tests were the only investigation tool that could not be obtained from the VSD data arrays and required additional simulation. Groundwater extraction from a well specified by a DM team, and decreases in hydraulic head at specified observations wells, were simulated using DNAPL3D-RX. Up to three extraction rates were simulated in step-drawdown tests, and the reported data included a recovery period sufficient for hydraulic heads at the observation wells to return to near-pre-pumping conditions.

Hydrophobic dye test: Dye test results were based on DNAPL saturations, with very low showing 'negative; low showing 'weak positive; and medium-to-high showing 'positive.'

Groundwater analysis: Groundwater concentrations (for volatile organic compounds [VOCs], semi-volatile organic compounds [SVOCs], metals, inorganics, dissolved gases, organic carbon and Gene-trac) were based on a flux-weighted average of the dissolved concentrations at each model node over the specified screened interval, using the Darcy flux at the same model nodes. Multiparameter values were calculated using the same approach. Dissolved organic carbon (DOC) values were based on a fraction of the f_{oc}, and total organic carbon (TOC) values were based on the sum of the DOC and the TCE and cDCE concentrations in the VSD data array. Samples specified as low-flow samples were calculated at a single model node.

Soil analysis: VOC and SVOC concentrations were determined as a total concentration according to Kueper and Davies (2009), using the dissolved concentration, sorbed concentration, DNAPL saturation, bulk density and porosity. For metals, sorbed concentrations were assumed to be negligible. TOC and f_{oc} were based on the f_{oc} values in the VSD data array. Samples were assumed to be collected from within a single 0.15 m vertical interval (one model node).

Grain size distribution curve: A series of grain size distribution curves were created manually for each of the 13 USCS classifications used in the borehole logs and were assigned based on the intrinsic permeability at the location of the soil sample for which a curve was requested. Samples were assumed to be collected from within a single 0.15 m vertical interval (one model node).

4.4.3 Investigation Tracking

DM team requests and response times were tracked by the DIVER team using an internal quality assurance and quality control (QA/QC) spreadsheet. The spreadsheet catalogued the following information: DM team, VSD site, reference project number, summary description of the request, date that the request was received, dates tracking the correspondence between the DIVER and DM teams to clarify/resolve issues, and the date of request fulfillment. 90 query requests were received and completed during the DM team virtual site investigation timeline for VSDs 1 to 3. The response times to the DM teams varied depending on the query request type and the number of installation/sampling locations (e.g., 1 business day for a MIP-HPT request at 6 locations, 11 business days for a pumping test request where the model was run to obtain water level measurements during an 8-hr aquifer pumping test and 24-hr recovery period). Additional QA/QC for DM team mobilizations included visual tracking of DM team query request locations and overlaying these coordinates onto the VSD raster images in RStudio. The northing and easting coordinates for each query request type were entered and updated on a frequent basis in order to filter out any discrepancies between the DM team requests and the DIVER team interpretations.

4.5 CSM parameters and Assessment

The DIVER Project Team established parameters that were used to evaluate the performance of the DM Teams site investigation approaches based on their developed CSMs. The parameters were established through several rounds of consultation, discussion, and literature review, and are focused on what the Project Team concluded were the most critical aspects of CSMs for the virtual sites related to decisions on remediation design. The parameters were provided to the DM Teams in a reporting template (Appendix E) which was designed to give the DM Teams an opportunity to describe their CSM in a semi-quantitative manner and allowed the CSMs from each of the DM Teams to be compared consistently. The CSM template included the following reporting elements:

- Identification of Contaminants of Concern
- Description and quantification of geology, hydrogeology and hydraulics
- Understanding of biogeochemical conditions

The specific quantitative parameters for assessment at each site are:

- Identification of the presence or absence of DNAPL and the identification of the locations of “confirmed” and “potential” DNAPL
- DNAPL mass present at the site
- Total contaminant mass in the plume(s) – both aqueous phase and sorbed
- Mass discharge immediately downgradient of the source and at a location of their choice further downgradient
- Estimation of first- order biodegradation rates

4.5.1 CSM Parameter Importance and Scoring

In developing their CSMs, each DM team was asked to investigate both the DNAPL source zone and the plume for the purpose of designing an EISB remedy. The DM team CSMs were therefore evaluated across multiple parameters. These performance parameters included both quantitative, qualitative and graphical parameters (Table 4-9). Quantitative parameters are those that are directly represented by a single numerical value (e.g., DNAPL mass). Qualitative parameters are those that require a word answer (e.g., is there DNAPL present at the site?). Graphical parameters are those that encompass elements of a CSM that are depicted in plan view or cross-section view, and include multiple values distributed over a large area (e.g, plume footprint). The methods used to evaluate each parameter are described below. For all parameters, the 'estimate' refers to the response (values, answer, or outline) provided by a DM team and the 'truth' refers to information in the corresponding VSD data array. True values for each quantitative and qualitative parameter are listed in Table 4-10. The importance of key parameters for site investigation and remediation is discussed further in Section 7.

Table 4-9: CSM Parameters and rationale for inclusion

Quantitative parameters	Importance
DNAPL mass	Many remedy designs are a function of DNAPL Mass (e.g. EISB)
Dissolved mass	Understanding of mass loading to downgradient receptors
Sorbed mass	Understanding of plume longevity
Average groundwater velocity	Critical in remedy design (e.g., thermal)
Mass discharge (2 locations)	Important in evaluating risk to receptors
Decay coefficient	Important in evaluating risk to receptors
Qualitative parameters	
Contaminants of concern	Missing a CoC can result in remedy failure or incomplete risk assessment
Average flow direction	Important for understanding amendment migration
DNAPL Presence	Presence/Absence of DNAPL will be important for remedy selection
Biodegradation Occurrence	Required information for MNA assessment as a component of remedy
Graphical parameters	
Plume footprint	
Source footprint	Important for remedy design targeting the source
Plume cross-section (parallel to flow)	
Plume cross-section (perpendicular to flow)	

Table 4-10: True values for CSM parameters

Parameter	VSD1	VSD2	VSD3
Quantitative parameters			
Average groundwater velocity (ft/yr)[a]	20.31	50.83	33.46
DNAPL mass (kg)[b]	10,160	14,923	21,440
Dissolved TCE mass (kg)	890	1363	859
Dissolved cDCE mass (kg)	285	155	180
Sorbed TCE mass (kg)	425	760	490
Sorbed cDCE mass (kg)	86	54	63
TCE Mass discharge (location 1)[c] (kg/yr)	93.8-142.5	0.02-519.9	52.9-156.6
TCE Mass discharge (location 2)[c] (kg/yr)	3.1-54.8	13.9-506.5	1.5-77.7
Decay coefficient (1/yr)	0.14	0.14	0.14
Qualitative parameters			
Contaminants of concern	TCE and cDCE	TCE and cDCE	TCE and cDCE
Average flow direction	to South	to North	to West
DNAPL presence	Yes	Yes	Yes
Biodegradation occurrence	Yes	Yes	Yes

[a] Based on the applied hydraulic head gradient and the geometric mean intrinsic permeability.
[b] Mass at the end of the plume generation time, which is less than the mass released (Table 4-6).
[c] Locations were selected by the DM teams during their virtual site investigation, therefore true value is different for each DM team.

4.5.2 Parameter Scoring

Quantitative parameters: All quantitative parameters were evaluated as the ratio of the estimate to the known true value:

$$\mathbf{Score_Q = Re/Rt} \qquad \textbf{[4-1]}$$

where $Score_Q$ is the score for the quantitative parameter, R_e is the DM Team estimate, and R_t is the true value. Therefore, a score of 1 represents a perfectly accurate answer, a score of 10 is an overestimate by one order-of-magnitude and a score of 0.1 is an underestimate by one order-of-magnitude.

Qualitative parameters: Most qualitative parameters were assigned a score of 1 if the DM team response matched the true conditions of the VSD. That is, values of 1 were assigned for correctly identifying TCE and cDCE as contaminants of concern, for indicating that there is DNAPL present at the site, and that biodegradation is occurring. The average groundwater flow direction was scored as the cosine of the angle between the estimated and true directions. Therefore, a score of 1 was assigned for no difference in direction, a value of 0.92 for a difference of 22.5°, and a score of 0 for a difference of 90° (cross-gradient).

Graphical parameters: Graphical parameters were based on an outline of a CSM feature (plume or DNAPL) depicted in a two-dimensional plan view or cross-section. There are two elements required for accuracy: (i) the area of the feature and (ii) the location of that area. Inaccuracies with respect to either element are detrimental to an accurate CSM. False negatives (estimated absence of DNAPL or dissolved VOC where true DNAPL or dissolved VOC exists) result in missed mass and poorly defined remediation targets, and false positives (estimated presence of DNAPL or dissolved VOC where true DNAPL or dissolved VOC does not exist) result in over design and increased cost. To account for this, graphical parameters were scored based on a difference in two area ratios, one that defines presence of the feature and one that defines its absence:

$$\mathbf{Score_G = A_{correct} / A_{tp} - A_{incorrect} / A_{ta}} \qquad \textbf{[4-2]}$$

where $Score_G$ is the score for the graphical parameter, $A_{correct}$ is the area of overlap between the estimated presence of the feature and the true presence, $A_{incorrect}$ is the area estimated to contain the feature but does not overlap with the true presence, A_{tp} is the true area where the feature is present, and A_{ta} is the true area where the feature is absent. Equation 4-2 penalizes both false positives and false negatives. It gives a score of 1 for perfect overlap between the estimated and true location of the feature ($A_{correct} = A_{tp}$ and $A_{incorrect} = 0$), a score of zero for estimates that the feature is present everywhere ($A_{correct} = A_{tp}$ and $A_{incorrect} = A_{ta}$), and score of zero for estimates that the feature is not present anywhere ($A_{correct} = 0$ and $A_{incorrect} = 0$). For all calculations, A_{ta} is based on a target area defined to extend outside of the true feature by half the feature width on either lateral edge, half the feature length on the upgradient edge, one feature length on the downgradient edge, and half the feature depth on the top and bottom edges. Selection of too large of a target area increases the denominator in the second term of Equation 4-2, which substantially reduces the penalty for false positives. A graphical scoring example is shown in Table 4-9.

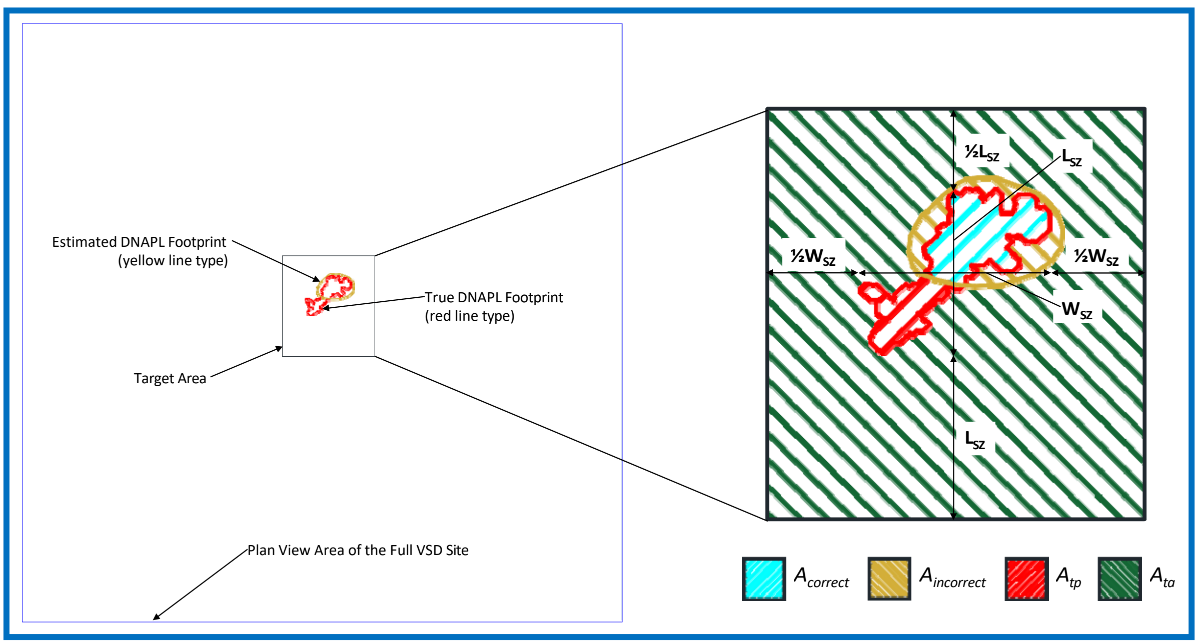


Figure 4-9: Illustration of the areas used to score graphical parameters, for example, the DNAPL footprint of VSD1. L_{SZ} is the length of the true DNAPL footprint, W_{SZ} is the width of the true DNAPL footprint.

4.6 Experience Based (EB) Remediation Design, Simulation, and Scoring

4.6.1 Overview

Following the conclusion of their EB virtual site investigations and the development of their CSMs, the DM teams were tasked with the development of an enhanced in situ bioremediation (EISB) remedy for all three VSD sites. EISB was chosen as the remedy for the site based on its suitability for the contaminants, long history of success at chlorinated solvent contaminated sites, availability as a remedy in SCOToolkit, and understanding of the process by the DM Teams. A single remedy approach was chosen to allow for consistent comparisons across the DM Teams as well as to allow for a single set of reaction kinetics to be utilized in all remedy simulations. Based on the data and information obtained from their virtual site investigations and CSMs, DM teams designed their EISB remedies to meet the functional POs established for each VSD. Functional POs were established from DIVER team EISB remedy model simulations where the perfect information of each virtual site was known; these are referred to as the optimal remedies. The DM teams submitted their EISB remedy designs to the DIVER team for model simulation. It was clearly communicated that the DM team remedy strategies would be applied to the true VSD sites and not to the developed VSD CSMs submitted by the DM teams, which allowed for a comparable remedy evaluation.

DM teams were given a period of 5 years to implement an active EISB remedy at each of the 3 VSDs. Within this timeframe, the DM teams were provided monitoring data upon their request and allowed one modification to their initial remedy design. The modification could involve any aspect of the design. Following this modification action(s), the modified remedies were simulated to the 5-year point without any further DM team correspondence (no additional changes allowed). No limitations were placed upon the DM Teams in terms of design with the exception that re-circulation systems could not be used.

The remedial performance of each DM team's design was evaluated 5 years post-completion of the EISB remedy (i.e., after 5 years of post-remedy dissolution, reaction, and transport for a total of 10 years since remedy inception) to determine if they had met the functional POs for each VSD site. The total costs of the DM team remediation designs were calculated over the 5-year active EISB remediation timeframe, which includes the costs associated with any remedy optimization/modification and accounted for the remedial operations and maintenance costs.

4.6.2 Remediation Modeling

The DM teams' remediation designs were simulated using the numerical model DNAPL3D-RX (also described in Section 4.2.2). The EISB modeling capabilities of DNAPL3D-RX were developed and further discussed by West (2009). Multi-Monod reaction kinetics (different from those described in Section 4.2.2) were implemented into DNAPL3D-RX to model the EISB designs submitted by the DM teams for VSDs 1 to 3 to allow for more realistic simulation of dichlorination all the way to ethene. The DNAPL3D-RX model utilized for the simulation of the

EISB remedies included the following additions compared to the model version described in Section 4.2.2:

- Additional solute transport parameters for the following chemical species: lactate, hydrogen (H_2), vinyl chloride (VC), ethene (ETH) and chloride (Cl^-). These input parameters are listed in Table 4-11;
- Multi-Monod kinetics to simulate the growth and decay of multiple bacteria species (lactate fermenters, methanogens and dechlorinators) and the sequential reductive dechlorination of TCE → cis-DCE → VC → ETH (Christ and Abriola, 2007). A full list of the Monod kinetics equations utilized by DNAPL3D-RX can be found in Appendix B. H_2 electron donor competition existed between methanogenic and dechlorinating species. Additionally, competitive inhibition terms were incorporated into each of the individual dechlorinating reaction steps. EISB Monod kinetic input parameters are listed in Appendix B;
- Multiple "pulse" type boundary conditions to simulate the operation (injection on/off) of substrate injection wells throughout the duration of the active remedy; and
- External bioaugmentation algorithms which allowed DM teams to bioaugment at requested locations anytime during the 5-year active remedy period.

To utilize the same modeling parameters for each VSD remedy, DM teams were constrained to using lactate as the organic substrate source. DM teams could request EISB performance monitoring results no more frequently than monthly. In terms of substrate delivery approaches, DM teams were given the following options based on the modeling limitations of DNAPL3D-RX:

- Continuously operating vertical water injection wells with a regular frequency of lactate dosing;
- Periodic injection of lactate solution into vertical injection wells at a regular frequency and dose; and
- Injection of lactate solution using Direct push technology (DPT) (push and drift) at a regular frequency and dose.

These delivery approaches (i.e., flow and/or concentration boundary conditions) were initially tested and found to be compatible with the DNAPL3D-RX model.

Table 4-11: Additional solute transport parameters required for VSD remedy simulations

Model Parameter	Value	Reference
VC Soil Organic Carbon-Water Partitioning Coefficient (mL/g)	11	TRRP (2005)
VC Free-Water Diffusion Coefficient (m^2/s)	1.23×10^{-9}	TRRP (2005)
Chloride Free-Water Diffusion Coefficient (m^2/s)	2.00×10^{-9}	West et al. (2008)
Ethene Free-Water Diffusion Coefficient (m^2/s)	1.34×10^{-9}	Christ and Abriola (2007)
Lactate Free-Water Diffusion Coefficient (m^2/s)	6.70×10^{-10}	[a]
Hydrogen Free-Water Diffusion Coefficient (m^2/s)	3.30×10^{-9}	West (2009)
First-Order Ethene Half-Life (days)	1.0	[b]

[a] Determined using reference values from Lide (2012) and an approximate correction factor from Poling et al. (2001).
[b] Developed for this study.

4.6.3 Remediation Objectives and Assessment

Remediation guideline documents were provided to the DM teams outlining the functional POs for each VSD site; remediation guidelines documents are presented in Appendix F. The functional POs established for each VSD included performance parameters for the following:

- Reduction of DNAPL mass,
- Reduction of dissolved phase, total chlorinated VOC (TCE + cDCE + VC) mass discharge downgradient of the DNAPL, and
- Reduction of TCE concentrations in groundwater downgradient of the DNAPL.

The focus of the functional POs established for the DIVER project was directed more towards DNAPL source zone remediation and reduction of source zone mass discharge rather than downgradient VOC plume(s) remediation to meet absolute numeric remedial objectives such as Maximum Contaminant Levels (MCLs) assuming a drinking water source. The DM teams were directed to develop their EISB remedies and apply these to the DNAPL source zone in each VSD. DM teams were provided site-specific (i.e., VSD-specific) POs that were determined from DIVER team remediation modeling of VSDs 1 to 3 where the "perfect" information of each VSD was known; these are referred to as the optimal remedies. These optimal remedies are further described in Section 4.6.6. The POs and performance assessment criteria established for each site were included in each VSD remedy guidance document and followed the same template outline listed below:

- Achieve a VSD-specific PO percentage reduction in DNAPL mass to be evaluated 5 years after the completion of the EISB remedy.
- Achieve a VSD-specific PO percentage reduction in the total chlorinated VOC (TCE + cDCE + VC) dissolved phase mass discharge across the vertical control plane oriented perpendicular to the mean groundwater flow direction, located 10 m downgradient of the

true DNAPL source zone. The mass discharge is evaluated 5 years after the completion of the EISB remedy.

- Achieve a VSD-specific PO percentage reduction in the average maximum TCE groundwater concentration in a sub-section of the vertical control plane oriented perpendicular to the mean groundwater flow direction, located 10 meters downgradient of the true DNAPL source zone.

This TCE dissolved phase plume sub-section width is equal to half of the source zone width and represents the average maximum TCE groundwater concentration within the core of the TCE dissolved phase plume ("TCE plume core"). The average maximum TCE groundwater concentration is calculated for the TCE plume core by calculating the maximum TCE groundwater concentrations of each 10-ft well screen interval spaced 4 ft apart (i.e., equal to the model discretization of 1.2 m) inside the TCE dissolved phase plume core and computing the mean of these individual 10-ft well screen maximum concentrations. The position of the TCE plume core along the vertical control plane (located 10 m downgradient of the source zone) is not temporally or spatially fixed and is dependent on the location where the highest average maximum TCE groundwater concentration is calculated. The average maximum TCE groundwater concentration is evaluated 5 years after the completion of the EISB remedy. Additional details are provided in Section 5.2.1.

- Total cost of the remediation, inclusive of EISB remedy-specific costs associated with pre-installation, installation, operations and maintenance, performance monitoring, and decommissioning activities. The total cost of remediation will also include any costs associated with the optimizations or modifications to the initial remedy designs specified by requests from the DM teams. The total cost of remediation is calculated over the 5-year period of the EISB remedy in constant dollars (i.e., not a net present value calculation).

The quantitative values that were specified for the POs for each VSD are presented in Table 4-12. The quantitative evaluation of the DM team remedy designs against these POs was conducted by the DIVER team, which knew the perfect information about each VSD. Further discussion on the quantitative assessment of the DM team remedies is described in Section 5.2.1.

Table 4-12: Performance objectives for each VSD

Remedial Performance Objective	PO		
	VSD1	VSD2	VSD3
Percentage reduction in DNAPL mass	30%	25%	25%
Percentage reduction in total chlorinated VOC dissolved phase mass discharge	50%	50%	50%
Percentage reduction in average maximum TCE groundwater concentrations	60%	50%	50%

4.6.4 Remediation Design and Implementation

After reviewing the guidance document and with the prior knowledge of each VSD from their earlier site investigations and developed CSMs, DM teams submitted their initial EISB remedy designs to the DIVER team to be modeled in DNAPL3D-RX. The submitted remedy designs from the DM teams included instructions with regards to the following detail(s) specific to their EISB remedies:

- Remediation well network
  - DM teams specified locations for their injection wells. New boring/well logs for their newly installed injection wells were provided by the DIVER team.
  - Fluid injection tests at the injection wells were completed by the DIVER team using the hydraulic conductivity fields of VSDs 1 to 3 and MODFLOW. Based on the measured water levels during active injection, DM teams finalized their injection flow rates, injection durations/schedules and lactate concentrations.
- Direct injection locations
  - DM teams specified direct injection locations where lactate was applied via DPT. Design information provided for direct injection included the number of direct injection points and the volume/mass of lactate to be added at each direct injection location.
- Baseline sampling and monitoring (prior to remedy)
  - Initial baseline monitoring results at injection and/or (new or existing) monitoring wells were provided based on DM team request. DM teams finalized their performance monitoring well network (locations and sampling frequency) based on these issued results.
- Bioaugmentation
  - DM teams specified the injection well and/or direct injection locations where bioaugmentation was to be implemented. The DM teams provided the volume(s) of dechlorinating culture that was to be added at each of the bioaugmented well(s).
- Performance monitoring well network (during the 5-year active remedy period)
  - DM teams specified well locations and biogeochemical analytes to be sampled for during the remediation timeframe. Both injection and monitoring (new or existing) well locations were requested to be sampled at a frequency no shorter than monthly for performance monitoring purposes by the DM teams. In the cases where new monitoring wells were installed, new boring/well logs were provided.

DM teams were permitted to revise their initial EISB designs once during the 5-year active remedy period. Performance monitoring results were only submitted to the DM teams as requested, as specified in their initial EISB designs. Based on the analysis of their performance monitoring results, DM teams could modify their EISB remedies by making direct adjustments to their existing initial design (e.g., injection rates, injection durations, lactate concentrations, bioaugmentation, well decommissioning) and/or by installing new remediation well locations. DM team remedies were considered finalized once revised EISB remedy designs were submitted to the DIVER team. The revised EISB remedy designs were modeled in DNAPL3D-RX from the timepoint where the

DM team requested the remedy revision to the end of the 5-year active remedy period. In the cases where DM teams did not request a revision to their initial EISB remedies, the DM teams' initial EISB remedies were implemented (i.e., modeled in DNAPL3D-RX) over the 5-year active remedy period. Performance monitoring results were not issued after the commencement of the revised EISB remedy since DM teams could not further revise their EISB remedy designs. A brief description and detailed table summarizing the EISB remedy designs submitted from each DM team are presented in Section 5.2.1.

4.6.5 Remediation Performance Objectives

The remediation performance objectives (described in Section 4.6.3) were quantitatively assessed following the completion of the EISB remedy, simulated as 5 years post initiation of the EISB remedy. The methods used to evaluate each objective are described below.

DNAPL Mass Reduction: The DNAPL masses remaining in each VSD model domain following the conclusion of each EISB remedy was evaluated against the initial pre-remedy VSD DNAPL masses presented in Table 4-6. DNAPL3D-RX calculates and tracks the DNAPL mass by converting nodal non-wetting phase saturations to masses, then sums all non-wetting phase nodal masses within the finite difference model grid (West and Kueper, 2012).

Total Chlorinated VOC Dissolved Phase Mass Discharge Reduction: The total chlorinated VOC (TCE + cDCE + VC) dissolved phase mass discharge measured following the conclusion of each EISB remedy was evaluated against the initial pre-remedy total chlorinated VOC dissolved phase mass discharge(s) for each respective VSD (Table 4-10). Mass discharge (M_D^n) is evaluated across the vertical control plane oriented perpendicular to the mean groundwater flow direction, located 10 m downgradient of the true DNAPL source zone in each VSD. Total chlorinated VOC dissolved phase mass discharge ($M_D^{Total\,VOC}$) is calculated and tracked by DNAPL3D-RX by summing the local scale mass discharge at each model node located along the vertical control plane:

$$M_D^n = \sum_{i=1}^{N} C_i^n q_i A_i \qquad [4\text{-}3]$$

$$M_D^{Total\,VOC} = M_D^{TCE} + M_D^{cDCE} + M_D^{VC} \qquad [4\text{-}4]$$

where i denotes an individual model node located along the vertical control plane 10 m downgradient of the true DNAPL source zone (with respect to each VSD), n is the dissolved phase VOC species of interest (TCE, cDCE, VC), q is the nodal wetting phase Darcy flux oriented in the direction of mean groundwater flow (extracted from the model), C is the nodal aqueous concentration, and A is the cross-sectional area of each individual finite difference grid block oriented perpendicular to the mean groundwater flow direction which contains the i model node(s).

Average Maximum TCE Groundwater Concentration Reduction: The average maximum TCE groundwater concentration within the post-remedy TCE plume core measured following the conclusion of each EISB remedy was evaluated against the initial pre-remedy average maximum TCE groundwater concentration within the pre-remedy TCE plume core(s) for each respective VSD (Table 4-13). As illustrated in Figure 4-10, the location(s) of the TCE plume core(s) and their respective 10-ft screen intervals of maximum TCE groundwater concentrations vary laterally, vertically, and temporally (e.g., pre-remedy conditions, post-remedy conditions following an applied remedy). The TCE groundwater concentration for a 10-ft well screen interval ($C^{TCE}_{well,j}$) and the average TCE groundwater concentration along the TCE plume core(s) (C^{TCE}_{core}) were calculated using the following equations:

$$C^{TCE}_{well,j} = \frac{\sum_{i=1}^{N} C_i^{TCE} q_i}{\sum_{i=1}^{N} q_i} \qquad [4\text{-}5]$$

$$C^{TCE}_{core} = \frac{\sum_{j=1}^{N} C_{well,j}}{N} \qquad [4\text{-}6]$$

where i denotes a model node located within the TCE plume core, q is the nodal wetting phase Darcy flux oriented in the direction of mean groundwater flow, C^{TCE} is the nodal TCE aqueous concentration, and j denotes an individual 10-ft well screen interval located within the TCE plume core.

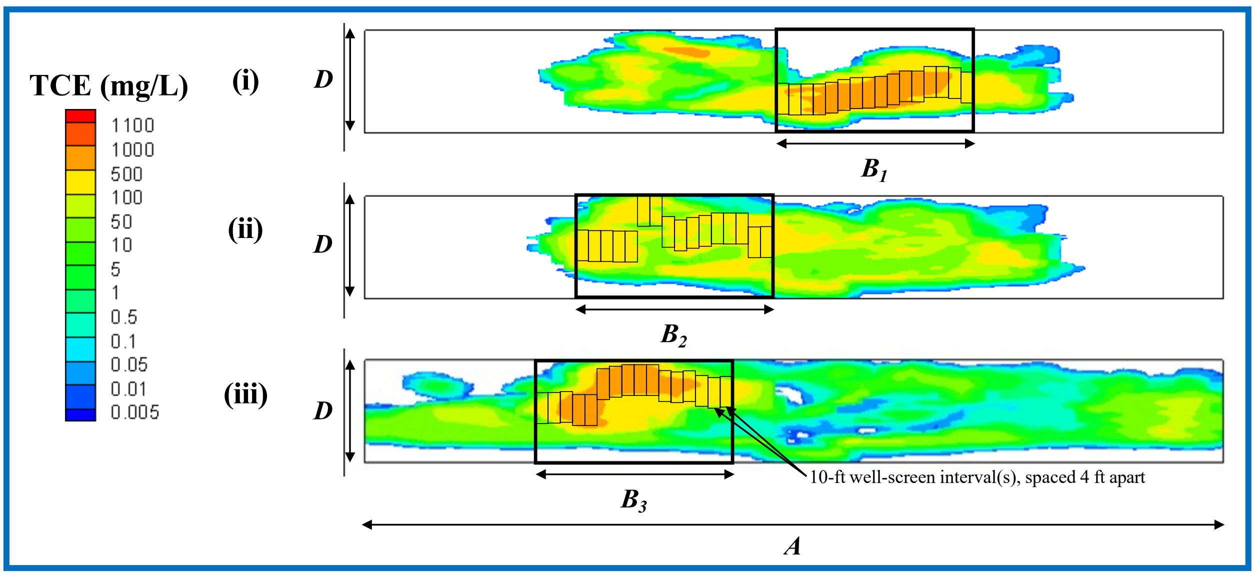


Figure 4-10: Illustration of the TCE plume core method for evaluating the average maximum TCE groundwater concentration. In this example, the location of the TCE plume core(s) (i.e., outlined using the dashed line type) along the vertical control plane oriented perpendicular to the mean groundwater flow direction (i.e., in these figures, mean groundwater flow direction is out of the page), 10 meters downgradient of the pre-remedy true DNAPL source zone in VSD2 are presented for the following scenarios: (i) Pre-remedy TCE plume core location for VSD2; (ii) TCE plume core location, 5 years following the conclusion of the optimal EISB remedy; and (iii) TCE plume core location, 5 years following the conclusion of Team D's EISB remedy. *A* is the width of the vertical control plane for VSD2. *B1*, *B2*, and *B3* are the TCE plume core widths for scenarios (i), (ii), and (iii), respectively. *B1*, *B2*, and *B3* are equal widths, and are equivalent to half of the true DNAPL source zone width for VSD2.

Table 4-13: DNAPL and dissolved phase mass, concentration, and mass discharge

VSD	TCE DNAPL Mass (kg)	TCE Dissolved Phase Mass Discharge (kg/day)[a]	cDCE Dissolved Phase Mass Discharge (kg/day)[a]	Total Chlorinated VOC Dissolved Phase Mass Discharge (kg/day)[a]	Average Maximum TCE Groundwater Concentration Within The TCE Plume Core (mg/L)[b]
1	10,160	0.30	0.12	0.42	547
2	14,923	0.65	0.10	0.75	590
3	21,440	0.25	0.07	0.32	434

[a] Mass discharge(s) is measured with respect to the vertical control plane(s) perpendicular to the mean groundwater flow direction, 10 meters downgradient of the true DNAPL source zone.

[b] Concentration(s) is measured within the TCE plume core(s) of the VSD-respective vertical control plane(s) perpendicular to the mean groundwater flow direction, 10 m downgradient of the true DNAPL source zone.

Total Cost of The EISB Remedy: The total costs of each EISB remedy were calculated over the 5-year active remedy period. EISB remedies were costed for expenditures associated with the following EISB remedy design activities:

- Pre-installation activities (permitting, planning, procurement);
- Installation activities:
  - Contractor/driller labor/mobilization/demobilization;
  - Borehole drilling, remedy/monitoring well installation, remedy/monitoring well headworks/in-well and plumbing components, direct-push injection boreholes;
  - Commissioning and reporting; and
  - Purchase of frac tanks.
- Operations and maintenance:
  - Rental of on-site injection trailers;
  - On-site utilities (water, electricity);
  - Lactate masses/volumes;
  - Bioaugmentation culture volumes; and
  - Contractor labor and equipment needed for maintenance and injection events.
- Performance monitoring activities:
  - Contractor labor and equipment needed for remediation performance monitoring;
  - Costs associated with DM team-requested laboratory analyses of groundwater samples;
  - Costs associated with containment and disposal of on-site purge water; and
  - Reporting with respect to performance monitoring results.
- EISB remedy decommissioning (flat rate dependent on the scope of the EISB remedy design).

4.6.6 Optimal Remedies

Optimal remedies (achieving the POs at minimum cost) were developed by the DIVER team for VSDs 1 to 3. Model sensitivity EISB remedy runs were performed for each VSD, varying the different components of EISB remedy design (e.g., number and location of injection wells, injection rate, lactate concentration, continuous/periodic injection schedules). A list of the optimal EISB remedies used to develop the POs for each VSD determined from the model sensitivity runs is presented below (the injection well networks implemented in the optimal remedies for VSDs 1 to 3 are illustrated in Figure 4-11).:

- VSD1 Optimal EISB Remedy Design
  - Remediation well network: 8 injection wells were installed within the true DNAPL source zone. Lactate was injected using a flow rate of 0.6 gallons per minute (gpm) for a duration/schedule of 1 day per week over the five-year active remedy period. A lactate concentration of 27 gram per liter (g/L) was used at each injection well.
  - Performance monitoring well network, sampling and analytical plan.
- VSD2 Optimal EISB Remedy Design
  - Remediation well network: 20 injection wells were installed within the true DNAPL source zone. Lactate was injected using a flow rate of 0.1 gpm for a duration/schedule of 1 day per week over the five-year active remedy period. A lactate concentration of 19 g/L was used at each injection well.
  - Performance monitoring well network, sampling and analytical plan.
- VSD3 Optimal EISB Remedy Design
  - Remediation well network: 26 injection wells were installed within the true DNAPL source zone. Lactate was injected using a flow rate of 0.15 gpm for a duration/schedule of 2 days per week over the five-year active remedy period. A lactate concentration of 19 g/L was used at each injection well.
  - Performance monitoring well network, sampling and analytical plan.

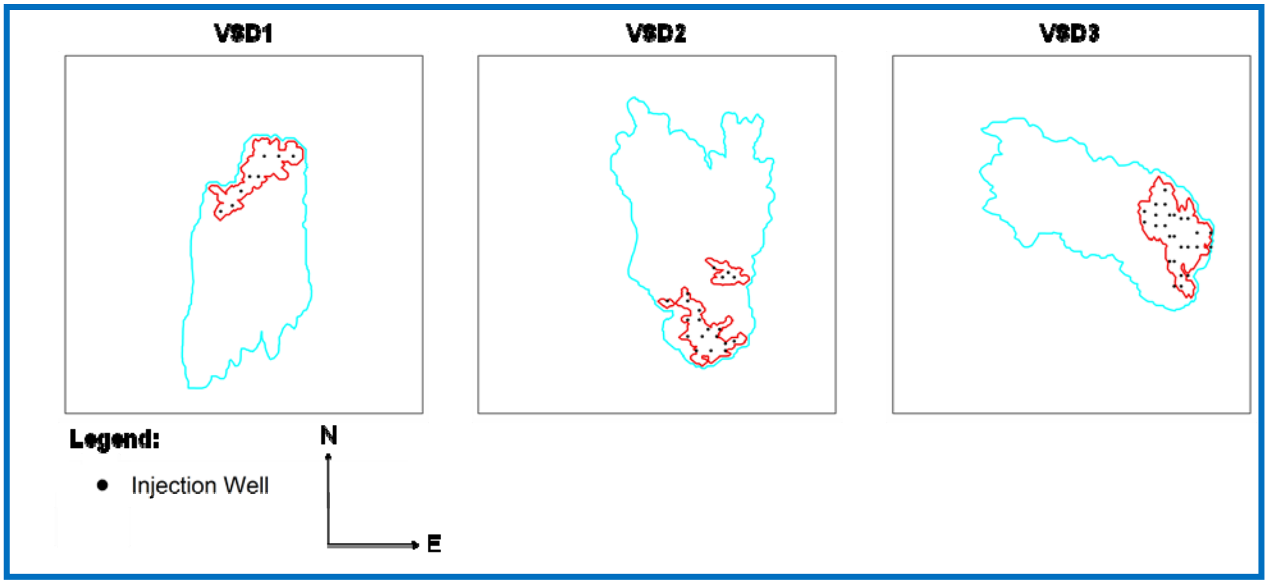


Figure 4-11: Injection well networks for the optimal EISB remedies. Red line type depicts the areal footprint of the true DNAPL source zones. Cyan line type depicts the areal footprint of the true VOC plumes.

The DM Team EISB remedies for VSDs 1 – 3 were quantitatively assessed against the optimal EISB remedies via an approach described in Section 4.6.3.

4.7 Decision Theoretic (DT) Remediation Design, Simulation, and Scoring

Remediation designs were optimized for VSD 1 and VSD 2 using SCOToolkit to assess the effects of increasing site characterization information on remediation strategy, success, and cost. The CSMs prepared for VSD1 and VSD2 by the DM teams formed the basis for the analysis using a two-step stochastic modeling approach to:

7) Calibrate uncertain site parameters (e.g., hydraulic conductivity, source mass and discharge, biodegradation rates etc.) modeled through probability distributions; and

8) Identify the best remediation strategy for minimal cost. Optimal remediation of the calibrated models was achieved by minimizing a cost function for enhanced in-situ bioremediation (EISB).

The amount of site information used to estimate model parameters was increased stepwise to determine the effects on remediation success and cost. The central component of this approach is a semi-analytical mathematical model used to simulate DNAPL source depletion and dissolved phase transport over time in response to natural and engineered conditions. Additional details on the SCOToolkit model can be found in Parker et al (2018). The CSM data provided by the DM teams were used to calibrate the simulation model and to estimate parameter covariances and residual prediction error. Forward predictions of remediation performance and cost were performed for defined remediation strategies, operating rules, and remediation criteria. Stochastic design optimization was performed to determine values of remediation design variables that minimize the expected cost.

4.7.1 Design

The DT evaluation for VSD1 and VSD2 was performed using the SCOToolkit, which couples semi-analytical DNAPL source depletion and transport models with parameter estimation (calibration), error propagation, and stochastic optimization (Parker et al., 2018). Model parameters may be calibrated to field observations/data (plume concentrations, source mass and/or source mass discharge) based on prior estimates of those parameters and their uncertainty. Monte Carlo simulations are then performed to identify optimal remediation decisions that minimize the expected cleanup cost while achieving specified reductions in source mass, source mass discharge and plume concentrations at compliance wells.

Dissolution of TCE DNAPL and reactive transport of a single component dissolved phase under natural and EISB conditions were simulated. DM Team CSMs for VSD1 and VSD2 were reproduced in simplified, reduced order (two-dimensional [2D]) homogeneous and isotropic model domains with uniform 1D groundwater flow fields, rotated through 90 or 270 degrees and rectilinear source terms (Figure 4-12).

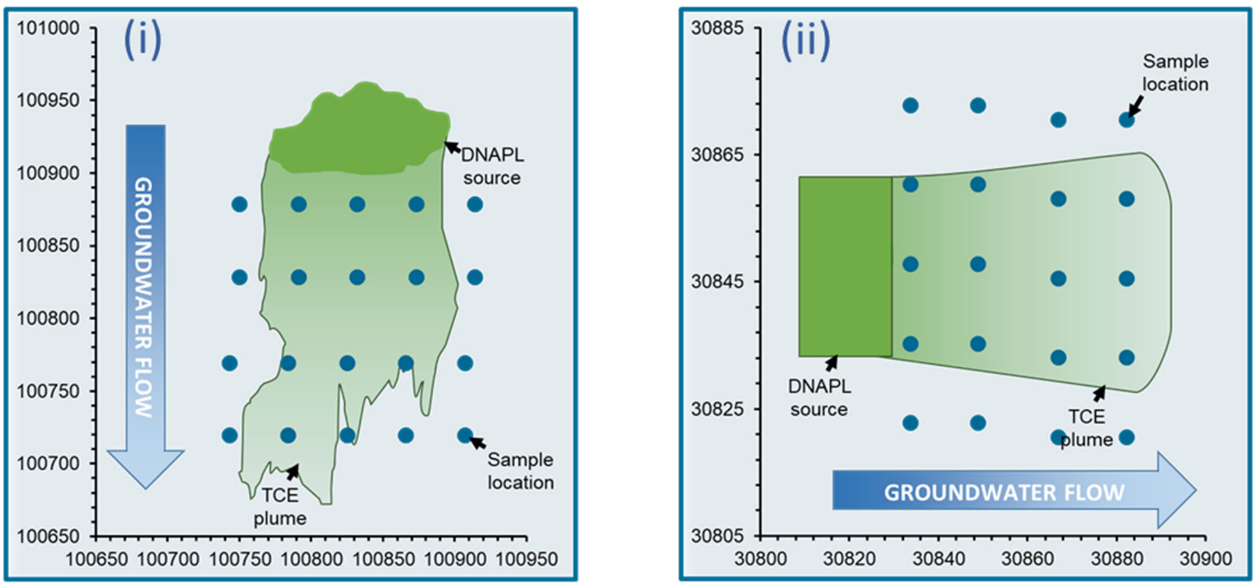


Figure 4-12: Converting DM Team VSD CSM (i) to SCOToolkit model domain (ii)

The source and plume attenuation processes represented in the SCOToolkit models included:

- DNAPL dissolution – a power law (β) relating source mass removal with source mass discharge to assumed source architecture (residual, pooled or mixed DNAPL);
- Plume attenuation – dispersivity (2D), retardation (reversible linear sorption) and biotic degradation (1^{st} order).

Remediation was simulated by a single, constant rate electron donor injection via a gallery in the upgradient edge of the DNAPL source (Figure 4-13) with implicit simulation of DNAPL dissolution and biodegradation rate enhancements. Optimization of remedy design variables (injection rate and duration) aimed to identify the lowest cost solution satisfying all remediation criteria.

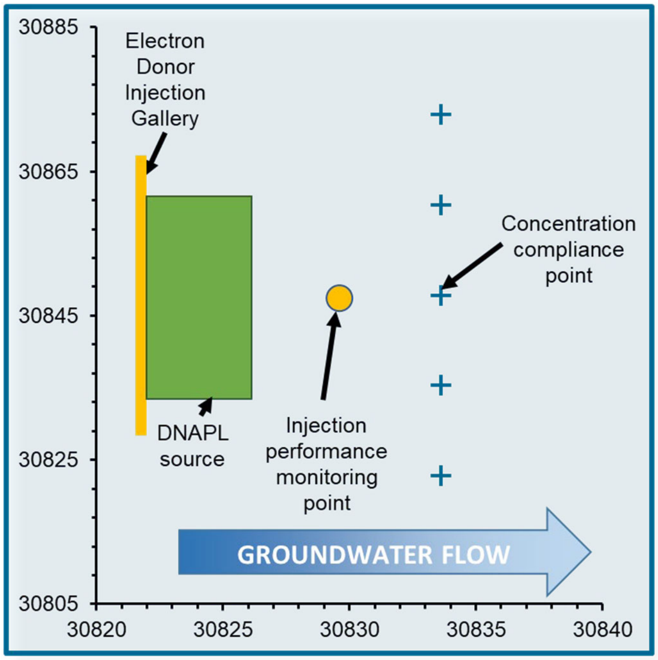


Figure 4-13: EISB Remediation implementation in SCOToolkit

Since the POs were percentage-based, two optimization routines were assessed:

- Relative criteria based on the flow and transport models for the DM Teams' CSMs (i.e., a percent reduction from each DM Team's estimate). Success would be indicated despite not achieving the actual objectives if the R_e was inaccurate.
- Fixed target criteria based on the actual percent reductions (i.e., percentage reduction from the true value). Rather than achieve a 25% reduction the remediation design must achieve an actual value (e.g., 100 kilogram per day [kg/day]).

The DT evaluation of the DM Teams' CSMs was performed in three modeling phases (Table 4-14).

Table 4-14: Phased decision theoretic evaluation

Modeling Phase	Modeling Parameter and Data Sources	Flow and Transport Model Calibration	Remediation*
1. Deterministic	Phase I and DM Team CSM report	Not performed	Optimize remedy based on parameterized DM Team CSM
2. Stochastic	Phase I and DM Team CSM reports, considering parameter uncertainty	Performed with plume concentration timeseries	Optimize remedy across 100 realizations of the calibrated flow and transport models of the DM Teams' CSMs
3. Stochastic	All available data from the DNAPL3DRX model	Performed with plume concentration, source mass and source mass discharge timeseries	Optimize remedy across 100 realizations of the calibrated flow and transport model

* The optimal remedy is the lowest cost solution that meets the remediation criteria within bounds of remediation design variables (injection rate, duration) based on 1 (deterministic) or 100 (stochastic) realizations. For Modeling Phases 2 and 3, the result is average of lowest cost solutions across 100 realizations.

Modeling Phases 1 through 3 were performed for all four DM Teams' CSMs and the DNAPL3DRX model (perfect information) for VSD1. Only Modeling Phases 1 and 2 were completed for the CSM of VSD2 provided by one of the DM Teams. Phase 3 modelling was not completed for VSD2 due to challenges representing the apparent complexity of this VSD with SCOToolkit as regardless of the flexibility of parameter distributions provided to SCOToolkit effective calibration could not be achieved. This is potentially due to the heterogeneity within VSD2 being too extreme to simulate with a vertically averaged analytical model such as SCOToolkit.

4.7.2 Simulation

The DT Evaluation for each phase comprised a 4-step process of model parameterization; calibration; optimization; and assessment.

<u>Model Parameterization</u>

Flow and transport model parameters (Table 4-15) were identified, calculated, or inferred from review of the Phase I and DM Team CSM reports for VSD1 and VSD2. Where required, model parameterization was supported with literature or default model values.

Table 4-15: Key flow and transport model parameters

Aquifer	Source	Plume
Darcy velocity*	Mass* Mass discharge* DNAPL architecture* Length (parallel with flow) Width (transverse to flow)*	Dispersivity* Decay rate* Retardation

* Variable parameters subjected to calibration

Some aquifer, source and transport model parameters are inherently variable. For Modeling Phases 2 and 3 (stochastic), variability in seven parameters (denoted with a * in Table 4-15) was represented using probability density functions (PDFs, normal or lognormal distributions[1]). The PDFs were defined by mean, standard deviation, lower and upper bound values based on parameter datasets reported by the DM Teams, or on consistent sets of assumed values for teams that did not report ranges or uncertainty in their CSMs. Summaries of the model parameterization for each DM Team for VSD1 and VSD2 are included in Appendix G.

Calibration

Field observation data (e.g., plume concentrations, source mass and source mass discharge) are a function of the flow and transport model parameters and their uncertainty. Calibration was performed during Modeling Phases 2 and 3 to improve upon *prior* estimates of parameters and their uncertainty, given field observation data (e.g., groundwater concentrations as demonstrated in Figure 4-14).

1 Variable parameters can only be represented in SCOToolkit by normal or lognormal PDFs. PDF selection was based on observed or reported variability for specific parameters and the requirement for model simulations to use non-negative values ($x \geq 0$) for certain parameters. PDF selection was standardised for simulation of VSD1 and VSD2.

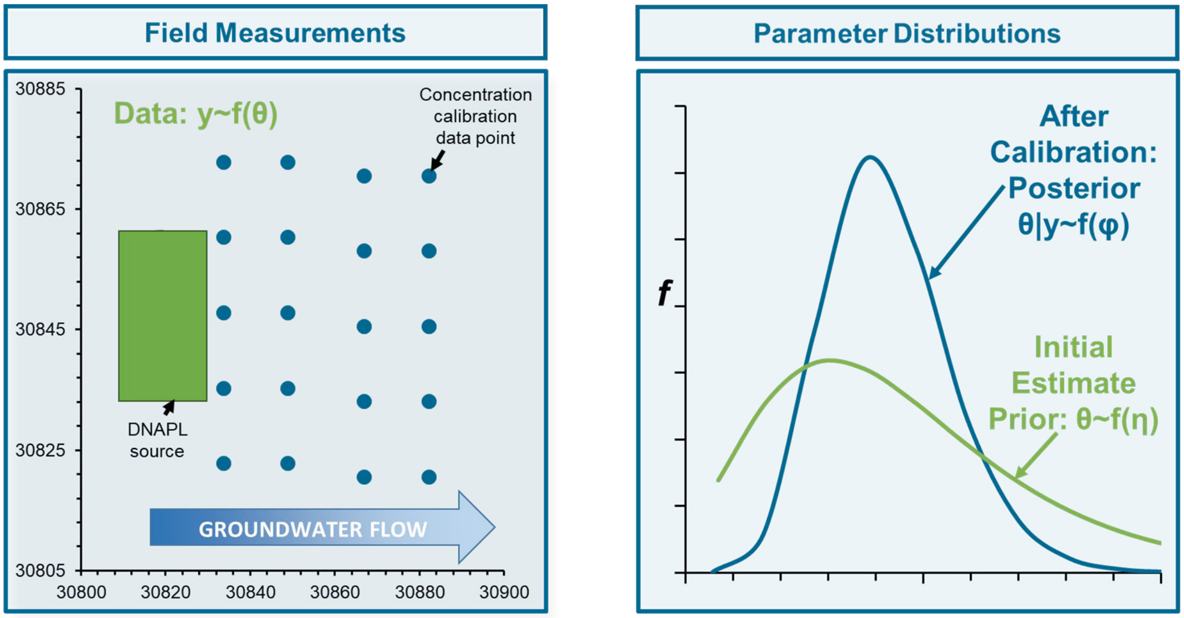


Figure 4-14: Posterior distribution derivation with groundwater concentration data

In Modeling Phase 2, the field observation data comprised plume concentration timeseries data from groundwater monitoring wells; in Modeling Phase 3, the observation data were extended to also include source mass and source mass discharge timeseries data (Table 4-16). In both phases, noise in the plume concentration data was considered using the average natural log (*ln*) standard deviation of concentrations in the timeseries (*SlnC*):

$$SlnC = \frac{s_{ln}}{N^{1/2}} \quad [4\text{-}7]$$

Where s_{ln} is the sample *ln* standard deviation and N was the number of samples.

Table 4-16: Modeling phase 2 and 3 calibration datasets

Modeling Phase	VSD1	VSD2
2. Stochastic	• TCE concentrations in groundwater for 20 single-depth interval wells arranged in four transects • Timeseries data provided for up to four sampling events (years 2006, 2010, 2011 and 2012) • Initial estimate of noise in concentration data (SlnC 0.1)	• TCE concentrations in groundwater for 27 single-depth interval wells arranged in four transects • Time series data provided for up to nine sampling events (years 2008 to 2015 inclusive plus a second event in 2015 corresponding to the DM Teams' CSM investigations) • Noise applied to concentration data (SlnC 0.02)
3. Stochastic	• TCE concentrations (TCE) from DNAPL3DRX model for 20 full aquifer thickness/vertically averaged wells arranged in 4 transects for 2006, 2010, 2011 and 2012 with noise (SlnC 0.1) • Source mass (DNAPL) depleted 1992 to 2012 • Source mass discharged 1992 to 2012	Not performed

Posterior distributions of the variable parameters were derived through the calibration process, with revised estimates for their uncertainty (Figure 4-14).

Remediation Cost Optimization

Remediation was simulated by a single, constant rate sodium lactate electron donor injection via a gallery in the upgradient edge of the DNAPL source (Figure 4-13). DM Team-specific and consistent remediation design parameters were applied (Table 4-17). Summaries of the model remediation parameters for each DM Team for VSD1 and VSD2 are included in Appendix G.

Table 4-17: Remediation design parameters

Assumptions applied to all DM Teams	Based on DM Team CSM or Flow and Transport Model Calibration
• Infiltration rate (based on hydraulic testing) • Maximum sodium lactate electron donor concentration (solution density ≤1.05 kg/L) • Background aquifer geochemistry/ electron donor demand • Maximum duration of injections (≤5 years) • DNAPL mass transfer enhancement coefficient • Performance monitoring strategy (quarterly in 5 well compliance transect) • Compliance regime • Remediation costs • Monitoring costs	• Electron donor gallery width and thickness (1.5x width and 1x thickness estimates) • Maximum injection rate (based on electron donor gallery width) • Maximum DNAPL dissolution enhancement (based on pre-remedy source mass discharge estimates) • Compliance well location (10 m downgradient of DNAPL source) • Penalty date (based on estimated plume velocity)

The injection rate and duration (≤5 years) were optimized to deliver the lowest cost remedy that achieved all three remedial criteria. Compliance with the remedial criteria was measured using a regression-based confidence limit rule. Compliance was achieved if the 95% upper confidence limit (UCL) over a 5-year lookback period was below the remedial criteria, at which point the simulated injection would be terminated.

The remediation scenarios required that compliance should be achieved a maximum 5 years after completion of EISB, else a penalty would be incurred. However, the arrival times for treated groundwater in the compliance well transect based on some DM Teams' CSMs exceeded this timeframe. This aspect of the remediation scenarios had to be relaxed for the DT evaluation, which applied penalty remediation cost on penalty dates based on the sum of:

- The maximum duration of injections (+5 years),
- Estimated TCE travel time between the electron donor gallery and compliance well transect (years), and
- Lookback period (+5 years).

4.8 Summary

A significant amount of the effort of the DIVER project (greater than 50%) went into the development of VSD1 – 4 to provide perfect data, the translation of the data to investigation results for the DM Teams and the simulation of the 12 remedies submitted for VSD1 – 3. This has been summarized in the preceding sections. The remaining sections of this report present the data gathered from the CSM development and assessment as well as the remediation design, modelling, and comparison between EB, DM, and perfect information approaches.

5 CSM AND REMEDIATION RESULTS AND ASSESSMENT

5.1 Experience Based CSM

5.1.1 Investigation Strategies

The approaches used by the DM teams for investigation of VSDs 1 to 3 are illustrated in Figure 5-1. Symbols are used to represent different investigation tools (boreholes, monitoring wells, CMT wells, MIP and DyeLIF), colors are used to represent the sequence of installation (by mobilization number rather than by individual tool location), and the placement relative to the 'true' DNAPL and plume is given by the symbol location. Each panel in Figure 5-1 is also presented individually in Appendix H for clarity.

Overall, Figure 5-1 shows that there was more variation between DM team approaches than between the implementation of those approaches at different sites (greater differences between rows rather than columns in Figure 5-1). This suggests that DM teams have a particular strategy for site investigation and make only minor modifications for site complexity (keeping in mind all VSDs 1 to 3 shared similar attributes as TCE-impacted sites in unconsolidated geological material). In general, the approaches were similar in their use of multiple (2-4) mobilizations, and their substantial use of MIP-HPT (19-74 locations) in early mobilizations. Differences between approaches were predominantly in their use of boreholes, CMT and DyeLIF, as well as the number of groundwater and soil samples analyzed. Post-investigation discussions with the DM Teams indicated that each approach was based on their experience in site investigation projects, the results of previous rounds of sampling, and development of a CSM for the site. No team used any form of modeling (other than graphical CAD-type modeling) or any VOI approaches to support their investigation strategy. It is possible that the budgets allocated to the DM Teams did not allow for extensive modeling to be performed.

Figure 5-2 and Figure 5-3 summarize the investigation tools and sample analyses conducted by the DM teams across all VSDs 1 to 3. Corresponding plots of investigation tools and sample analyses for each VSD are presented in Appendix I. The strategies of each DM teams are summarized in the sections below.

It is also important to note that DM teams appeared to refine their investigative approach as they progressed from VSD1 to VSD2 to VSD3 (which were investigated in order). This is apparent in both a decreased density of tool placement (e.g., DM Team B VSD1 to VSD3) and fewer tools placed far from the 'true' DNAPL and plume (e.g., DM Team C VSD1 to VSD3). This is not the case for every team and every VSD, but it suggests that performance on VSDs 1 and 2 may be more representative of industry practice. However, learning through the progression of VSDs did not necessarily result in improved parameters. The role of overconfidence effects and intuition bias may account for this (Clayton, 2017). Of 15 graphical parameters estimated at more than one VSD by a DM team, 8 were lowest for VSD1 (53%) (Figure 5.8). However, of 33 quantitative parameters estimated at more than one VSD by a DM team, only 12 were lowest for VSD1 (36%).

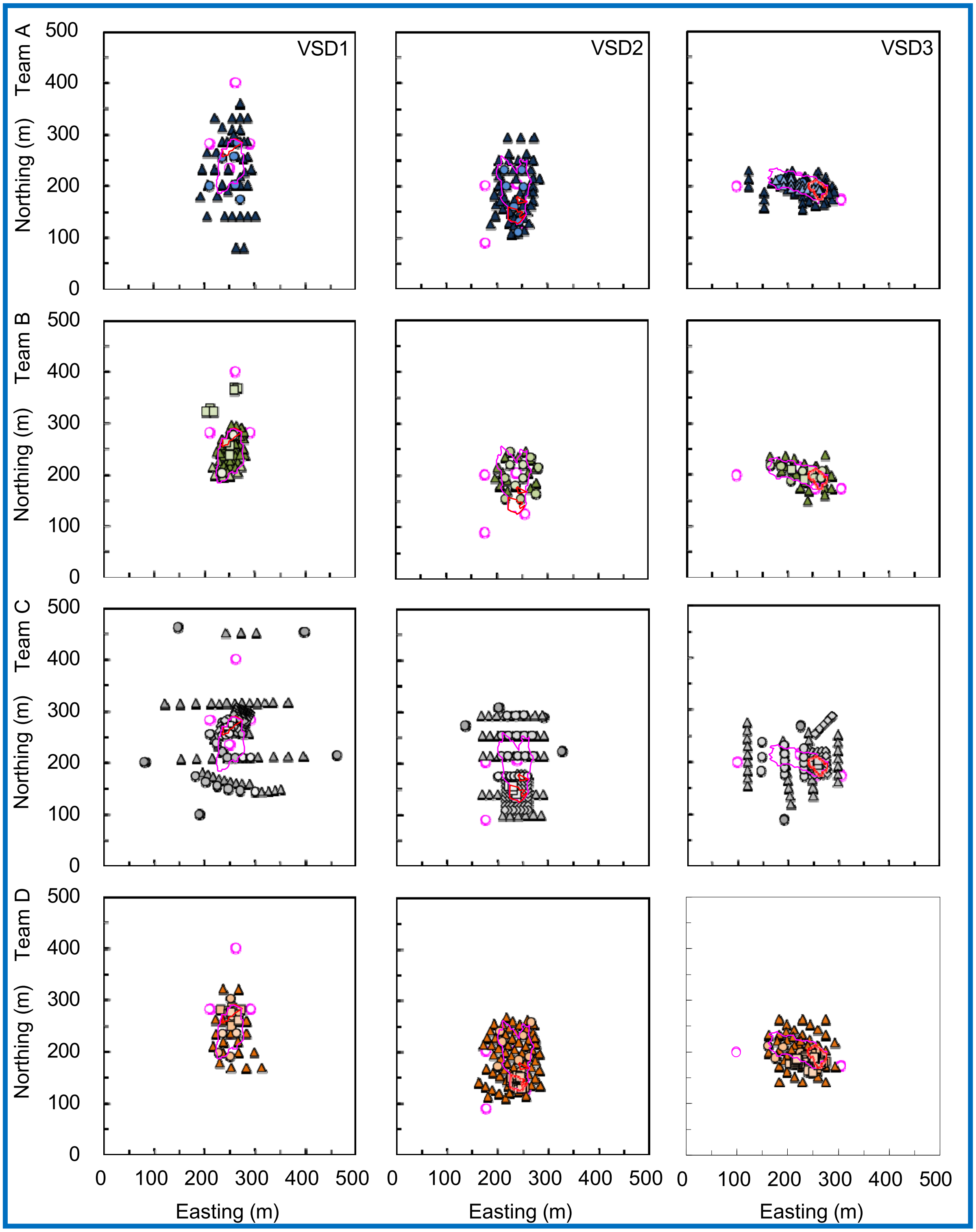


Figure 5-1: Deployment of site investigation tools by DM Teams during the investigation of VSD1-3, where darker shades represent tools deployed during earlier mobilizations. Pink circles represent monitoring wells installed as part of the Phase 1 ESA, and the true DNAPL source (red) and chlorinated ethene plume (pink) are outlined. Different symbols represent boreholes (■), MIP-HPT (▲), monitoring wells (●), DyeLIF (♦), and CMT wells (○).

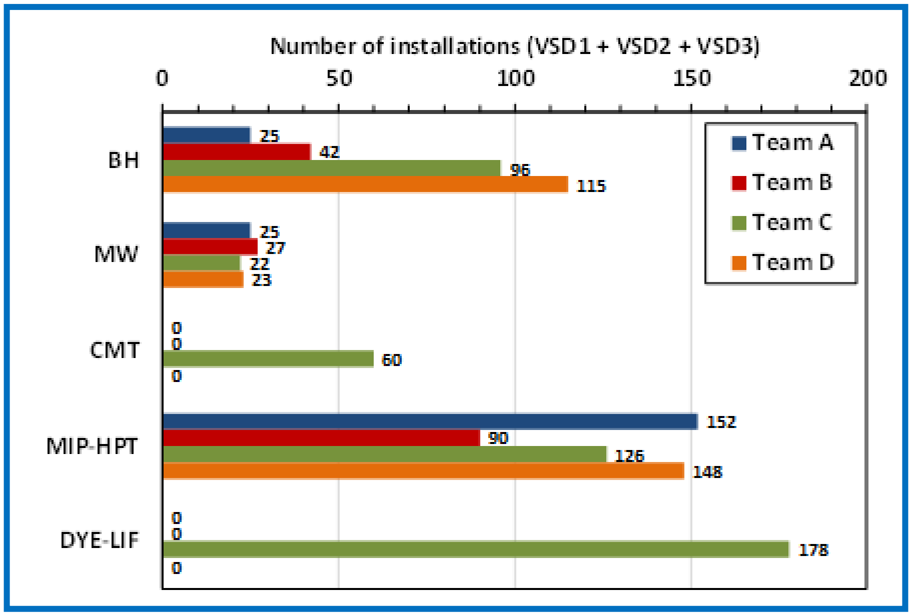


Figure 5-2: Tool deployments by DM Teams

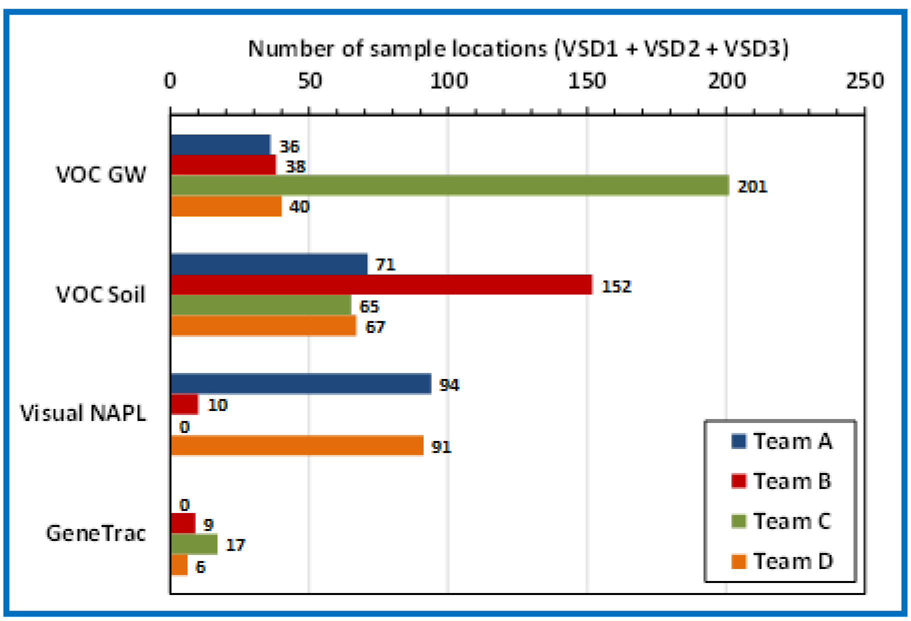


Figure 5-3: Samples taken by all DM Teams

<u>Team A Investigation Strategy:</u> Overall, DM team A used lines of MIP-HPT perpendicular to groundwater flow (as calculated from monitoring well water levels) for delineation of the plume followed by the installation of monitoring wells in the suspected plume and source zone over few mobilizations. Quantification focused on correlations to MIP-HPT results. Their approach is summarized in Table 5-1, Table 5-2, and Table 5-3.

Table 5-1: Summary of Team A approach for VSDs 1 to 3

Number of mobilizations:	- two or three (depending on VSD)
Step 1:	- MIP-HPT at 43-55 locations at a spacing of 25-50 ft. installed in a series of closely spaced transects, generally starting downgradient of REC locations and moving upgradient towards the suspected source zone, followed by additional locations within the suspected plume. - All MIP-HPT were installed during the first mobilization.
Step 2:	- Monitoring wells installed at 6-12 locations within the suspected plume and source zone, often immediately adjacent to previous MIP-HPT locations. - Pumping test at one newly installed monitoring well. - Monitoring wells and pumping test conducted during the second mobilization.
Step 3:	- Additional MIP-HPT at 17 locations at VSD3.

Table 5-2: Summary of Team A mobilizations for VSDs 1 to 3.

VSD	Mobilization	
1	1	- 43 MIP-HPTs (S1-MH-01 to S1-MH-43)
	2	- 6 Sonic MWs (MW-05 to MW-10) - Pumping test at MW-07 (pumped well); MW-3S, MW-4S, MW-05 and MW-06 were used as observation wells
	3	- Sampling only
2	1	- 54 MIP-HPTs (MiHPT-01 to MiHPT-54)
	2	- 7 Sonic MWs (MW-05 to MW-11) - Pumping test at MW-09 (pumped well); MW-07, MW-08, MW-11 and MW-4S were used as observation wells
3	1	- 55 MIP-HPTs (MiHPT-01 to MiHPT-55)
	2	- 12 Sonic MWs (MW-05, MW-06, MW-07 D/S to MW-11 D/S) - Pumping test at MW-10S (pumped well); MW-3S, MW-09S, MW-09D, MW-10D, MW-11S and MW-11D were used as observation wells
	3	- 17 MIP-HPTs (MiHPT-56 to MiHPT-72)

Table 5-3: Summary of Team A data analysis approach for VSDs 1 to 3.

Analysis	
Hydraulic conductivity:	- Pumping test data.
Groundwater velocity:	- Estimated hydraulic conductivity from pumping test, assumed porosity, and estimated hydraulic gradient.
DNAPL location:	- Threshold PID result from MIP-HPT, using a threshold of 20 V (VSD1), 29 V (VSD2) or 28 V (VSD3). - Combined with NAPL dye test results at VSD2 and VSD3.
DNAPL mass:	- Assumed 10% NAPL saturation in regions above the chosen PID threshold.
Plume location:	- PID results from MIP-HPT.
Dissolved concentrations:	- Aqueous concentrations correlated to PID response from MIP-HPT.
Plume mass:	- Integrated plume concentrations using Leapfrog model, with sorbed concentrations based on an estimated distribution coefficient.
Mass discharge:	- Based on concentrations measured in one monitoring well for each of two downgradient locations.

5.1.2 Team B Investigation Strategy

Overall, DM team B used a high-density, inside-out, unstructured MIP-HPT grid for delineation of the plume followed by borehole and monitoring well installation over multiple mobilizations. Quantification focused on correlations of DNAPL and dissolved phase presence and concentrations to MIP-HPT results. Their approach is summarized in Table 5-4, Table 5-5, and Table 5-6.

Table 5-4: Summary of Team B approach for VSDs 1 to 3

Number of mobilizations:	- Three to four (depending on VSD)
Step 1:	- MIP-HPT at 19-48 locations at a spacing of 20-80 ft. installed in an unstructured grid pattern, generally starting near REC locations identified in the Phase I report and moving outwards (upgradient, cross-gradient and downgradient). - Divided into two mobilizations at VSD1 to obtain additional detail at the downgradient edge of the plume.
Step 2:	- Borings at 5-12 locations installed either adjacent to or between previous MIP-HPT locations. - Monitoring wells at all boring locations at VSD2 and VSD3. - Slug tests at 3-4 locations at VSD2 and VSD3.
Step 3:	- Borings at 3-11 locations within the region defined by the MIP-HPT but away from previous boring locations. - Monitoring wells installed at most boring locations.

Table 5-5: Summary of Team B mobilizations for VSDs 1 to 3

VSD	Mobilization	
1	1	- 42 MIP-HPTs (MIP-B01 to MIP-B42)
	2	- 6 MIP-HPTs (MIP-B43 to MIP-B48)
	3	- 12 DPT borings (BH-05 to BH-13, MIP-B1, MIP-B10 and MIP-B20)
	4	- 3 Sonic MWs (MIP-B23, MIP-B36 and BH/MW-14)
2	1	- 19 MIP-HPTs (MIP-B01 to MIP-B19)
	2	- 7 DPT MWs (MW-05S to MW-11S) - Slug tests at MW-06S, MW-07S, MW-08S
	3	- 4 DPT MWs (MW-12S to MW-15S)
3	1	- 23 MIP-HPTs (MIP-B01 to M123)
	2	- 5 DPT MWs (MW-05 D/S to MW-6 D/S, MW-07S)
	3	- 11 DPT borings and 8 MWs (MW-08S, MW-09S, MW-10D/S, MW-11S, MW-12 D/S, MW-15S were installed wells; MW-08D, BH-13S and BH-14S were DPT borings only) - Slug tests at MW-10S, MW-05S, MW-08S, MW-06S

Table 5-6: Summary of Team B data analysis approach for VSDs 1 to 3

Analysis	
Hydraulic conductivity:	- MIP-HPT data at VSD1, slug test data at VSD3, and a combination of MIP-HPT and slug test data at VSD2
Groundwater velocity:	- Estimated hydraulic conductivity (geometric mean at VSD1 and VSD2 and median at VSD3), estimated horizontal gradient and assumed porosity (0.30-0.35).
DNAPL location:	- Multiple lines of evidence for DNAPL presence including observations of DNAPL from borehole logs, dye testing, soil concentrations that exceeded a threshold concentration (1,000 mg/kg), and aqueous concentrations greater than 10% of solubility. - Delineation based on threshold MIP-HPT ECD response established through comparison to nearby aqueous concentrations greater than 10% of solubility (1,280 mg/L or 1,472 mg/L depending on the site) and observed DNAPL.
DNAPL mass:	- Correlation between ECD response and soil concentrations used (VSD1), a DNAPL saturation of 6% throughout the delineated volume (VSD3), or an estimate based on the sum of aqueous and sorbed masses (VSD2).
Plume location:	- MIP-HPT with confirmation of concentrations at some locations by analysis of groundwater samples from monitoring wells.

Analysis	
Dissolved concentrations:	- Analysis of groundwater samples from monitoring wells (VSD3). - Relationship between total VOC soil concentrations and MIP-HPT ECD response used with average measured f_{oc} (assume also used estimated K_{oc} values) to determine equilibrium dissolved concentrations, assuming TCE and cDCE concentrations based on TCE to cDCE ratios from groundwater samples from nearby monitoring wells (VSD1 and VSD2).
Plume mass:	- Total plume mass, dissolved and sorbed, determined by integrating estimated concentrations over the delineated plume volume.
Mass discharge:	- Calculated using average groundwater flow rate and either the maximum concentration at one monitoring well (VSD3), estimated concentrations along a transect based on the ECD response correlation (VSD1), or the geometric mean of concentrations measured in 3 monitoring wells along a transect (VSD2).

5.1.3 Team C Investigation Strategy

Overall, DM team C used multiple MIP-HPT transects followed by CMT transects and a high-density DYE-LIF grid in the suspected source location over multiple mobilizations. Quantification focused on groundwater samples from CMT and correlations to DYE-LIF. Their approach is summarized in Table 5-7, Table 5-8, and Table 5-9.

Table 5-7: Summary of Team C approach for VSDs 1 to 3

Number of mobilizations:	- Three to four (depending on VSD)
Step 1:	- Monitoring wells at 4-5 locations (shallow-deep pairs at VSD1 and VSD2) away from existing monitoring wells. - Locations were upgradient and downgradient (VSD1), downgradient (VSD2) or cross-gradient (VSD3) depending on the site.
Step 2:	- MIP-HPT at 34-50 locations on 3-4 transects approximately perpendicular to groundwater flow, at a spacing of 40-50 ft. (up to 100 ft. at VSD1) between locations and with one transect located upgradient of the suspected source zone. - MIP-HPT installed during the second mobilization (VSD2 and VSD3) or a combination of the first and second mobilization (VSD1).
Step 3:	- CMT wells at 14-24 locations installed in transects, some of which coincided with the MIP-HPT (installed between MIP-HPT locations). - CMT installed during the third (VSD3), second and third (VSD1), or third and fourth (VSD2) mobilization.
Step 4:	- DYE-LIF at 47-66 locations in a grid pattern at 25-30 ft. spacing within the suspected source zone. - DYE-LIF installed during the third (VSD2 and VSD3) or second and third (VSD1) mobilization.

Step 5:	- Additional borings (10-13) with some completed at CMT wells (6-8) during the final mobilization. - Slug tests at selected (4-6) CMT and monitoring well locations.

Table 5-8: Summary of Team C mobilizations for VSDs 1 to 3

VSD	Mobilization	
1	1	- 41 MIP-HPTs (HA-01 to HA-41) - 10 Sonic MWs (MW-05 D/S to MW-09 D/S)
	2	- 9 MIP-HPTs (HA-42 to HA-50; mislabeled HA-41 to HA-49) - 15 DPT CMT wells (CMT-01 to CMT-15) - 49 DYE-LIFs (LIF-01 to LIF-49)
	3	- 3 DPT CMT wells were installed (CMT-16 to CMT-18) - 16 DYE-LIFs were requested (LIF-101 to LIF-116) - Slug tests at MW-4S, CMT-01-20.5 ft, CMT-02-13 ft, CMT-03-30 ft
	4	- 10 DPT borings and 6 CMT wells (CMT-19 to CMT-24 for CMT wells; GP-01 to GP-04 for DPT borings only)
2	1	- 8 DPT MWs (MW-05 D/S to MW-08 D/S)
	2	- 42 MIP-HPTs (MIP-01 to MIP-42; mislabeled MIP-33 to MIP-41)
	3	- 14 DPT CMTs (CMT-01 to CMT-14) - 66 DYE-LIFs (LIF-001 to LIF-066)
	4	- 13 DPT borings and 8 CMT wells (CMT-15 to CMT-22 for CMT wells; DP-01 to DP-05 for DPT borings only) - Slug tests at MW-1S, MW-06S, CMT-04-20 ft, CMT-05-10 ft, CMT-05-20 ft, CMT-05-30 ft
3	1	- 4 DPT MWs (MW-05 D/S to MW-06 D/S)
	2	- 34 MIP-HPTs (MIP-01 to MIP-34)
	3	- 19 DPT borings and 14 CMT wells (CMT-01 to CMT-14 for CMT wells; DP-01 to DP-05 for DPT borings only) - 47 DYE-LIFs (LIF_001 to LIF_047) - Slug tests at MW-1S, MW-2S, CMT-01-45.5 ft, CMT-03-18.5 ft, CMT-04-45.5 ft, CMT-05-45.5 ft

Table 5-9: Summary of Team C data analysis approach for VSDs 1 to 3

Analysis	
Hydraulic conductivity:	- MIP-HPT and slug test data were used to estimate hydraulic conductivity.
Groundwater velocity:	- Range reported based on different hydraulic conductivity estimates.
DNAPL location:	- DNAPL location was determined using DYE-LIF, with DYE-LIF inferences confirmed using co-located soil samples.
DNAPL mass:	- DNAPL saturations in soil samples were determined using partitioning relationships and were correlated to the DYE-LIF response to map the DNAPL saturations in 1 ft. intervals.
Plume location:	- Interpolation of concentrations measured in samples from CMT wells.
Dissolved concentrations:	- Interpolation of concentrations measured in samples from CMT wells.
Plume mass:	- Dissolved and sorbed mass estimates were based on published K_{oc} values, and estimated porosity and an average measured f_{oc}.
Mass discharge:	- Calculated using the GSI Mass Flux Toolkit, with hydraulic conductivity values from slug tests correlated to soil classifications on boring logs and dissolved concentrations from individual CMT well screens. In some cases, estimates of mass discharge were compared to estimates using Thiessen polygon calculations (VSD1), or EVS Studio (VSD3) with hydraulic conductivity values based on MIP-HPT. Transect locations were based on estimates of the downgradient edge of the source zone (first transect) and another 150 feet downgradient (second).

5.1.4 Team D Investigation Strategy

Overall, DM team used a MIP-HPT grid followed by a high-density of boreholes in the suspected source zone over multiple mobilizations. Quantification focused on soil samples in the source zone and correlations to MIP-HPT results. Their approach is summarized in Table 5-10, Table 5-11, and Table 5-12.

Table 5-10: Summary of Team D strategy for VSDs 1 to 3.

Number of mobilizations:	- Three
Step 1:	- MIP-HPT at 20-74 locations at a spacing of 50-80 ft. installed in a grid pattern.
Step 2:	- Monitoring wells at 4-9 locations throughout the suspected plume. - Borings (without monitoring wells) at 10-30 locations at a spacing of 15-25 ft. in the suspected source zone.
Step 3:	- Additional borings at 5-25 locations in between or adjacent to previous borings in the suspected source zone. - Monitoring wells installed at 3 of these locations at VSD1 (1 in the suspected source zone and 2 downgradient). - Slug tests at 3 locations at VSD2.

Table 5-11: Summary of Team D mobilizations for VSDs 1 to 3

VSD	Mobilization	
1	1	- 20 MIP-HPTs (MIP-1-01 to MIP-1-20)
	2	- 4 Sonic MWs (MW-D1 to MW-D4) - 10 DPT borings (BH-D2-N, BH-D2-S1, BH-D2-S2, BH-D2-E1, BH-D2-E2, BH-D2-W1, BH-D2-W2, BH-D2-S3, BH-D2-SE1, BH-D2-SW1)
	3	- 5 DPT borings and 3 MWs (wells at BH-D2-S4, BH-4S-SO1, BH-4S-SO2 and only DPT borings at BH-D2-SO1 and BH-D2-S1-SO1)
2	1	- 74 MIP-HPTs (MIP-P1-01 to MIP-P3-74)
	2	- 9 Sonic MWs (BH-D1-01 to BH-D2-09) - 18 DPT borings were drilled (DPT-1-01 to DPT-2-18)
	3	- 7 DPT borings were drilled (DPT-3-19 to DPT-3-25) - Slug tests at BH-D1-04, BH-D2-09, MW-1S
3	1	- 54 MIP-HPTs (MIP-1-01 to MIP-3-54)
	2	- 7 Sonic MWs (MW-1-01, MW-1-02, MW-1-03 D/S, MW-1-04 D/S, MW-1-05) - 30 DPT borings (DPT-1-01 to DPT-3-30)
	3	- 25 DPT borings (DPT-4-31 to DPT-5-55; mislabeled DPT-4-30 to DPT-5-54)

Table 5-12: Summary of Team D data analysis approach for VSDs 1 to 3

Analysis	
Hydraulic conductivity:	- MIP-HPT data. - Slug test data used at VSD2
Groundwater velocity:	- Estimated hydraulic conductivity from MIP-HPT data (VSD 1 and VSD3) or slug test data (VSD2), porosity calculated from soil sample bulk density measurements. - Range reported based on range of hydraulic conductivities measured.
DNAPL location:	- Multiple lines of evidence for DNAPL presence including observations of DNAPL in borehole logs and partitioning threshold calculations.
DNAPL mass:	- At VSD 1, DNAPL mass was estimated assuming a 15 ft. diameter cylinder around two boreholes with observed pooled DNAPL (approximately half the distance to an adjacent clear borehole) and assuming a DNAPL saturation of 100% of the pore space over those vertical intervals. - At VSD2 and VSD3, DNAPL mass was estimated using a Thiessen polygon method applied to DNAPL observations in the borehole logs, with a saturation of 15% applied to residual and 50% applied to pooled.
Plume location:	- Interpolation of MIP-HPT results.
Dissolved concentrations:	- Assumed correlation to MIP-HPT results.
Plume mass:	- Integration of isoconcentration contour intervals with measured f_{oc} and literature K_{oc}.
Mass discharge:	- Interpolated concentrations used to assign concentrations to regions of transects together with estimated Darcy flux.

5.1.5 Virtual Site Investigation Cost

As described in Section 4.4.3, the cost of the virtual investigation conducted by each of the DM teams was tracked based on unit costs for investigation tool deployment, mobilization, and sample analyses. The total cost for each investigation is shown in Figure 5-4. Investigation costs incurred by DM team C were substantially greater than other DM teams, due primarily to the extensive use of DyeLIF and CMT wells. However, it is important to note that of the 12 estimates of DNAPL footprint (DM teams A-D and VSDs 1-3) all 3 estimates by DM team C were in the top 5 most accurate (Figure 5-13a), and all 3 estimates of plume footprint by DM team C were in the top 7 most accurate (Figure 5-13b). No other DM team showed that consistent accuracy over all VSDs 1 to 3. However, this accuracy was not reflected in estimates of DNAPL or dissolved TCE mass, with all three estimates of DNAPL mass in only the top 9 of 12 and one estimate of dissolved TCE mass being the least accurate.

Trends of site investigation costs with increased complexity (from VSD1 to VSD3) were as expected for DM teams A and D, which showed increased cost with increased geologic complexity. However, DM team C costs decreased, and DM team B costs were similar for the same progression. There is likely an element of "learning" seen in DM Team C; however, this did not necessarily translate to increased accuracy (see Section 5.1).

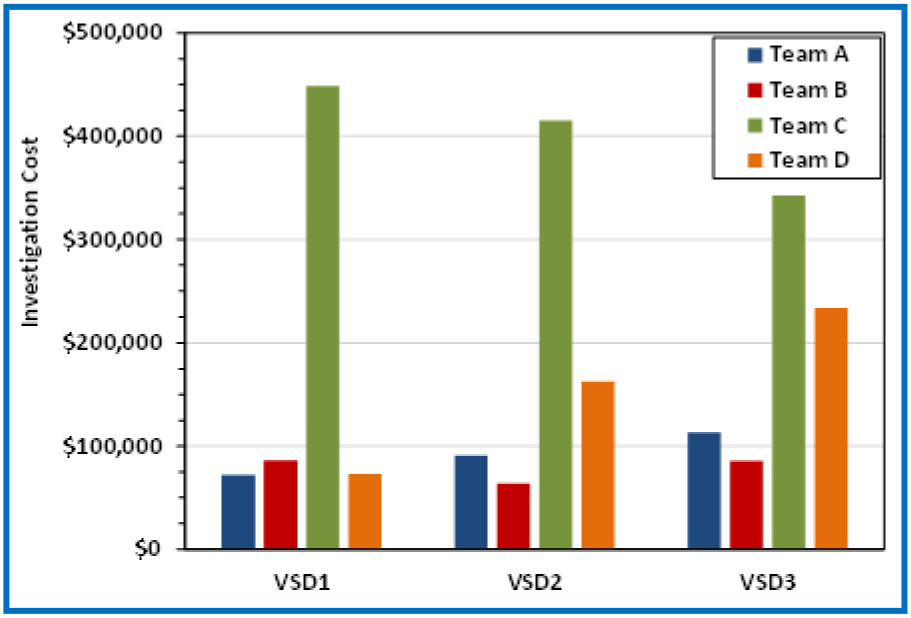


Figure 5-4: Investigation costs for each DM Team at VSDs 1 to 3

5.1.6 CSMs for VSDs 1 to 3

CSMs for each of VSDs 1 to 3 prepared by DM teams A-D are presented in Appendix J (12 CSMs in total). Each CSM report includes: (i) descriptions of the hydrogeology, biogeochemical conditions and risk drivers, (ii) estimates of DNAPL mass in the source zone, VOC mass (dissolved and sorbed) in the plume, and VOC mass discharge, and (iii) figures depicting estimated locations and extents of the DNAPL and plume. Information contained in these CSM reports was used by the Project Team to evaluate the performance parameters against the true values in each VSD using Equations 4-1 and 4-2. Values reported by each of the DM teams are listed in Appendix J for the qualitative, quantitative, and graphical parameters, which are discussed further below.

<u>Qualitative parameters:</u> All DM teams correctly identified the qualitative parameters. DNAPL was present in each of VSDs 1 to 3 and was correctly identified by all DM teams. Biodegradation was occurring in each of VSDs 1 to 3 and was correctly identified by all DM teams. Contaminants of concern at each of VSDs 1 to 3 were TCE and cDCE, which were correctly identified by all DM teams. Groundwater flow direction accuracy was slightly lower. It was correctly identified in six of the 12 CSM reports, and was within 22.5° (e.g., reported as to S-SW when the true direction was directly to S) in the remaining six CSMs. Based on these results, the various investigation approaches used by all teams to identify these qualitative attributes of a CSM were likely sufficient for the future design of a remedy (with the possible exception of groundwater flow direction).

<u>Quantitative parameters:</u> The scores for each of the quantitative parameters (calculated using equation 1) are listed in Table 5-13, Table 5-14, and Table 5-15 for VSDs 1, 2 and 3, respectively.

The scores are also shown in Figure 5-5 to facilitate comparison between parameters (vertically) and between DM teams (horizontally). Each score represents a ratio of the DM Team calculated value to the true value.

Table 5-13: Quantitative parameter scores for VSD1 for all DM Teams

Parameter	True value	A	B	C	D
Average groundwater velocity	20.31 ft/yr	1.77	0.52	0.74	3.02
DNAPL mass	10,160 kg	0.21	0.04	0.54	0.70
Dissolved TCE mass	890 kg	0.29	0.70	1.38	0.32
Dissolved cDCE mass	285 kg	0.29	1.32	0.46	0.33
Sorbed TCE mass	425 kg	0.05	0.78	1.94	0.25
Sorbed cDCE mass	86 kg	0.05	0.54	0.26	0.38
TCE Mass discharge (location 1)	93.8-142.5 kg/yr	NR	0.35	3.37	15.83
TCE Mass discharge (location 2)	3.1-54.8 kg/yr	NR	0.35	NR	4.85
Decay coefficient	0.14 yr^{-1}	7.3	NR	0.9	2.14

NR: Not reported in the CSM report.

Table 5-14: Quantitative parameters scores for VSD2 for all DM Teams

Parameter	True value	A	B	C	D
Average groundwater velocity	50.83 ft/yr	0.68	0.43	1.30	1.02
DNAPL mass	14,923 kg	5.34	1.61	1.26	2.4
Dissolved TCE mass	1363 kg	1.64	1.99	0.32	0.27
Dissolved cDCE mass	155 kg	1.64	2.24	0.45	0.51
Sorbed TCE mass	760 kg	0.93	1.34	0.16	0.34
Sorbed cDCE mass	54 kg	0.93	0.67	0.23	0.45
TCE Mass discharge (location 1)	0.02-519.9 kg/yr	NR	0.61	0.26	483
TCE Mass discharge (location 2)	13.9-506.5 kg/yr	NR	0.35	0.0001	0.37
Decay coefficient	0.14 yr^{-1}	1.23	NR	0.67	0.13

NR: Not reported in the CSM report.

Table 5-15: Quantitative parameters scores for VSD3 for all DM Teams

Parameter	True value	A	B	C	D
Average groundwater velocity	33.46 ft/yr	0.95	0.93	2.15	1.26
DNAPL mass	21,440 kg	0.33	0.1	0.19	2.77
Dissolved TCE mass	859 kg	0.5	1.26	0.17	0.72
Dissolved cDCE mass	180 kg	0.5	1.43	0.28	0.82
Sorbed TCE mass	490 kg	0.76	0.15	0.08	0.69
Sorbed cDCE mass	63 kg	0.76	0.31	0.43	0.01
TCE Mass discharge (location 1)	52.9-156.6 kg/yr	NR	1.28	1.95	1.53
TCE Mass discharge (location 2)	1.5-77.7 kg/yr	NR	0.25	3.97	1.02
Decay coefficient	0.14 yr^{-1}	2.31	NR	0.28	5.43

NR: Not reported in the CSM report.

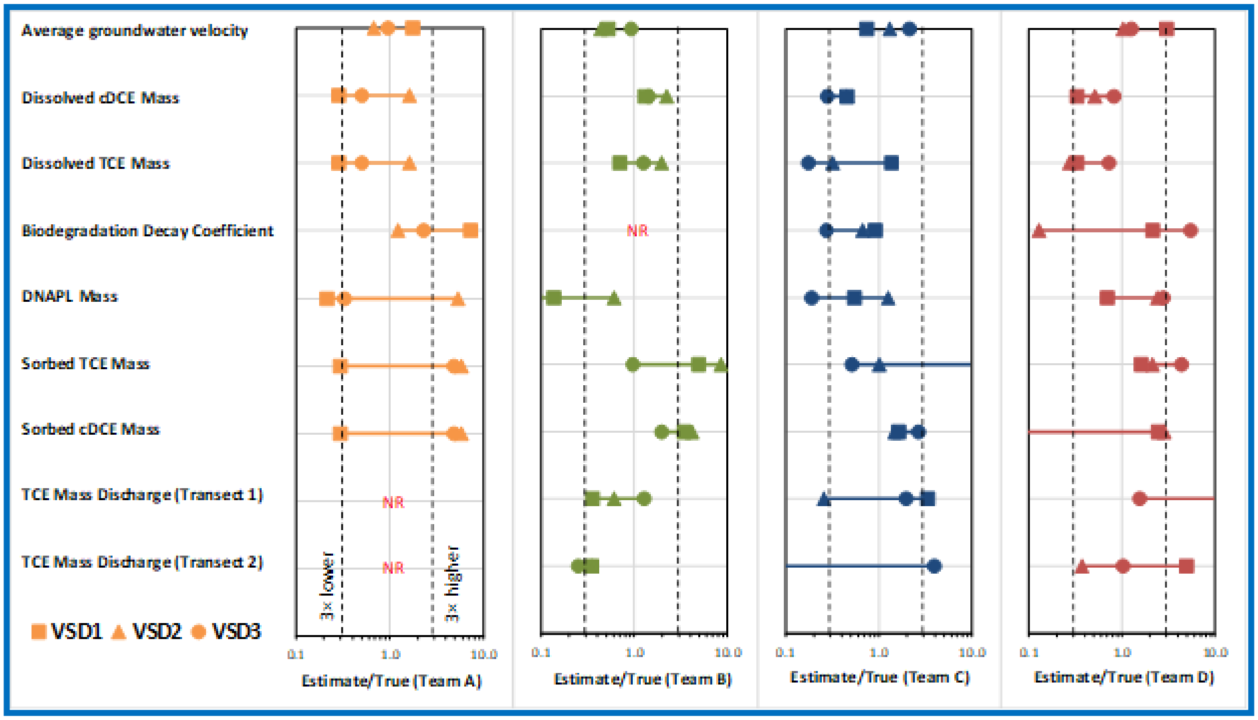


Figure 5-5: Quantitative parameter scores for VSDs 1 to 3 based on the CSM reports from all DM teams (NR – Not Reported)

The scores shown in Table 5-13 to Table 5-15 and Figure 5-5 show that all DM teams performed well (64% were within a factor of 3 (scores between 0.33 and 3), and 92% were within a factor of 10 (score between 0.1 and 10)).

The list of parameters in Table 5-13 to Table 5-15 and Figure 5-5 has been ordered such that the parameter that was scored best (i.e., closest to a ratio of 1) is listed first. This ranking was based on the absolute value of the logarithm of quantitative parameter score, such that a score of 10 (a one order-of-magnitude overestimate) was treated equally to a score of 0.1 (a one order-of-magnitude underestimate).

It is difficult to determine the importance of a factor of 3 error versus a factor of 10 error in an absolute sense. It is likely the importance will be different for each parameter, for the end use of each parameter (e.g., remedy design versus risk assessment) and at individual sites.

Graphical parameters:

Example graphical parameters for the plume footprint and DNAPL source footprint are shown in Figure 5-6 to Figure 5-8 and Figure 5-9 to Figure 5-11, respectively. The method used to develop the actual size for each is detailed in Section 4.2.4. A comparison of the plume and DNAPL footprints, as well as the graphical parameter scores listed in Table 5-16 to Table 5-18, shows that estimates of plume location were more accurate than estimates of DNAPL location, likely given the ease of identifying dissolved phase contamination as compared to DNAPL contamination. DNAPL estimates included both overestimations of the footprint (e.g., Figure 5-10b), underestimations of the footprint (e.g., Figure 5-11a), misplacement of the DNAPL (e.g., Figure 5-10a) and missed DNAPL location (e.g., Figure 5-9d, Figure 5-10c and Figure 5-10d).

The scores, which represent a weighted difference between the correct and incorrect plume or DNAPL locations, are also shown in Figure 5-12 to facilitate comparison between parameters (vertically) and between DM teams (horizontally). Figure 5-12 shows that estimates of plume footprints were more accurate (average score of 0.82 across all VSDs and all DM teams) than estimates of plume cross section (average score of 0.66) and estimates of DNAPL footprint (average score of 0.55).

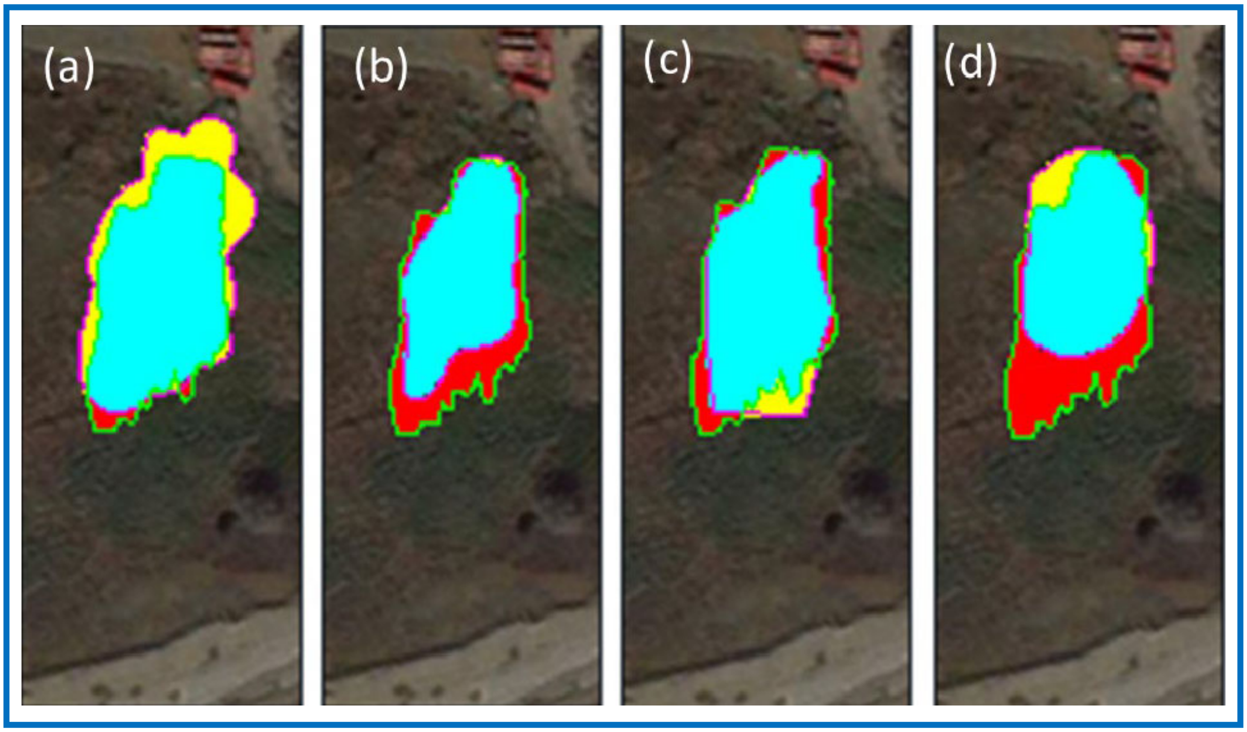


Figure 5-6: Estimated and true plume (to 0.5 ppb) footprints for VSD1, based on CSM reports from DM teams (a) A, (b) B, (c) C and (d) D. Red is actual not identified by the DM Team, blue is actual identified by the DM Team and yellow is region identified as plume by DM Team that was not actual plume

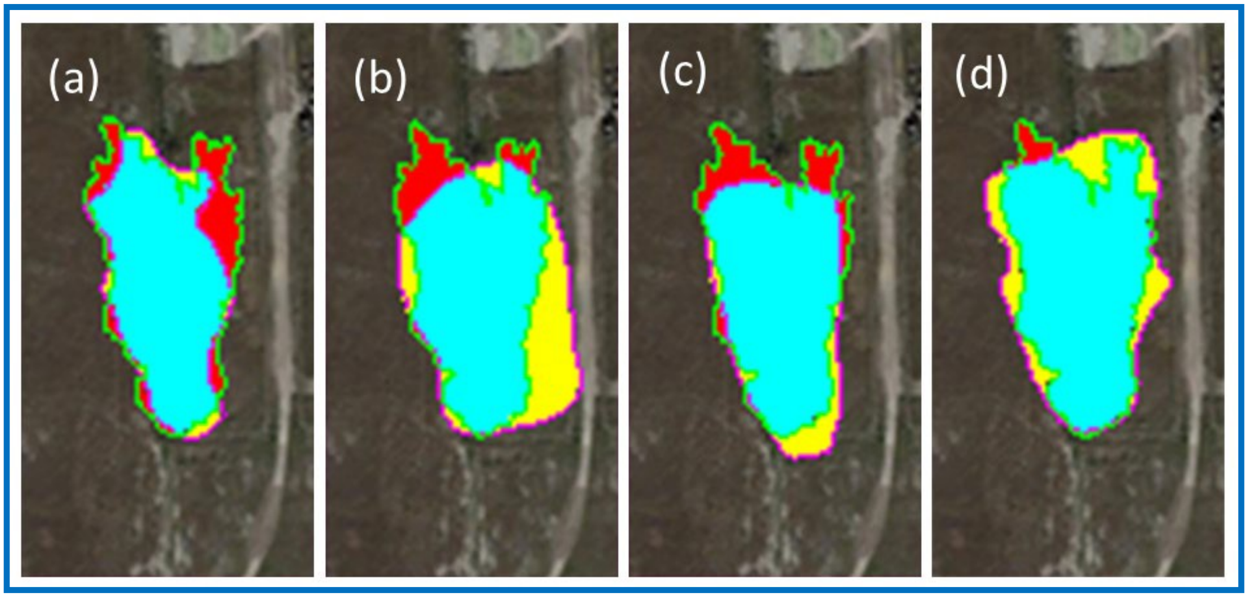


Figure 5-7: Estimated and true plume (to 0.5 ppb) footprints for VSD2, based on CSM reports from DM teams (a) A, (b) B, (c) C and (d) D. Red is actual not identified by the DM Team, blue is actual identified by the DM Team and yellow is region identified as plume by DM Team that was not actual plume

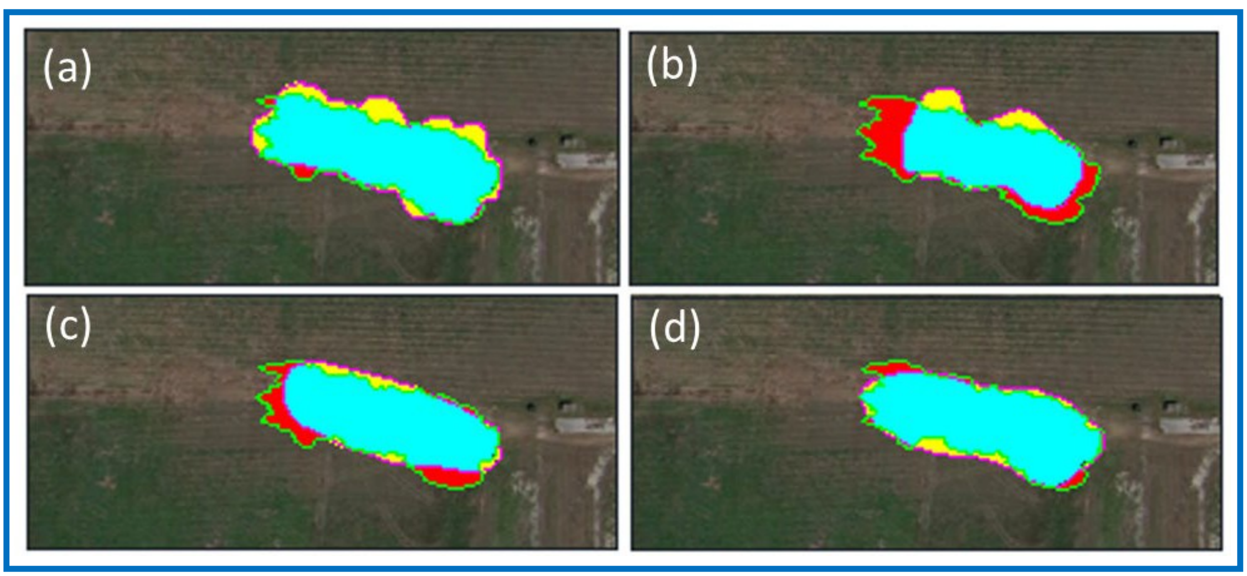


Figure 5-8: Estimated and true plume (to 0.5 ppb) footprints for VSD3, based on CSM reports from DM teams (a) A, (b) B, (c) C and (d) D. Red is actual not identified by the DM Team, blue is actual identified by the DM Team and yellow is region identified as plume by DM Team that was not actual plume

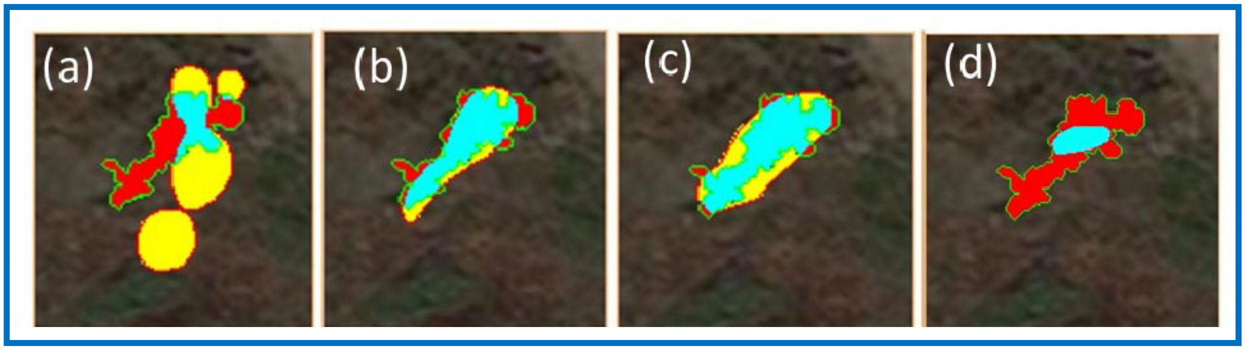


Figure 5-9: Estimated and true (Snw > 0.01) DNAPL footprints for VSD1, based on CSM reports from DM teams (a) A, (b) B, (c) C and (d) D. Red is actual not identified by the DM Team, blue is actual identified by the DM Team and yellow is region identified as DNAPL by DM Team that was not actual DNAPL

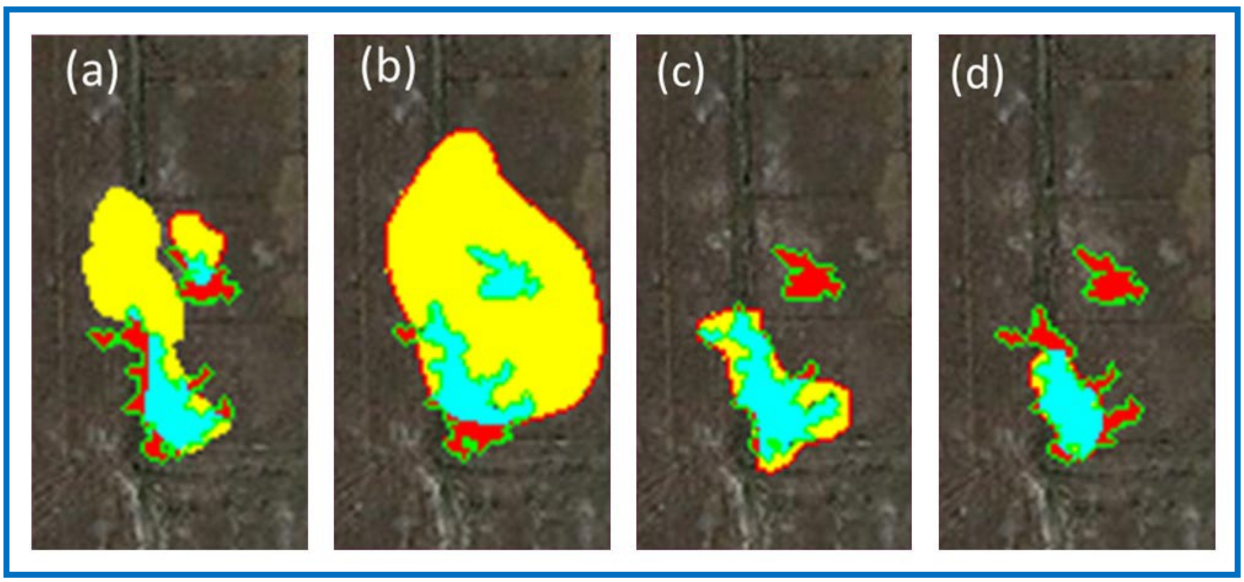


Figure 5-10: Estimated and true (Snw > 0.01) DNAPL footprints for VSD2, based on CSM reports from DM teams (a) A, (b) B, (c) C and (d) D. Red is actual not identified by the DM Team, blue is actual identified by the DM Team and yellow is region identified as DNAPL by DM Team that was not actual DNAPL

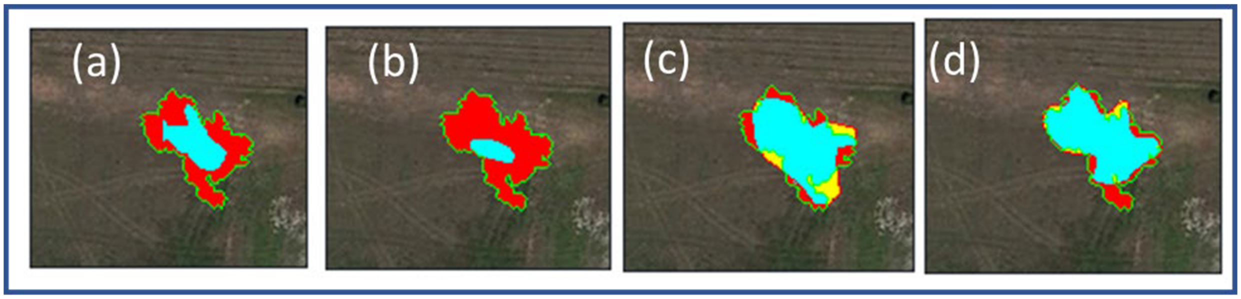


Figure 5-11: Estimated and true (Snw > 0.01) DNAPL footprints for VSD3, based on CSM reports from DM teams (a) A, (b) B, (c) C and (d) D. Red is actual not identified by the DM Team, blue is actual identified by the DM Team and yellow is region identified as DNAPL by DM Team that was not actual DNAPL

Table 5-16: Graphical parameters scores for VSD1 for all DM Teams

Parameter	A	B	C	D
Total VOC plume footprint	0.91	0.70	0.84	0.65
Total VOC plume cross-section (parallel to flow)	NR	0.40	0.64	0.69
Total VOC plume cross-section (perpendicular to flow)	NR	0.64	0.51	0.61
DNAPL source zone footprint	0.23	0.76	0.87	0.21

NR: Not reported in the CSM report.

Table 5-17: Graphical parameters scores for VSD2 for all DM Teams

Parameter	A	B	C	D
Total VOC plume footprint	0.78	0.81	0.81	0.92
Total VOC plume cross-section (parallel to flow)	NR	0.83	NR	0.54
Total VOC plume cross-section (perpendicular to flow)	NR	0.60	0.79	0.75
DNAPL source zone footprint	0.50	0.54	0.70	0.47

NR: Not reported in the CSM report.

Table 5-18: Graphical parameters scores for VSD3 for all DM Teams

Parameter	A	B	C	D
Total VOC plume footprint	0.94	0.70	0.80	0.93
Total VOC plume cross-section (parallel to flow)	NR	0.77	NR	0.85
Total VOC plume cross-section (perpendicular to flow)	NR	0.61	0.51	0.81
DNAPL source zone footprint	0.36	0.12	0.79	0.82

NR: Not reported in the CSM report.

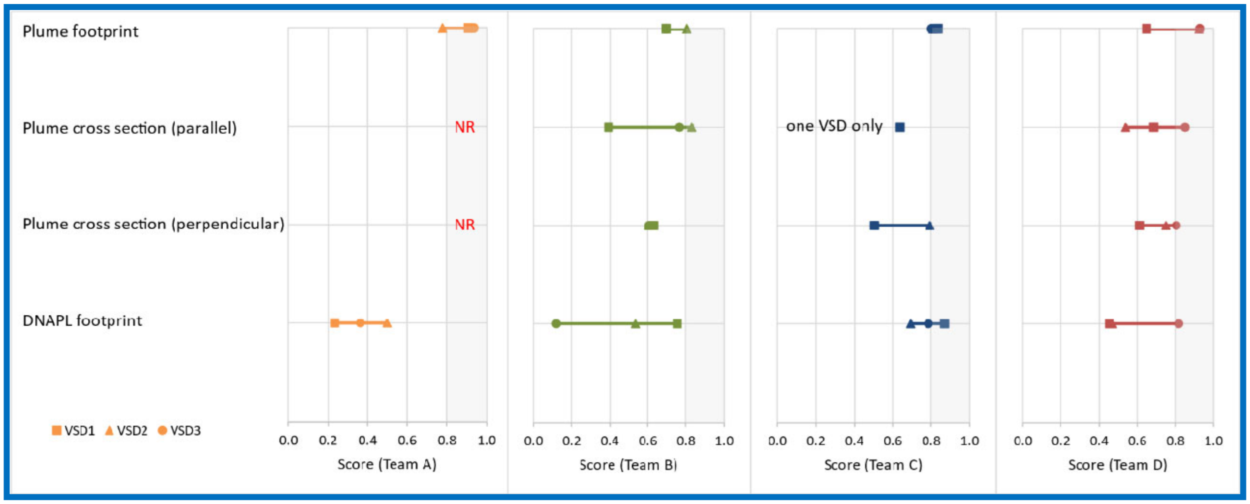


Figure 5-12: Graphical parameter scores for VSDs 1 to 3 based on the CSM reports from all DM Teams.

It is important not to limit any analysis of CSM accuracy to individual parameters because an effective CSM will incorporate multiple parameters. For example, Figure 5-13 shows two parameters associated with the DNAPL source and the VOC plume: the mass and the footprint, both of which are important for remediation design. In Figure 5-13, the true value is at coordinate (1, 1). In the case of DNAPL (Figure 5-13a) substantially less accurate estimates were reported, with estimates of mass ranging from underestimates by a factor of 10 to overestimates by a factor of 5, and scores for footprint ranging from 0.12 to 0.87. This contrasts with the estimates for the plume, with estimates of dissolved TCE mass ranging from underestimates by a factor of 6 to overestimates by a factor of 2, and scores for footprint ranging from 0.65 to 0.94. Overall, this demonstrates that the investigation strategies used by the DM teams were more accurate for plumes than for DNAPL source zones. This is not surprising given that identification of plumes is far more direct than identification of DNAPL. Any peak on a MIP will identify a plume, however DNAPL must be directly observed or measured quantitatively in a soil sample to confirm its existence.

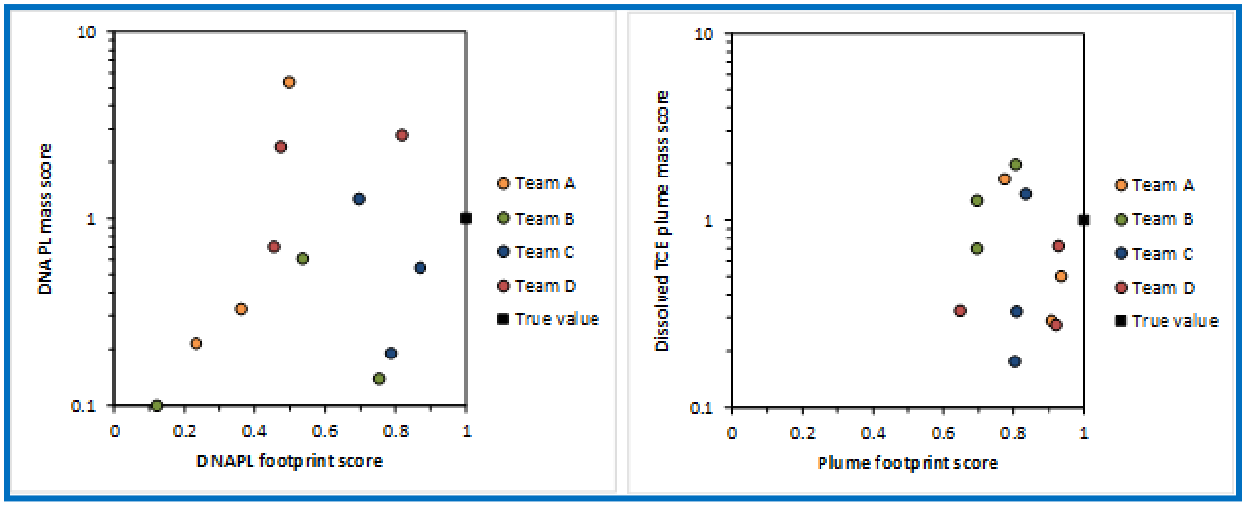


Figure 5-13: Scores for (a) DNAPL mass and DNAPL footprint, and (b) TCE plume mass and plume footprint for VSDs 1 to 3 based on the CSM reports from all DM Teams.

5.1.7 Overview of Findings Regarding Investigation

Inspection of the approaches and results of the investigations of VSD 1 to 3 by the DM teams offers a range of insight concerning strategies, costs, and expectations of accuracy, as described in the previous sections. In general, these results show that:

- The DM teams had different strategies for the investigation of the DNAPL-impacted sites represented by VSD 1 to 3 and made only minor modifications for site complexity.
- Investigation approaches made similar use of multiple (2-4) mobilizations, and substantial use of MIP-HPT (19-74 locations) in early mobilizations, but differed in their use of boreholes, CMT and DyeLIF.
- Many (92%) of the quantitative CSM metrics (e.g., dissolved TCE mass, DNAPL mass) were within a factor of 10 and 64% were within a factor of 3 of the true values, and both over- and underestimates of most metrics were reported.
- Estimates of plume footprint were often more accurate than estimates of DNAPL footprint, and a higher accuracy footprint did not necessarily result in a higher accuracy estimate of mass for either the plume or DNAPL source, suggesting that both the investigation strategy and the approach used to interpret the data are important in developing a CSM.
- None of the site investigation approaches resulted in a high accuracy for all CSM metrics, and the development of best-practices will likely require the incorporation of elements from multiple approaches used by the DM teams as well as from others.

5.2 Experienced Based (EB) Remediation for VSD1 to VSD3

The EISB remedy designs for VSDs 1 to 3 prepared by DM teams A-D are summarized in Table 5-19 to Table 5-21. Information provided by the DM teams pertaining to their EISB remedy design and monitoring was simulated by the Project Team in DNAPL3D-RX for the 5-year active remedy period. Out of the four DM teams, only Team D requested modifications to their initial EISB remedy designs for VSDs 1 to 3 during the period of remedy operation (ranging from 12 to 20 months). The EISB remedy approaches designed by DM teams A-D for VSDs 1 to 3 are illustrated in Figure 5-14.

Table 5-19: Remedy design summary for VSD 1

Design Element	Team A	Team B	Team C	Team D
Wells and Type	55 Injection wells injecting periodically	5 injection wells injecting continuously	77 DPT locations and 8 Injection wells injecting annually	38 Injection wells injecting 6 days per month. Decommissioned 20 wells in redesign and added 15 new wells
Injection Rate	0.75 – 1.5 gpm	0.1 to 0.26 gpm	1.2 gpm	0.15 gpm
Lactate Added (kg)	246,634	7,598	60,085	70,622
Lactate Concentration	38 g/L	0.8 g/L	99 g/L	7 g/L
Bioaugmentation	10L DhC per injection well	None	1.7 L DhC to each DPT location	1L DhC per injection well per event
Monitoring	10 Locations monthly for 6 months then 2 quarterly events then semi-annually	5 Locations monthly	10 CMT wells	38 Locations monthly
Parameters	VOCs, TOC, anions, metals, gases, GeneTrac	VOCs, anions, gases, alkalinity	VOCs, TOC, anions, metals, gases	VOCs, TOC, anions, gases

Table 5-20: Remedy design summary for VSD 2

Design Element	Team A	Team B	Team C	Team D
Wells and Type	45 Multi-port injection wells injecting semi-annually in years 1 and 2 and then annually in years 3 to 5	24 Injection wells injecting biennially	116 DPT locations and 8 injection wells injecting annually	21 Injection wells injecting 5 days out of every week. Redesigned after 1.5 years, decommissioned 11 of the original injection wells and added 12 more
Injection Rate	0.75 – 1.5 gpm	1.5 – 3.75 gpm	2.7 gpm	1 gpm
Lactate Concentration	42 g/L	3.7 g/L	250 g/L	2.2 g/L
Lactate Added (kg)	580,575	16,534	189,840	142,238
Bioaugmentation	1L DhC per foot of well screen	3.6 L DhC per injection well per event	1.4 L DhC per DPT location	2 L of DhC added to injection wells prior to first injection
Monitoring	9 Locations monthly for 6 months than 2 quarterly events then semi-annually	13 locations semi-annually	12 CMT wells monthly during the first year and then quarterly	21 wells monthly
Parameters	VOCs, TOC, anions, metals, gases, GeneTrac	VOCs, TOC, anions, gases, alkalinity, Genetrac	VOCs, TOC, anions, metals, gases	VOCs, TOC, anions, gases

Table 5-21: Remedy design summary for VSD3

Design Element	Team A	Team B	Team C	Team D
Wells and Type	63 Multi-port injection wells injecting semi-annually for first two years then annually for last 3 years	19 Injection wells injecting biennially	106 DPT locations and 8 injection wells injecting annually	39 Injection wells injecting 5 days per week. After 20 months decommissioned 20 injection wells.
Injection Rate	0.75 – 2.5 gpm	5 gpm	1.85 gpm	0.45 gpm
Lactate Concentration	41 g/L	5.5 g/L	99 g/L in DPT 150 g/L in injection wells	3 g/L
Lactate Added (kg)	253,215	5,518	50,018	103,218
Bioaugmentation	Total of 620 L of DhC added to injection wells prior to second injection event	1.2 L of DhC at each injection well at each injection event	1 L of DhC at each DPT location	2 L of DhC per injection well in the first injection event
Monitoring	10 Locations monthly for 6 months, quarterly for 2 events then semi-annually	11 Locations semi-annually	9 CMT wells monthly for first year then quarterly or semi-annually.	Monthly at 39 locations
Parameters	VOCs, TOC, anions, metals, gases, GeneTrac	VOCs, TOC, anions, gases, alkalinity, Genetrac	VOCs, TOC, anions, metals, gases	VOCs, TOC, anions, gases

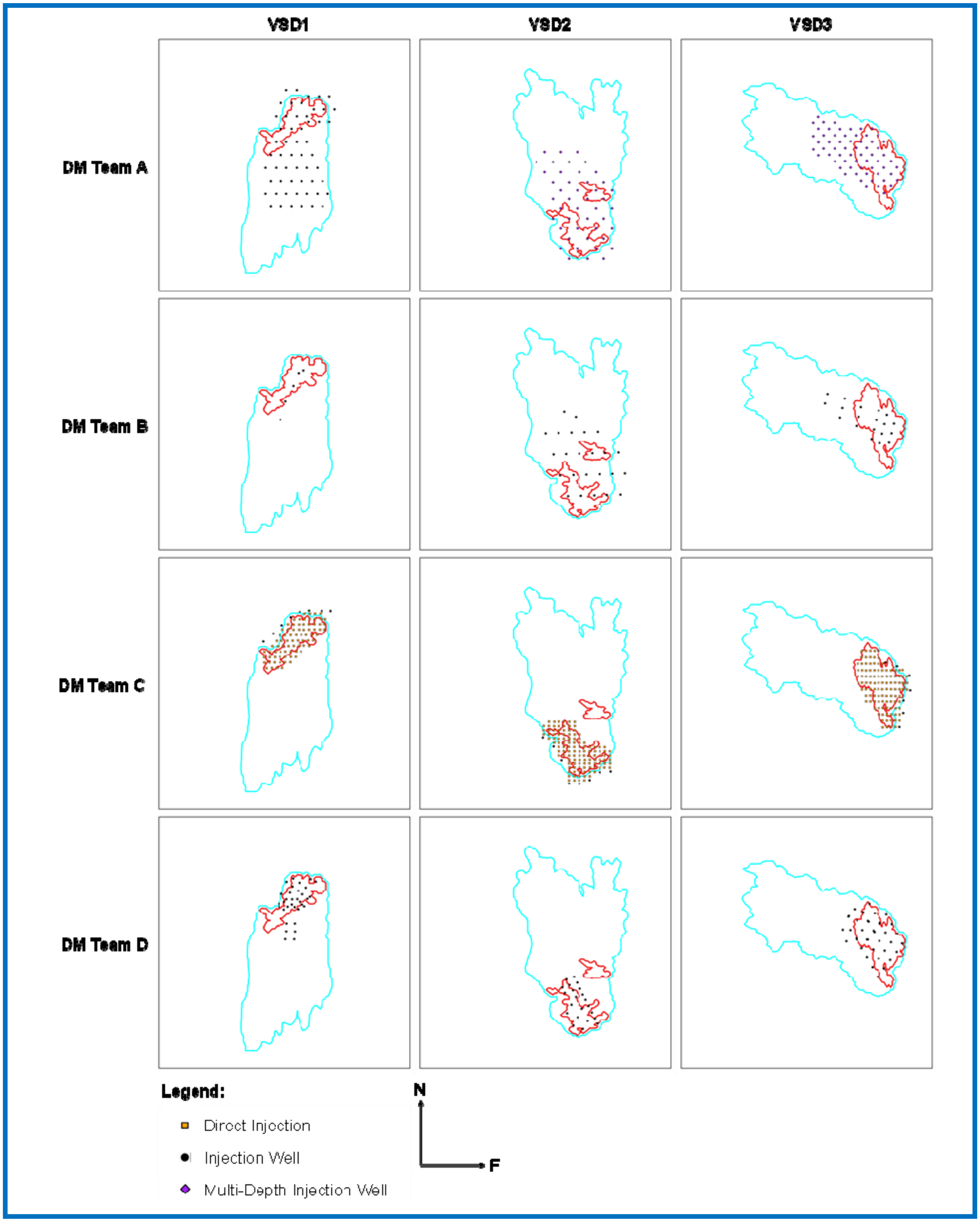


Figure 5-14: Final EISB remedy designs of DM teams A-D for VSDs 1 to 3 illustrating the locations of installed remediation wells and direct injection points. The true DNAPL and VOC plume footprints in each VSD are delineated in red and cyan, respectively.

5.2.1 Assessment of EB Remediation Designs for VSD1 to VSD3

The DM team EISB remedies for VSDs 1 to 3 were compared to the performance objectives after 10 years (5 years following the conclusion of the 5-year active remedy period to allow for source mass discharge decreases to manifest at measurement points downgradient). Modeled output parameters (e.g., DNAPL saturations, VOC concentrations, wetting phase fluxes) from DNAPL3D-RX for each DM team EISB remedy were used to evaluate the objectives against the true VSD pre-remedy conditions in Table 4-10 and VSD POs established for each VSD in Table 4-12. As described in 4.4.2, the costs associated with each DM team EISB remedy for VSDs 1 to 3 were calculated based on the unit costs for EISB remedy-specific activities for pre-installation, installation, operations and maintenance, performance monitoring and decommissioning. The optimal remedies for VSDs 1 to 3 described in Section 4.6.6 were also evaluated and costed to allow for a direct comparison to the DM team remedies. As noted in Section 4.6.6, the optimal EISB remedies were developed to determine the VSD-specific POs that could be achieved with access to perfect information for each VSD. The scores for each of the remedial performance objectives and the costs associated with each EISB remedy are listed in Table 5-22, Table 5-23, and Table 5-24, for VSDs 1, 2, and 3, respectively. DM Team A was the only DM team that achieved all VSD-specific POs from their implemented EISB remedies for VSDs 1 to 3 (due to a very high factor of safety employed in remediation design).

DNAPL Mass Reduction: Table 5-22 to Table 5-24 show that all DM teams performed reasonably well (met the parameter in 10 out of 12 cases) with respect to the DNAPL mass reduction performance objective. With the exception of DM Team C's and D's EISB remedies for VSD3, the remaining DM team remedies for VSDs 1 to 3 achieved the VSD-specific POs for DNAPL mass reduction specified in Table 4-12.

Total Chlorinated VOC Dissolved Phase Mass Discharge Reduction: Table 5-22 to Table 5-24 show that most DM teams performed poorly (met the objective in 4 out of 12 cases) with respect to this performance objective. With the exception of DM Team A's remedies for VSDs 1 to 3 and DM Team D's remedy for VSD2, the remaining DM team remedies for VSDs 1 to 3 failed to meet the VSD-specific POs as specified in Table 4-12.

Average Maximum TCE Groundwater Concentration Reduction: Table 5-22 to Table 5-24 show that most DM teams performed poorly with respect to the average maximum TCE groundwater concentration reduction performance objective. With the exception of DM Team A's remedies for VSDs 1 to 3 and DM Team D's remedy for VSD3, the remaining DM team remedies for VSDs 1 to 3 failed to meet the VSD-specific POs as specified in Table 4-12.

Total Cost of EISB Remedies: Table 5-22 to Table 5-24 show the variability in EISB remedy costs (undiscounted) between DM Teams A to D. The total costs of the DM team EISB remedies ranged from \$1.29M to \$3.36M, \$0.81M to \$6.34M, \$0.49M to \$5.07M, for VSDs 1, 2, and 3, respectively. The total costs of DM Team A's EISB remedies for VSDs 1 to 3 were substantially greater compared to the EISB remedies of DM Teams B to D. However, DM Team A was the only DM team that achieved all VSD-specific POs from their implemented EISB remedies for VSDs 1 to 3. The EISB remedies implemented by DM Teams B to D failed to achieve all three VSD-specific POs at VSDs 1, 2, or 3. The correlation of remedy cost to performance to investigation cost and strategy is explored in detail in Section 7.1.

Table 5-22: EISB remedy performance scores for VSD1, evaluated 5 years following the conclusion of the EISB remedy. Green shading indicates a success at meeting the PO.

Remedial Performance Objective	PO	Optimal	A	B	C	D
DNAPL Mass Reduction	30%	84%	64%	43%	41%	71%
Total Chlorinated VOC Dissolved Phase Mass Discharge Reduction	50%	75%	53%	-27%	25%	43%
Average Maximum TCE Groundwater Concentration Reduction	60%	62%	68%	2%	38%	37%
Total Cost of Remedy ($M)	--	1.75	3.36	1.29	1.34	2.38

Table 5-23: EISB remedy performance scores for VSD2, evaluated 5 years following the conclusion of the EISB remedy. Green shading indicates a success at meeting the PO.

Remedial Performance Objective	PO	Optimal	A	B	C	D
DNAPL Mass Reduction	25%	58%	63%	36%	53%	73%
Total Chlorinated VOC Dissolved Phase Mass Discharge Reduction	50%	53%	88%	-38%	49%	73%
Average Maximum TCE Groundwater Concentration Reduction	50%	64%	91%	-8%	21%	12%
Total Cost of Remedy ($M)	--	1.49	6.34	0.81	2.25	2.48

Table 5-24: EISB remedy performance scores for VSD3, evaluated 5 years following the conclusion of the EISB remedy. Green shading indicates a success at meeting the PO.

Remedial Performance Objective	PO	Optimal	A	B	C	D
DNAPL Mass Reduction	25%	48%	33%	16%	19%	68%
Total Chlorinated VOC Dissolved Phase Mass Discharge Reduction	50%	59%	83%	-38%	4%	-25%
Average Maximum TCE Groundwater Concentration Reduction	50%	64%	90%	9%	0%	55%
Total Cost of Remedy ($M)	--	2.64	5.07	0.49	1.33	3.62

Of the 36 scored remedy performance objectives across VSDs 1 to 3, only 10 (83%), 4 (33%), and 4 (33%) DM team EISB remedies achieved the DNAPL mass reduction, total chlorinated VOC dissolved phase mass discharge reduction, and average maximum TCE groundwater concentration reduction POs, respectively. The scores presented in Table 5-22 to Table 5-24 show that most DM teams failed to meet the VSD-specific POs established for total chlorinated VOC dissolved phase mass discharge reduction and average maximum TCE groundwater concentration reduction.

5.2.2 Overview of Findings Regarding Remediation

Inspection of the approaches and results of the remediation designs of VSD 1 to 3 by the DM teams offers a range of insight concerning strategies, costs, and expectations of performance, as described in the previous sections. In general, these results show that:

- Overdesign of the remedy could overcome limitations in the underlying CSM but at a significant cost
- At some level of error, inaccuracies in the underlying CSM could not be overcome by remedy overdesign
- DNAPL mass removal metrics were generally easier to achieve than mass discharge metrics

5.3 Decision Theoretic (DT) Remediation

5.3.1 VSD1 Phase 1

Assessment of the DT approach (using SCOToolkit) began with only consideration of the DM Team's CSM data in the remedy design (priors only). This is the Phase 1 approach as described in Section 4.7. The DM Teams' CSMs, in terms of inputs required for SCOToolkit, were compared to understand the main differences between each CSM (Table 5-25).

Table 5-25: Summary of VSD1 *Priors* (DM Team best estimates)

Parameter	Team A	Team B	Team C	Team D
Darcy velocity (m/day)	0.02	0.0029	0.0032	0.016
Source mass (kg)	18,200	1,400	10,300	7,100
Source mass discharge (kg/day)	2.6	0.065	0.49	1.2
DNAPL architecture (-)	Residual ($\beta > 1$)	Residual ($\beta > 1$)	Pooled ($\beta < 1$)	Pooled ($\beta < 1$)
Source width (m)	17	32	37	18
Longitudinal Dispersivity (m)	10	9.1	6.8	7.3
Decay rate (1/day)	3.7E-03	5.6E-04	2.0E-04	6.9E-04
Retardation factor (-)	4	4.3	4.7	4.3

Figure 5-15 presents the simulated plumes in 2012 predicted by SCOToolkit using the input parameters from Table 5-25.

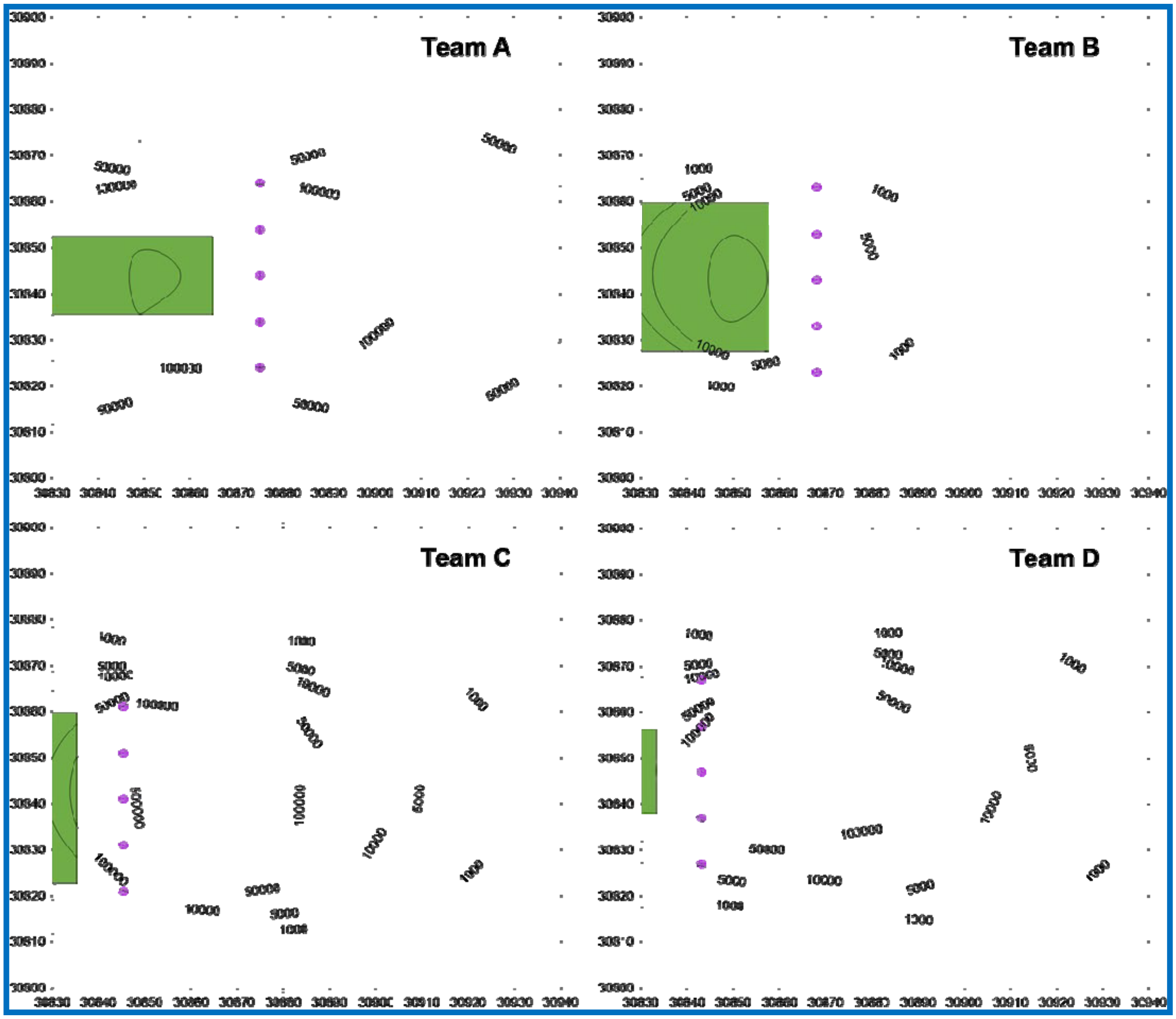


Figure 5-15: Simulated TCE plumes in 2012 using parameters (priors) from DM Teams' CSMs of VSD1. For each DM Team: TCE concentration contours (µg/L) from kriging modeled data. Concentration data plotted on similar axes (m). Green rectangles denote the downgradient extent of the DNAPL source zone (as defined in the DM Teams CSM shown in Figure 5-9 and normalized to the downgradient edge as specified in Team D's CSM).

Team A estimated the largest source area, projecting the leading edge of the source far downgradient compared to the other DM Teams (see Figure 5-9). This, coupled with the highest estimated source mass discharge, resulted in simulation of the longest and highest strength plume between the four teams. The source mass and source mass discharge estimated by Team B were between 1 and 2 orders of magnitude lower than Team A, resulting in a short, low strength plume based on their estimates of flow and transport parameters. Teams C and D provided similar estimates of source mass and architecture, with the exception of source width (Team C wider). Simulations of Teams C and D's conceptual models produced similar length plumes (based on the 50,000 µg/L contour).

These initial simulations (Phase 1 process) indicate that the DM Teams' estimates for key flow and transport parameters in VSD1 were broadly inconsistent with the plume extents delineated through their characterization and visualized in their CSM reports (see Figure 5-6). That is, flow and transport modeling based on their CSMs predicted very different plumes than they identified in their site investigations. Identification of this inconsistency through the use of simple analytical flow and transport modeling to check and/or refine parameter estimates against observed plume data would have resulted in improvements to the CSM before proceeding to design a remedy.

The identical Phase 1 process was performed using perfect information (access to all data used in DNAPL3D-RX to create VSD1). The plume simulated by the uncalibrated flow and transport model in SCOToolkit (Figure 5-16b) was quite similar to that produced by DM Teams C and D but overestimated concentrations in the plume fringe compared to "actual" concentrations (Figure 5-16a). The model used in Figure 5-16b was based on central tendency values (arithmetic means or geometric means) for variable parameters developed with access to perfect information for VSD1, as is a common approach for deterministic modeling. Even for a low complexity/heterogeneity site such as VSD1, this approach to model parameterization resulted in a poor match to observed data (compare Figure 5-16b to Figure 5-16a) that could mislead decisions for remediation.

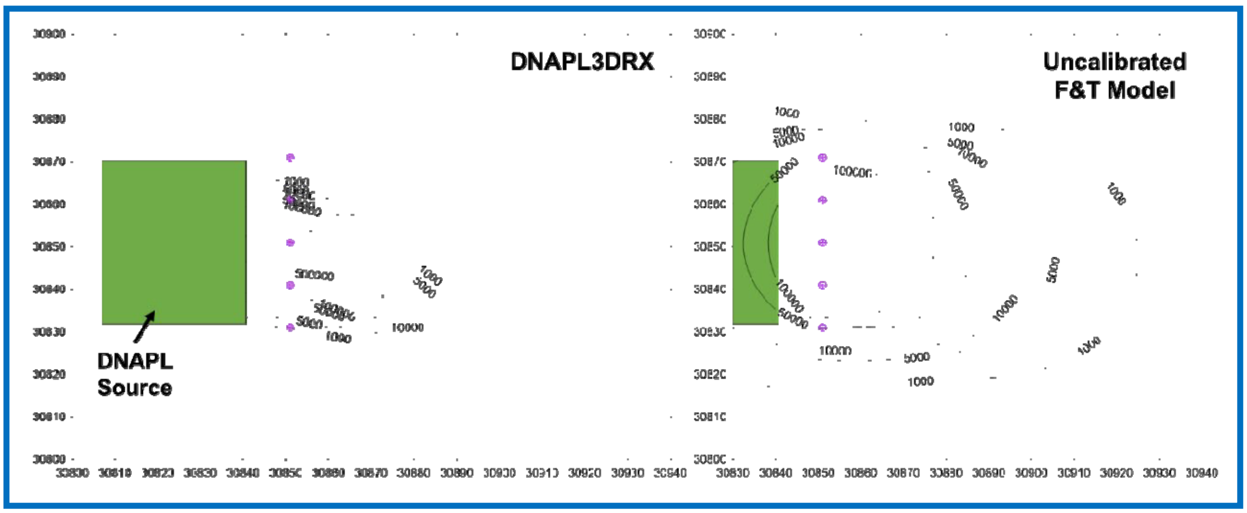


Figure 5-16: (a) TCE plume observed (perfect information) and (b) simulated with uncalibrated flow and transport model based on all available data from DNAPL3D-RX. TCE concentration contours (µg/l) from kriging observed and modeled data. Axes units are meters (m).

5.3.2 VSD1 Phase 2

Phase 2 consisted of calibrating the flow and transport model to the observed concentrations from each of the DM Team's CSM site investigations using the initial estimates from Phase 1 as priors. This process results in a set of posterior distributions for each SCOToolkit parameter. Prior and posterior distributions for key flow and transport parameters (Table 5-27 and Figure 5-17 to Figure 5-20) were compared to understand the effectiveness of calibration at improving the DM Teams' initial estimates from characterization and data analysis. To our knowledge none of the DM Teams used flow and transport modelling in the development of their CSMs of VSD1.

Table 5-26: Methodology for Creating Distributions for Phase 2

Parameter	Description	Distribution	Prior	Standard Deviation	Basis
ts	Initial source deposition date	Normal	1964	10	Judgment
t0	Final source deposition date	Normal	2006	10	Judgment
Jcal	Source mass discharge at tcal	Lognormal	From CSM report	Single est. = 1.0 to 1.2 Range = ln((max-min)/4)	Judgment Calculated
Mcal	Source mass at tcal	Lognormal	From CSM report	Single est. = 1.0 to 1.2 Range = ln((max-min)/4)	Judgment Calculated
β (beta)	Mass depletion-discharge coefficient	Lognormal	Pooled DNAPL (0.5) Residual DNAPL (1.5) Mixed/Not specified (1)	0.3 0.3 0.4	Judgment
N0	Source centroid northing	Normal	From CSM report	2	Judgment
Lx	Source width	Normal	From CSM report	1	Judgment
qw	Darcy velocity	Lognormal	From CSM report	Single est. = 0.6 Range = ln(K)/N^1/2	Judgment Calculated
Al	Longitudinal dispersivity	Normal	From CSM report	1	Judgment
AT/AL	Transverse/Longitudinal D ratio	Normal	0.1	0.5	Judgment
AV/AL	Vertical/Longitudinal D ratio	Normal	0.01	0.5	Judgment
lambda	Degradation coefficient	Lognormal	From CSM report	Single est. = 1.8 Range = ln((max-min)/4)	Literature Calculated

Table 5-27: Priors and posteriors for key flow and transport parameters

Parameter	pdf	Te m A							
		Prior							
Source Mass Discharge (kg/day)	LN	2.62 (1.47)	0.59 (0.55)	0.07 (1.47)	0.03 (0.35)	0.49 (1.65)	0.05 (0.44)	1.21 (1.49)	0.43 (0.41)
Source Mass (kg)	LN	6,060 (0.90)	16,167 (0.88)	1,400 (0.67)	384 (0.42)	10,300 (0.25)	10,211 (0.25)	7,133 (1.20)	4,214 (1.19)
Beta (-)	LN	1.5 (0.2)	1.43 (0.2)	1.5 (0.2)	4.94 (0.2)	0.5 (0.3)	0.51 (0.3)	0.5 (0.3)	1.0 (0.3)
Source width (m)	N	32 (1.0)	32.73 (0.49)	32 (1.0)	31.99 (1.0)	37 (1.0)	30.18 (0.8)	18.3 (1.0)	17.6 (0.84)
Darcy velocity (m/day)	LN	0.02 (0.51)	0.011 (0.46)	0.003 (0.51)	0.002 (0.16)	0.003 (0.91)	0.002 (0.3)	0.016 (0.57)	0.004 (0.21)
Long. Dispersivity (m)	N	10.3 (1.0)	9.82 (1.0)	9.14 (1.0)	7.53 (0.94)	6.8 (1.0)	5.81 (0.92)	7.25 (1.0)	3.74 (0.25)
Degradation coefficient $^{-1}$	LN	0.004 (1.8)	0.015 (0.49)	0.1 (0.68)	0.021 (0.67)	0.002 (1.15)	0.0001 (0.96)	0.0007 (1.15)	0.0017 (1.10)

PDF – probability density function form
LN – log normal
N – normal
Prior and posterior distributions defined by the mean (either arithmetic or geometric) and standard deviation (in parentheses)

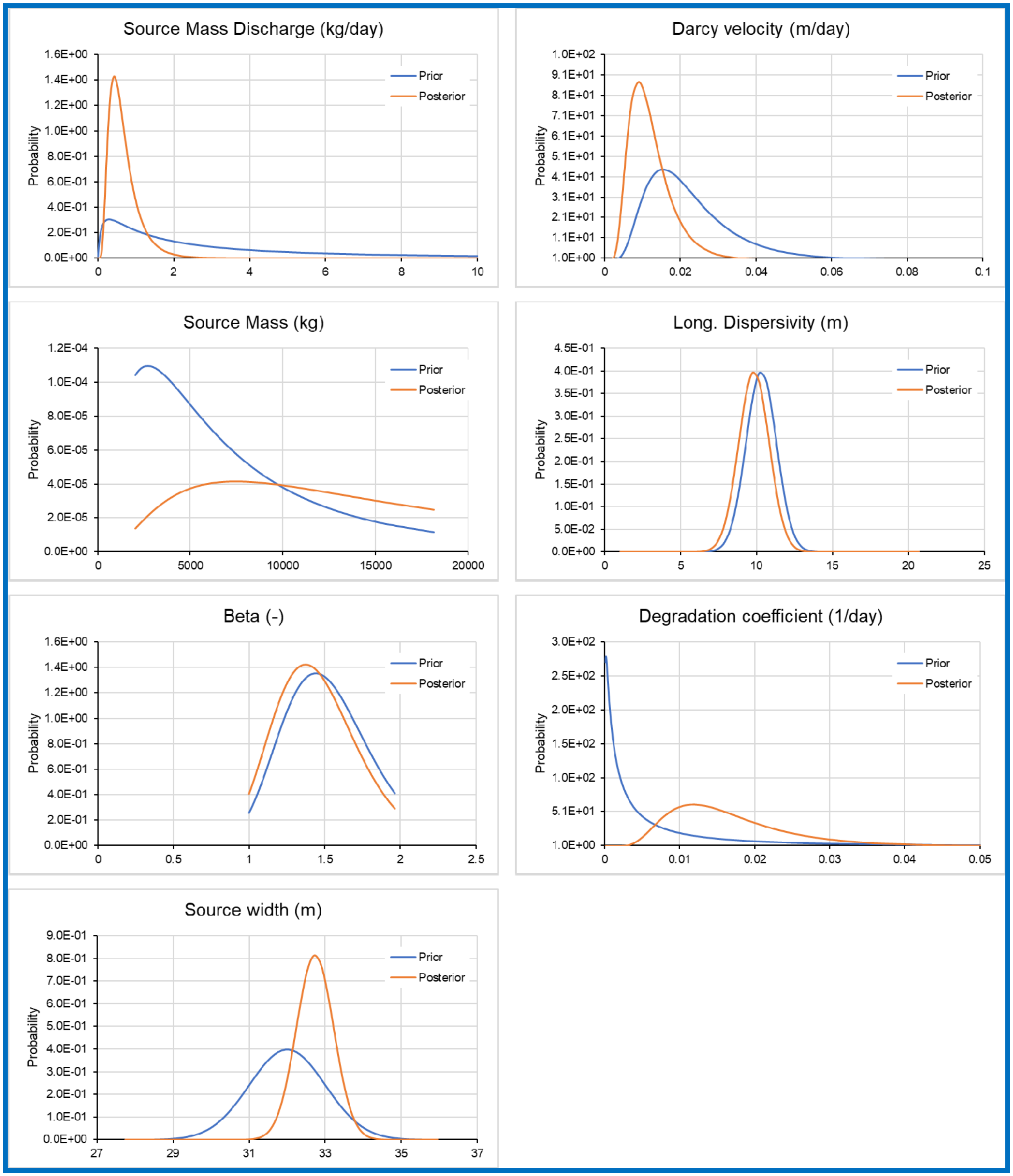


Figure 5-17: Comparison of prior and posterior distributions for key parameters, VSD1, Team A

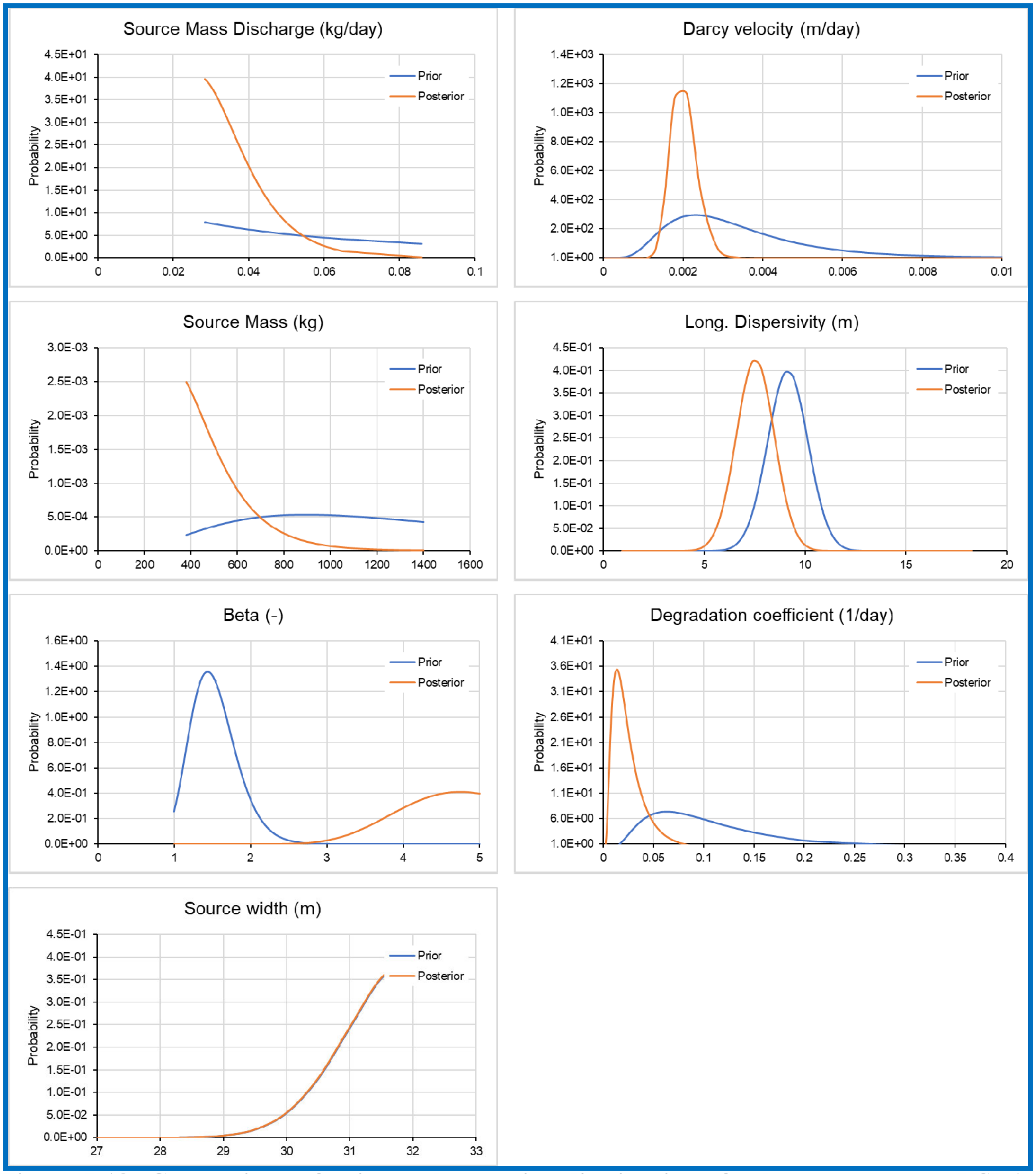


Figure 5-18: Comparison of prior and posterior distributions for key parameters, VSD1, Team B

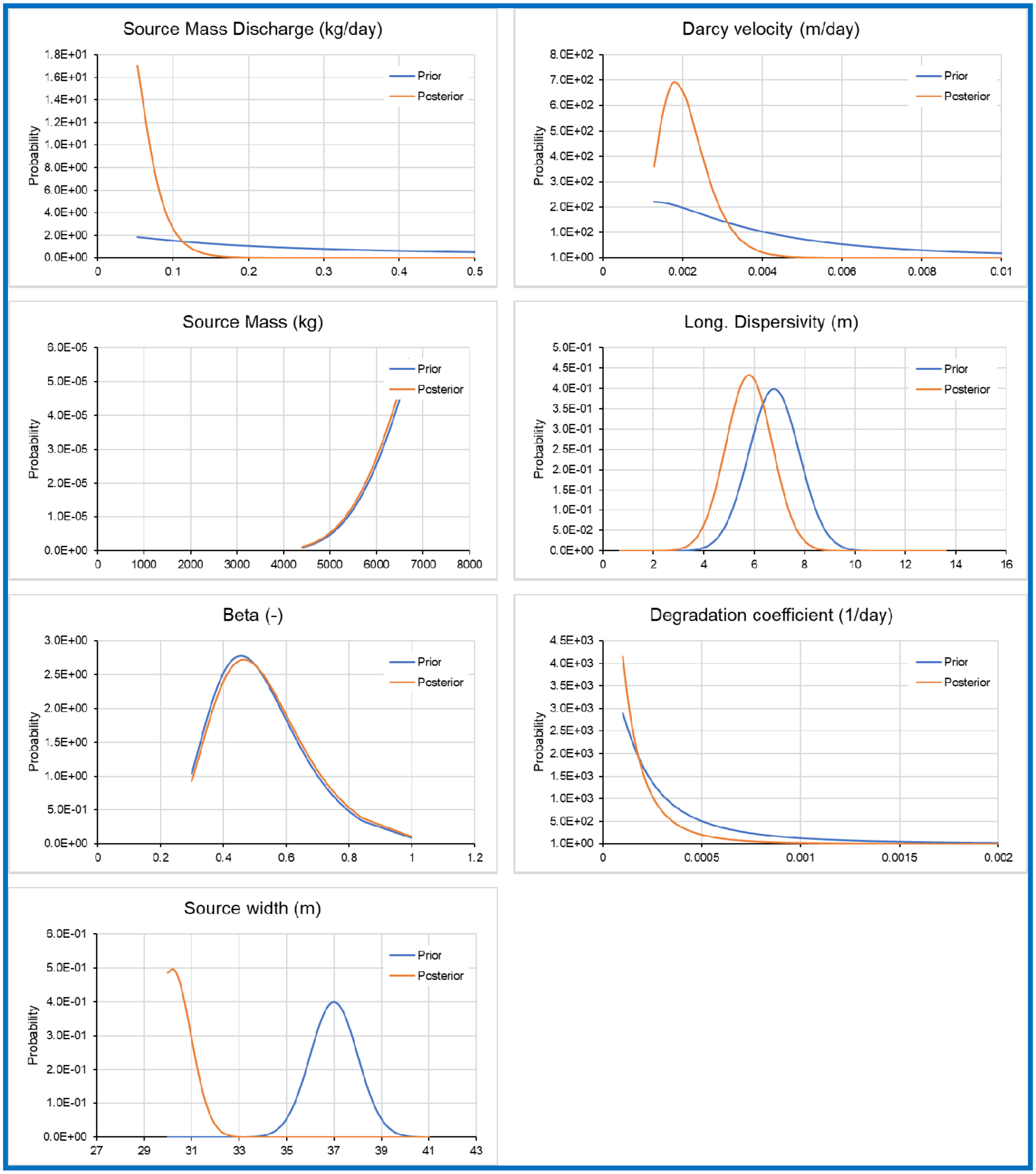


Figure 5-19: Comparison of prior and posterior distributions for key parameters, VSD1, Team C

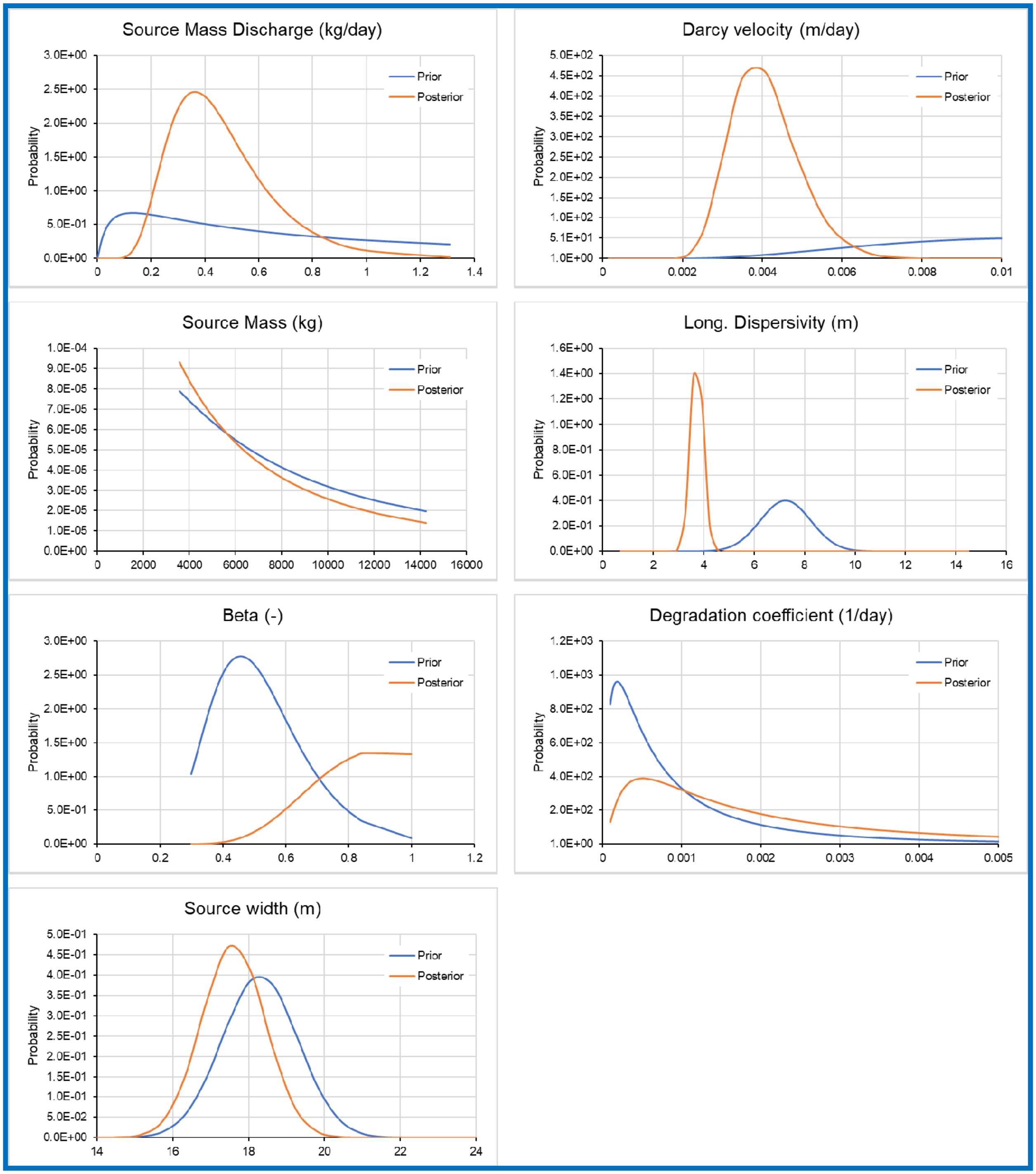


Figure 5-20: Comparison of prior and posterior distributions for key parameters, VSD1, Team D

Model calibration to groundwater concentration data (to create the posteriors) altered the estimates of key flow and transport parameters. Source mass discharge, source mass and Darcy velocity were the parameters estimated by the DM Teams that were most affected in terms of changes from priors to posteriors. Effects included shifts in the means and reduced uncertainty (smaller standard deviation) of flow and transport parameters. Team C defined ranges for several parameters, however the differences in prior and posterior distributions were relatively small. The greatest differences between prior and posterior distributions were noted for DM Teams A, B and D, who generally provided single value estimates for uncertain parameters (and thus uncertainty was added by the project team using approaches outlined in Appendix G). While uncertainty in the posterior distributions was reduced for nearly all parameters, the posterior means, in some cases (e.g., source mass, beta and degradation coefficient), were shifted by more than an order of magnitude to extreme values.

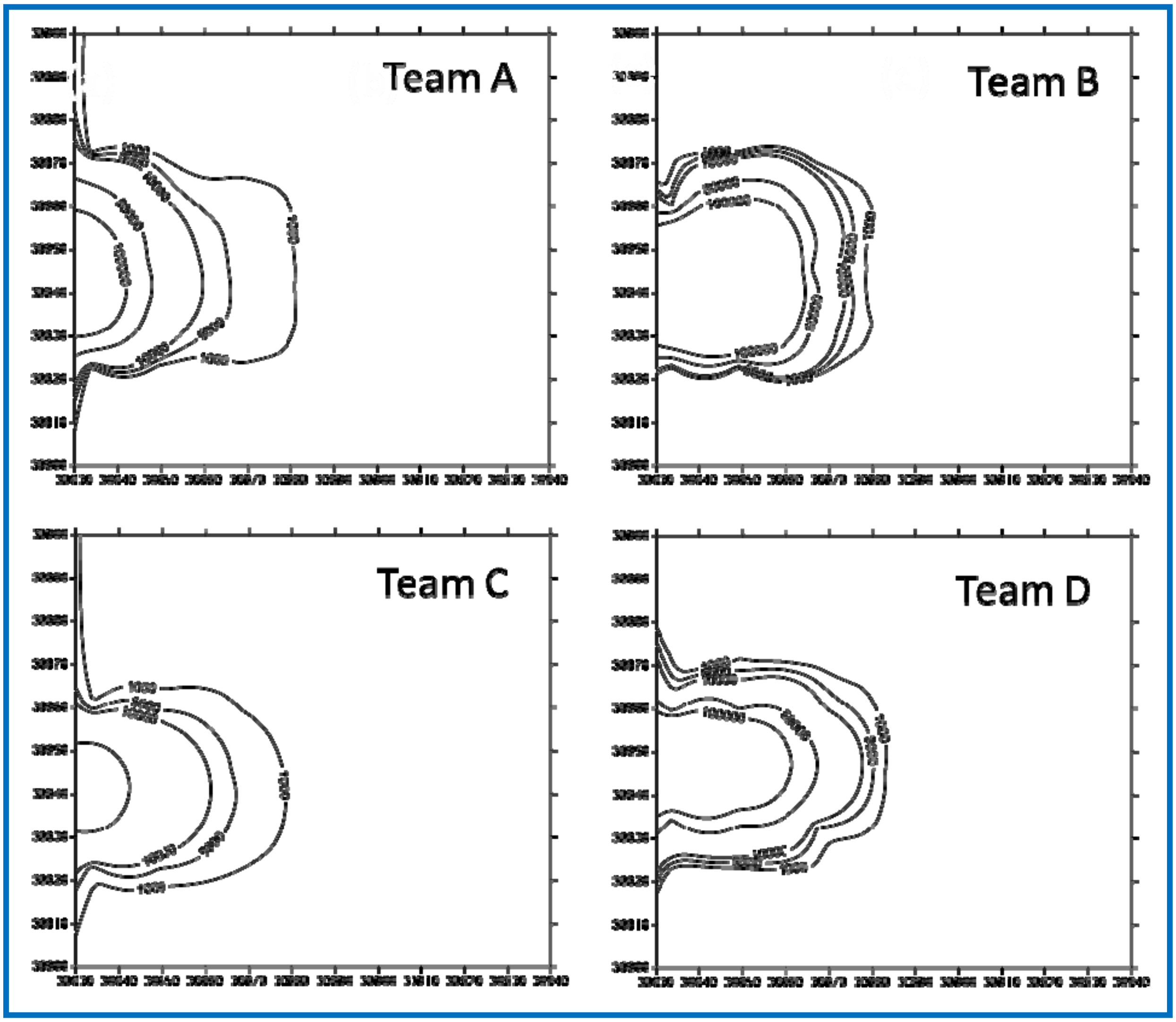


Figure 5-21: Simulated TCE plumes at start of remedy using posteriors (Figures 5-18 to 5-21). For each DM Team: TCE concentration contours (µg/L) from kriging modeled data. Concentration data plotted on similar axes (m).

Following Phase 2 calibration, the predicted plumes for each of the DM Teams were similar in extent (Figure 5-21) however still could not replicate the observed data of the "real" plume (Figure 5-16a). The correlation between observed and simulated TCE concentrations in groundwater was generally high (0.8 to 0.9 for Teams A, B and D). Poorer correlation was achieved for Team C (0.67). The priors for Teams A, B and D were more uncertain than for Team C, owing to the more limited information provided by those teams (the DM Teams were not required to provide quantitative estimates of flow and transport parameter uncertainties in their CSM reports). In this case, the information provided by Team C likely over constrained the calibration of certain parameters, reducing the model's ability to match the concentration data. This information suggests that while Team C considered uncertainty in its conceptualization of VSD1, the degree of uncertainty may have been underestimated resulting in artificial constraint of the model (forced to limit parameter uncertainty) and resulting in poorer performance than Teams that did not consider uncertainty.

5.3.3 Optimized EISB remedies based on Phase 1 and Phase 2 Approaches

Remedy optimization using the Phase 1 and Phase 2 approaches is summarized in Table 5-28 to Table 5-31 and Figure 5-22 to Figure 5-26 (Phase 2 only). Recall that the POs for the assessment are approached in two different ways. The first approach (relative) is to see if the designed remedy achieves the required percent reduction based on the estimates of the parameters using the DM Team's CSMs. As an example, imagine that the actual source mass discharge was 1000 grams per year (g/yr) but was predicted by the DM team to be 1 g/yr (i.e., their CSM was a poor estimate). If the PO was a 30% reduction, then if the remedy reduced the source mass discharge to 0.7 g/yr the relative PO is considered achieved. However, the system required to achieve a post-remediation 700 g/yr source mass discharge to meet the actual PO based on an accurate CSM (30% reduction from of 1000 g/yr) would be very different than the system required to achieve a 0.3 g/yr reduction. Because of this, the second approach (absolute) was implemented which evaluated the PO against the actual targets based on the actual site data. So, to meet the 30% PO in the absolute approach would require a mass discharge of 700 g/yr. If the DM Team CSM is predicting a mass discharge of 1 g/yr prior to any remedy being implemented, then SCOToolkit would decide that it was already compliant and thus pick monitored natural attenuation (MNA) as the remedial option. Thus, SCOToolkit would incorrectly identify MNA as the approach due to the poor CSM parameter estimate (not due to any limitations with the model).

Team A

Application of Team A's CSM for remediation planning in VSD1 would likely result in an incorrect remedy choice, even with calibration of the flow and transport model. Remedial simulation using Team A's best estimates of flow and transport parameters (Phase 1 modeling) indicated that plume concentrations, source mass and source mass discharge would achieve the target relative percent reductions through MNA and absolute reductions with only minor lactate injections. The overestimated source size (in the direction of groundwater flow) meant that Team A's concentration compliance well was located far downgradient of the actual source, in the distal, lower concentration portion of the plume. Despite the overestimated high source mass discharge, rapid depletion of source mass through dissolution combined with rapid degradation via an overestimated TCE degradation rate in the plume, led the model to predict the remediation criteria could be achieved within the timeframe for treated groundwater to migrate between the electron donor infiltration gallery and distant concentration compliance well (27 years), leading to incorrect remedy selection (MNA vs. active).

Model calibration (Phase 2 modeling) did not markedly improve Team A's estimates of key parameters and their uncertainties, nor identification of a remedy that would achieve high levels of certainty for compliance with the PO. Notably, calibration increased estimates of source mass and decreased source mass discharge to such an extent that achieving the relative percent reductions in these objectives would be challenging for EISB. As such, all three POs were only achieved in 16% of calibrated model realizations. TCE concentrations in groundwater at the compliance well (more than 35 m downgradient of the actual DNAPL source) were already in compliance with the absolute remediation concentration target, driving the model to identify MNA as the optimal remedy for this scenario. Under natural, non-injecting conditions, the absolute source mass and source mass discharge POs were achieved in higher proportions of calibrated model realizations, increasing the overall compliance performance of MNA. It is possible that were Team A to use the calibrated model to design the remedy, this would result in specifying a more aggressive strategy for VSD1, that achieved less and cost $0.72 million more compared to MNA. The low certainty (less than 30% of realizations meeting the objectives) in the adequacy of either remedial option (EISB or MNA) should prompt re-evaluation of the CSM, in particular revised delineation of the source, source mass discharge and TCE degradation rate, and modeling for VSD1 before redesigning the remedy to achieve higher rates of compliance with the remedial targets.

Table 5-28: Optimized remedies for VSD1 based on models of DM Team A's CSM report

Parameter	Deterministic, Uncalibrated F&T Model		Stochastic, Calibrated F&T Model	
Remediation Criteria[1]	**Relative**	**Absolute**	**Relative[4]**	**Absolute**
Target Concentration (µg/l)	95,276	180,050	-60%	180,050
Target Source Mass (kg)	3,254	7,000	-30%	7,000
Target Source Mass Discharge (kg/day)	1.08	0.2119	-50%	0.2119
Optimal remedy	MNA	EISB	EISB	MNA
Injection rate (kg/day)	---	0.5	50.9	---
Injection duration (years)	---	2	2.27	---
Compliance[2]	**Pass**	**Pass**	**16%**	**28%**
Concentration	Pass	Pass	13%	100%
Source Mass Discharge	Pass	Fail	59%	68%
Source Mass	Pass	Pass	2%	33%
Remedy Cost ($k)[3]	395	360	5,317	4,597

MNA – monitored natural attenuation (i.e., no active remediation required)

1 Relative remediation targets calculated for uncalibrated F&T model or for 100 realizations of calibrated F&T model based on Team A CSM report for VSD1. Absolute remediation targets from DNAPL3DRX model for VSD1

2 Compliance with remediation targets for single realization of uncalibrated F&T model or percent of 100 realizations of calibrated F&T model compliant with remediation targets

3 Remediation cost calculated by SCOToolkit including penalty for single realization of uncalibrated F&T model (Deterministic) or average of remediation costs for 100 realizations of calibrated F&T model (Stochastic)

4 Actual criteria calculated for each realization

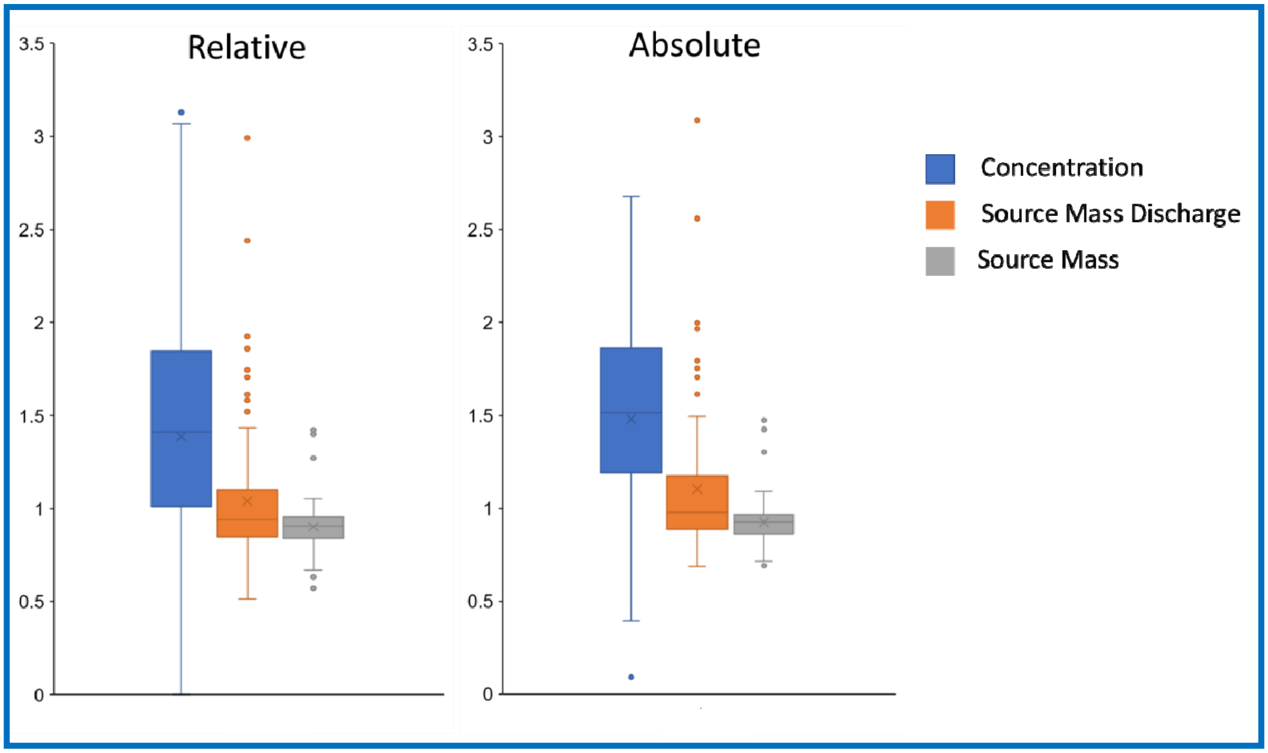


Figure 5-22: VSD1 remedy performance, Phase 2, Team A. The Y-axis is the ratio of the simulated value to PO: > 1 denotes Fail; ≤ 1 denotes Pass. The box represents the 25th to 75th percentiles of the 100 realizations with the line representing the 50th percentile. The "x" represents the arithmetic mean. Whiskers extend to 1.5 times the interquartile range with dots representing simulations that fall outside the whiskers.

Team B

EISB was the optimal remedy predicted by SCOToolkit using the relative percent reduction objectives for Team B's CSM (Phase 1 modeling). Team B's CSM included the lowest estimates of source mass and source mass discharge among the four DM teams. Due to an underestimated Darcy velocity, the remedial targets could be easily achieved with limited lactate injection (12,100 kg over 5 years). Source mass, source mass discharge and TCE concentrations in groundwater 10 m downgradient of the source were already lower than the absolute targets at the start of the proposed remedy (based on the incorrect R_es), causing SCOToolkit to select MNA as the optimal remedy for VSD 1.

Model calibration did not improve Team B's estimates of flow and transport parameters. Source mass, source mass discharge and Darcy velocity were calibrated to be lower than the true values (due to constraints imposed by the lack of information regarding uncertainty in Team B's CSM report), while an extreme posterior for beta was calibrated (indicating a high mass transfer rate) to match observed TCE concentrations in groundwater. Although the optimal remedy under relative percent reduction targets was again forecast to be EISB (the same as in Phase 1) and achieved high rates of compliance with source mass (89%) and source mass discharge (96%) relative remedial targets (Figure 5-23), the low strength plume simulated by the calibrated model was challenging to remediate and achieved target relative percent reductions in groundwater concentrations of TCE in far fewer realizations (15%). The model optimized remedy required more than 1,000 tonnes of lactate to be injected over 5 years which is not practical and an alternative approach would be needed.

When considering absolute remedial targets, the source mass, source mass discharge and TCE concentrations in groundwater for this scenario were low and easily achieved compliance within the five-year timeframe for remediation. Remedy optimization modeling therefore identified MNA as the preferred option to achieve the absolute remedy targets (Figure 5-23).

Table 5-29: Optimized remedies for VSD1 based on models of DM Team B's CSM report

Parameter	Deterministic, Uncalibrated F&T Model		Stochastic, Calibrated F&T Model	
Remediation Criteria[1]	**Relative**	**Absolute**	**Relative[4]**	**Absolute**
Target Concentration (µg/l)	6,542	180,050	-60%	180,050
Target Source Mass (kg)	964	7,000	-30%	7,000
Target Source Mass Discharge (kg/day)	0.032	0.2119	-50%	0.2119
Optimal remedy	EISB	MNA	EISB	MNA
Injection rate (kg/day)	6.63	---	578	---
Injection duration (years)	5	---	5	---
Compliance[2]	**Pass**	**Pass**	**13%**	**100%**
Concentration	Pass	Pass	15%	100%
Source Mass Discharge	Pass	Pass	96%	100%
Source Mass	Pass	Pass	89%	100%
Remedy Cost ($k)[3]	1,031	---	5,828	---

MNA – monitored natural attenuation (i.e., no active remediation required)

1 Relative remediation targets calculated for uncalibrated F&T model or for 100 realizations of calibrated F&T model based on Team B CSM report for VSD1. Absolute remediation targets from DNAPL3DRX model for VSD1

2 Compliance with remediation targets for single realization of uncalibrated F&T model or percent of 100 realizations of calibrated F&T model compliant with remediation targets

3 Remediation cost including penalty for single realization of uncalibrated F&T model or average of remediation costs for 100 realizations of calibrated F&T model

4 Actual criteria calculated for each individual realization

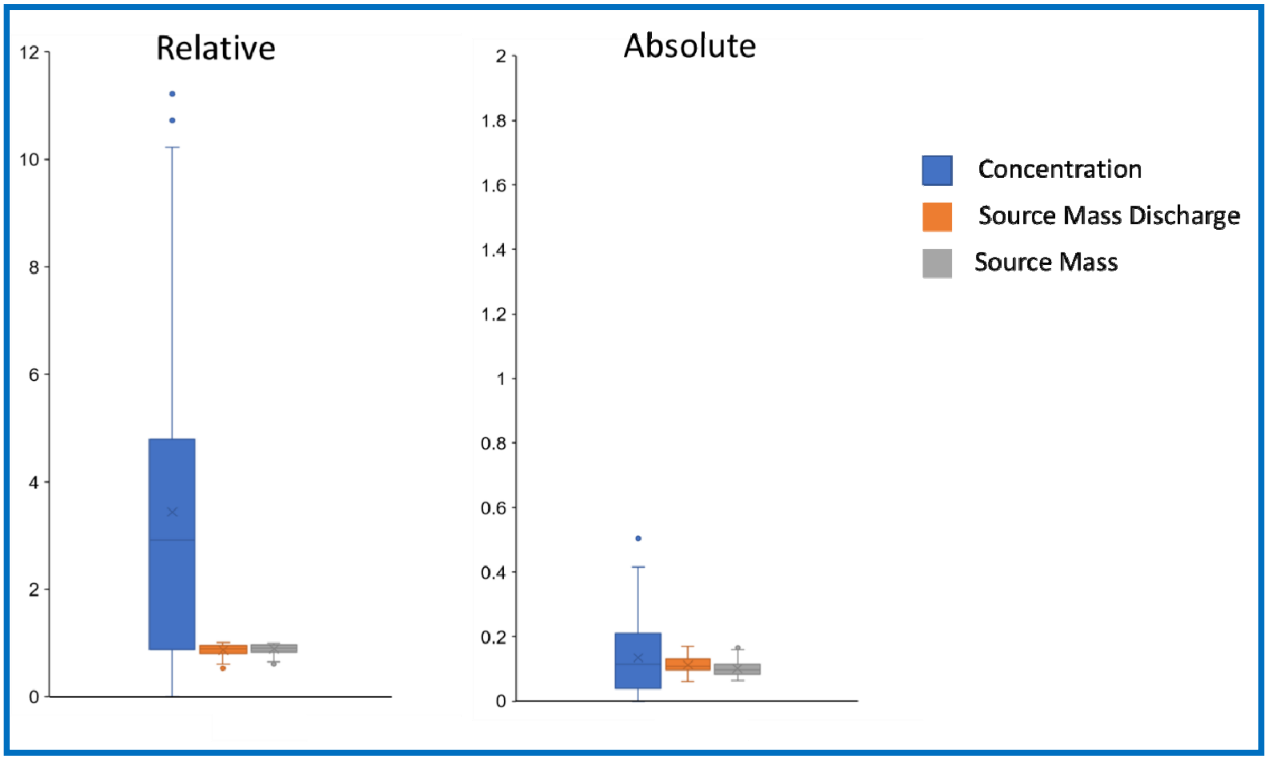


Figure 5-23: VSD1 remedy performance, Phase 2, Team B. The Y-axis is the ratio of the simulated value to PO: > 1 denotes Fail; ≤ 1 denotes Pass. The box represents the 25th to 75th percentiles of the 100 realizations with the line representing the 50th percentile. The "x" represents the arithmetic mean. Whiskers extend to 1.5 times the interquartile range with dots representing simulations that fall outside the whiskers.

Team C

An optimal EISB remedy could not be identified for either the relative or absolute targets for the uncalibrated (Phase 1) approach based on Team C's CSM report. Remedies could not be found to address both the high TCE concentrations in groundwater at the compliance well with the low estimated source mass. Relative percent reduction and absolute remedial targets for source mass and source mass discharge were achieved with no action (again based on the incorrect DM Team interpretation) but the concentration target was difficult to meet efficiently (an extreme, non-optimal EISB option (lactate injected at 761 kg/day over 5 years) was also simulated that achieved the concentration target but would likely not be selected as a viable remediation option). This is not due to any limitations within SCOToolkit rather highly inconsistent (and misaligned) priors from the CSM.

Model calibration (Phase 2 modeling) did not materially change the estimated source mass but reduced source mass discharge by nearly 2 orders of magnitude to reduce predicted TCE concentrations in groundwater downgradient of the source. The calibration process resulted in relative percent reduction remedial targets for source mass discharge and TCE concentrations that would be challenging for EISB to achieve efficiently within the remediation timeframe. The source mass relative percent reduction target was met in 93% of calibrated model realizations with no intervention, but only 10% of realizations met the criterion for source mass discharge and 0% of realizations for the TCE concentration criterion under these conditions (Figure 5-24). In comparison, SCOToolkit indicated the absolute remediation targets were met (based on the incorrect DM Team CSM) without need for active remediation.

The lack of a viable remedy from the modeling should trigger re-evaluation of the CSM. Specifically, the estimation of source mass, that was found to be incompatible with estimates for source mass discharge and calibrated values of beta, requires further investigation. Initial underestimates of source mass and, the presumption that DNAPL was pooled (beta ≤ 1), may have constrained source mass discharge through calibration such that elevated plume concentrations could not be simulated. Although Team C did examine ranges of some flow and transport parameters, it appears that more in-depth investigation of uncertainties associated with these parameters (and variability in observations informing these estimates) is warranted, even for relatively low complexity systems such as VSD1.

Table 5-30: Optimized remedies for VSD1 based on models of DM Team C's CSM report

Parameter	Deterministic, Uncalibrated F&T Model		Stochastic, Calibrated F&T Model	
Remediation Criteria[1]	**Relative**	**Absolute**	**Relative[4]**	**Absolute**
Target Concentration (µg/l)	249,980	180,050	-60%	180,050
Target Source Mass (kg)	3,725	7,000	-30%	7,000
Target Source Mass Discharge (kg/day)	0.242	0.2119	-50%	0.2119
Optimal remedy	NOR	NOR	NOR	MNA
Injection rate (kg/day)	<0.5	<0.5	<0.5	---
Injection duration (years)	>5	>5	4.98	---
Compliance[2]	**Fail**	**Fail**	**0%**	**100%**
Concentration	Fail	Fail	0%	100%
Source Mass Discharge	Pass	Pass	10%	100%
Source Mass	Pass	Pass	93%	100%
Remedy Cost ($k)[3]	>6,000	>6,000	>6,000	---

MNA – monitored natural attenuation (i.e., no active remediation required)
NOR – no optimal EISB remedy
1 Relative remediation targets calculated for uncalibrated F&T model or for 100 realizations of calibrated F&T model based on Team C CSM report for VSD1. Absolute remediation targets from DNAPL3DRX model for VSD1
2 Compliance with remediation targets for single realization of uncalibrated F&T model or percent of 100 realizations of calibrated F&T model compliant with remediation targets
3 Remediation cost including penalty for single realization of uncalibrated F&T model or average of remediation costs for 100 realizations of calibrated F&T model
4 Actual criteria calculated for each individual realization

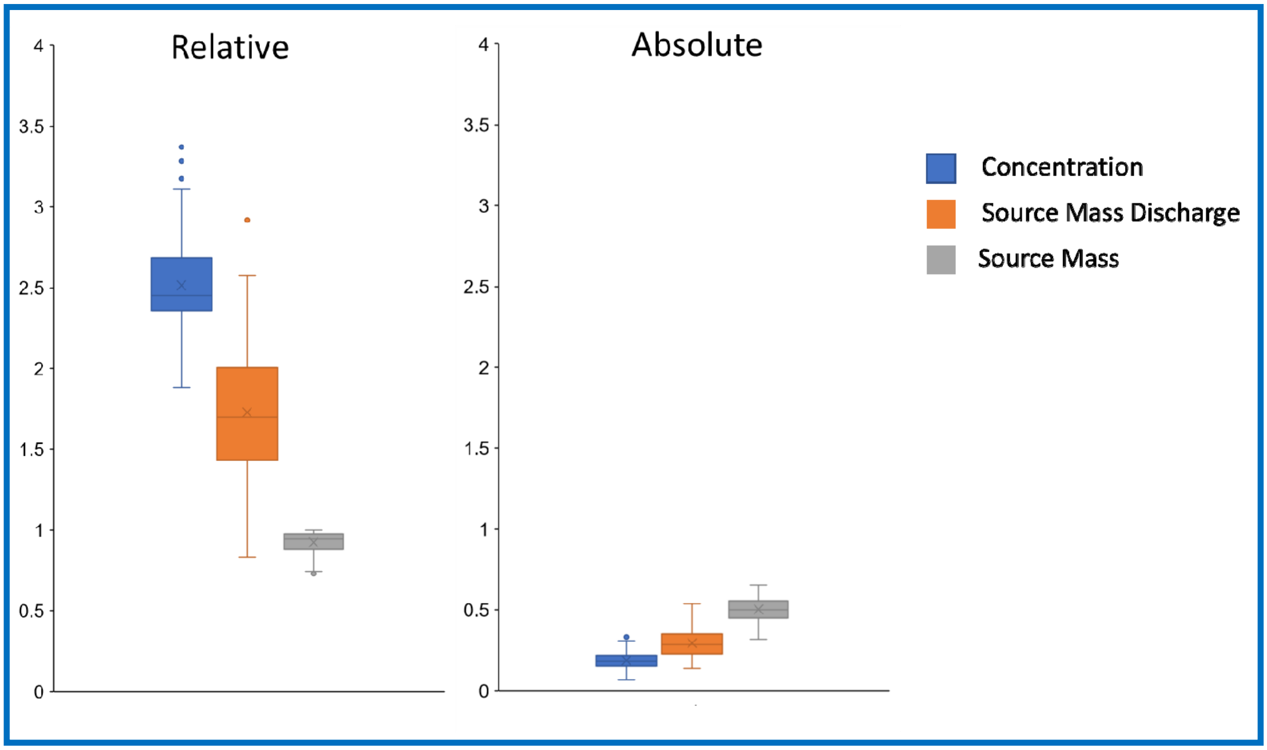


Figure 5-24: VSD1 remedy performance, Phase 2, Team C. The Y-axis is the ratio of the simulated value to PO: > 1 denotes Fail; ≤ 1 denotes Pass. The box represents the 25^{th} to 75^{th} percentiles of the 100 realizations with the line representing the 50^{th} percentile. The "x" represents the arithmetic mean. Whiskers extend to 1.5 times the interquartile range with dots representing simulations that fall outside the whiskers.

Team D

An optimal EISB remedy that met all objectives could not be identified (for either relative or absolute targets) based on Team D's conceptual model (Phase 1 modeling). Natural attenuation was predicted to achieve source mass discharge and source mass relative percent reduction remedial targets during the timeframe for remediation, but not concentration. This is likely linked to the relatively high rate of dissolution of the underestimated DNAPL source mass. Absolute source mass discharge and TCE concentration remediation targets could not be achieved even with implementation of highly aggressive active remedies.

Calibration of the model (during Phase 2) generated a posterior PDF for source mass discharge that bracketed the actual value for uncertainty but did not similarly improve estimates for source mass. The optimal remedies for achieving remedial targets for Team D's CSM of VSD1 used injection of lactate at 52.8 (relative) and 75.6 (absolute) kg/day over a 5-year period. The compliance rate for relative percent reduction remedial targets (compared to CSM data) was 12%, whereas the compliance rate for the absolute remedial targets was 83%. Given the similarity between the optimal remedies for relative and absolute objectives, this discrepancy is attributed to how compliance is measured in SCOToolkit. For the relative percent reduction remedial target, the compliance is assessed for each realization of the calibrated model. This means that for some realizations the magnitude of reduction required might be very small (to achieve the percent reduction) and in some cases the magnitude might be very high. This makes achieving high certainty that the remedy will achieve compliance challenging as the magnitude of the reductions can span an order of magnitude between realizations. When such large uncertainty is present in remedy design (also present in the priors and pre-posteriors) it should be a clear indicator that additional CSM refinement or checking is required.

The uncertainty in source mass and source mass discharge estimates (wide standard deviations in the distributions) drives the number of realizations with failure of relative targets for this remedy. This uncertainty could potentially be reduced with improved characterization of the source, including use of diagnostic methods for DNAPL delineation and in situ measurements of Darcy velocity.

Table 5-31: Optimized remedies for VSD1 based on models of DM Team D's CSM report

Parameter	Deterministic, Uncalibrated F&T Model		Stochastic, Calibrated F&T Model	
Remediation Criteria[1]	**Relative**	**Absolute**	**Relative[4]**	**Absolute**
Target Concentration (µg/l)	285,685	180,050	-60%	180,050
Target Source Mass (kg)	4,689	7,000	-30%	7,000
Target Source Mass Discharge (kg/day)	0.586	0.2119	-50%	0.2119
Optimal remedy	NOR	NOR	EISB	EISB
Injection rate (kg/day)	<0.5	<0.5	75.6	52.8
Injection duration (years)	>5	>5	5	5
Compliance[2]	**Fail**	**Fail**	**12%**	**83%**
Concentration	Fail	Fail	98%	99%
Source Mass Discharge	Pass	Pass	16%	97%
Source Mass	Pass	Fail	10%	85%
Remedy Cost ($k)[3]	>6,000	>6,000	5,185	1,768

MNA – monitored natural attenuation (i.e., no active remediation required)
NOR – no optimal EISB remedy
1 Relative remediation targets calculated for uncalibrated F&T model or for 100 realizations of calibrated F&T model based on Team D CSM report for VSD1. Absolute remediation targets from DNAPL3DRX model for VSD1
2 Compliance with remediation targets for single realization of uncalibrated F&T model or percent of 100 realizations of calibrated F&T model compliant with remediation targets
3 Remediation cost including penalty for single realization of uncalibrated F&T model or average of remediation costs for 100 realizations of calibrated F&T model
4 Actual criteria calculated for each individual realization

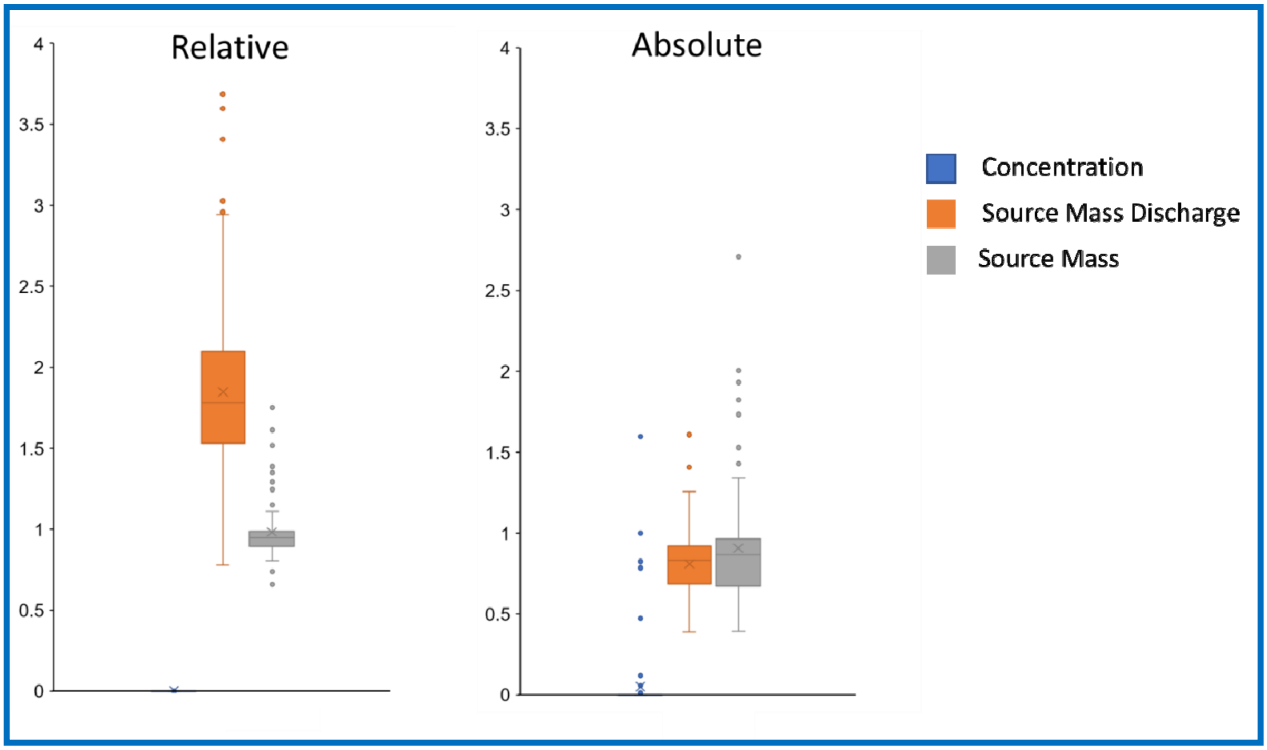


Figure 5-25: VSD1 remedy performance, Phase 2, Team D. Y-axis – simulated value to remediation criterion ratio: > 1 denotes Fail; ≤ 1 denotes Pass. The box represents the 25th to 75th percentiles of the 100 realizations with the line representing the 50th percentile. The "x" represents the arithmetic mean. Whiskers extend to 1.5 times the interquartile range with dots representing simulations that fall outside the whiskers.

5.3.4 Comparison with optimized remedies for flow and transport models based on all available data from DNAPL3DRX (Phase 3 – Perfect Information)

The uncalibrated flow and transport model (using priors estimated from access to perfect information) generated a plume that was a poor match for observed data (Figure 5-16). Therefore, reliance on a deterministic simulation using SCOToolkit resulted in incorrectly choosing MNA when active intervention was required (for both relative and absolute targets). This is primarily due to the differences between the 3-D process-based numerical model used to generate the VSDs and the analytical averaged model used within SCOToolkit. Field-scale variability in permeability, DNAPL saturation, and sorption, for example, result in differences that the simpler model is unable to rectify with the priors.

Calibration with priors estimated using known values from the heterogeneous domain improved the model performance and SCOToolkit indicated a low injection rate over 4.5 years achieves the remedial targets in 25 and 52% (relative and absolute respectively) of realizations. The performance of the optimal remedy as identified by SCOToolkit (ability to meet targets for both relative and absolute, Figure 5-26) is challenged by the source mass target and uncertainty in the source mass (high standard deviation in the pre-posterior), rather than source mass discharge and plume concentration targets that are met in a high proportion of model realizations. Closer inspection of the calibrated model shows that in more than 50% of the realizations, predicted concentrations at the compliance well location were at or below the target concentration at the start of active remediation (indicating no need for remediation to meet that target), which may explain why the optimal injection rate was low and did not achieve substantial source mass reduction resulting in non-compliance with that target. While parameter variability is considered by SCOToolkit, the spatial distribution of variable parameters, that likely contributed to the differences between the SCOToolkit and DNAPL3D-RX simulations, is not.

Even with all available data and consideration of uncertainty, the analytical model could not consistently match observation data sufficiently to identify a remedy that would achieve all three remediation targets more than approximately 50% of the time (Figure 5-26). The modeling suggests that, while analytical models can and should be used to support the development of site conceptual models (provide a holistic check), they may not be suited to remedy design even for low complexity/low heterogeneity sites, such as VSD1. A numerical model that can account for spatial variability of key parameters is preferred if (and only if) the level of site characterization can support developing such a model.

Table 5-32: Optimized remedies for VSD1 based on models of all available data from DNAPL3DRX

Parameter	Deterministic, Uncalibrated F&T Model		Stochastic, Calibrated F&T Model	
Remediation Criteria[1]	**Relative**	**Absolute**	**Relative[4]**	**Absolute**
Target Concentration (µg/l)	64,432	180,050	-60%	180,050
Target Source Mass (kg)	7,005	7,000	-30%	7,000
Target Source Mass Discharge (kg/day)	0.209	0.2119	-50%	0.2119
Optimal remedy	MNA	MNA	EISB	EISB
Injection rate (kg/day)	---	---	0.5	0.5
Injection duration (years)	---	---	4.45	4.45
Compliance[2]	**Fail**	**Pass**	**25%**	**52%**
Concentration	Fail	Pass	25%	82%
Source Mass Discharge	Pass	Pass	58%	70%
Source Mass	Pass	Pass	100%	53%
Remedy Cost ($k)[3]	>6,000	---	4,597	3,082

MNA – monitored natural attenuation (i.e., no active remediation required)

1 Relative remediation targets calculated for uncalibrated F&T model or for 100 realizations of calibrated F&T model for VSD1. Absolute remediation targets from DNAPL3DRX model for VSD1

2 Compliance with remediation targets for single realization of uncalibrated F&T model or percent of 100 realizations of calibrated F&T model compliant with remediation targets

3 Remediation cost including penalty for single realization of uncalibrated F&T model or average of remediation costs for 100 realizations of calibrated F&T model

4 Actual criteria calculated for each individual realization

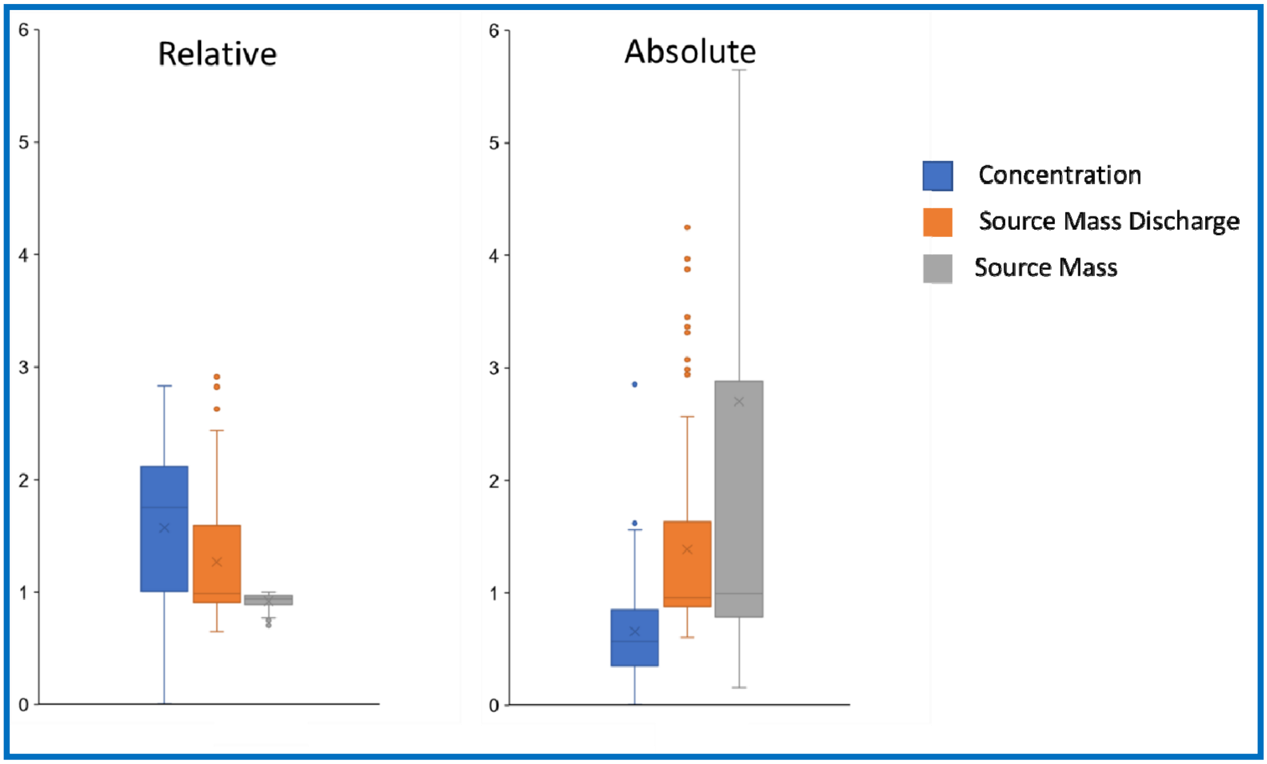


Figure 5-26: VSD1 remedy performance, all data, Phase 2. Y-axis – simulated value to remediation criterion ratio: > 1 denotes Fail; ≤ 1 denotes Pass. The box represents the 25th to 75th percentiles of the 100 realizations with the line representing the 50th percentile. The "x" represents the arithmetic mean. Whiskers extend to 1.5 times the interquartile range with dots representing simulations that fall outside the whiskers.

5.3.5 VSD2

Overall, the parameters estimated by DM Team C were a reasonable representation of the actual VSD2 conditions. Calibration of the fate and transport model did not substantially change priors or uncertainties for source mass, source mass discharge or Darcy velocity (Figure 5-27). The most marked parameter changes introduced by calibration were for beta, source width and longitudinal dispersivity. The prior for beta ($\beta \leq 1$) presumed DNAPL was pooled in the source, but calibrated values indicated $\beta > 1$, indicating residual DNAPL, which achieved better matches with observed TCE concentration data in groundwater downgradient of the source. The general size and shape of the plume predicted with the posteriors (Figure 5-28) is similar to the observed (DNAPL3D-RX) data, however the high concentrations in the core of the plume are not well matched.

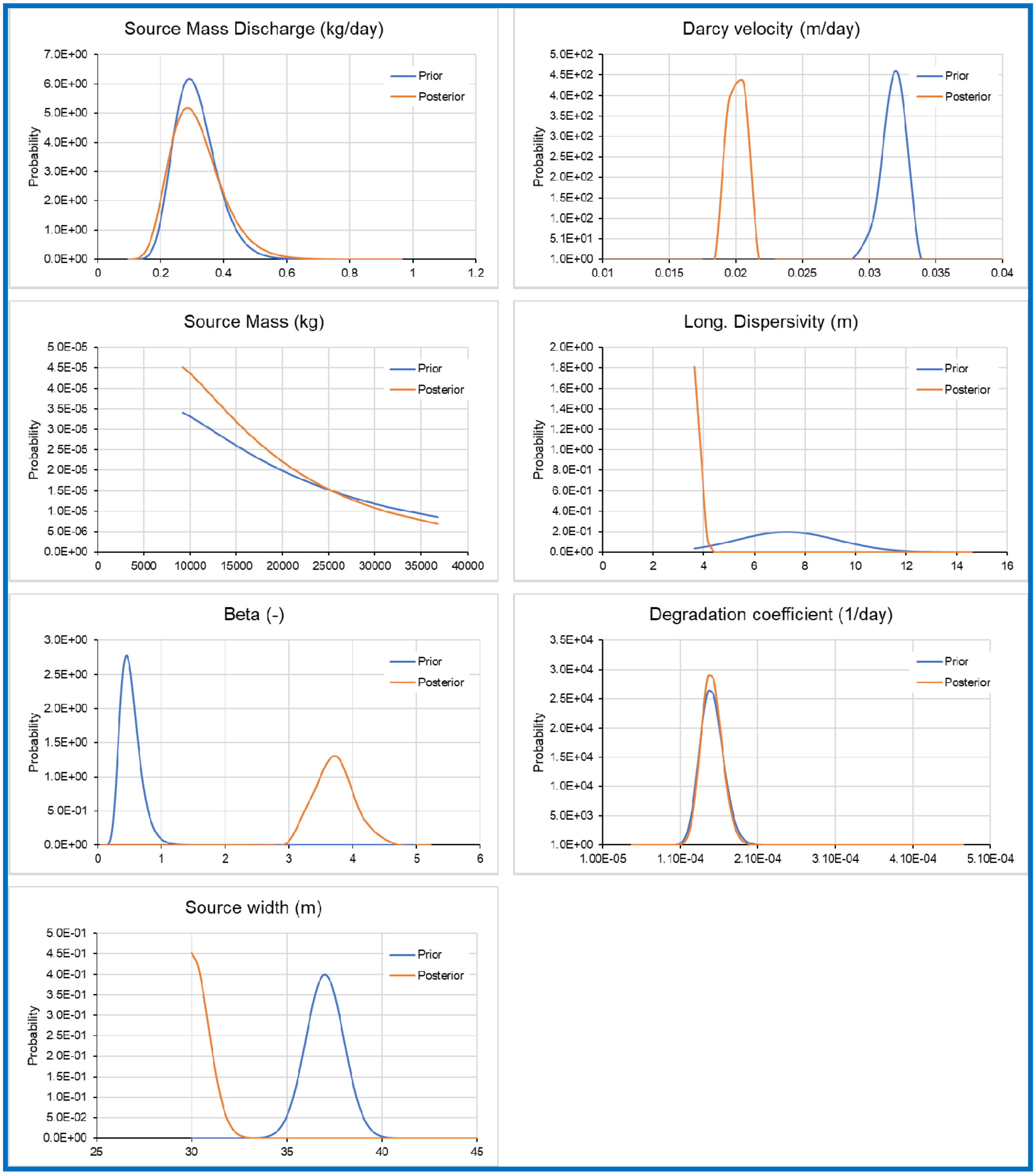


Figure 5-27: Comparison of prior and posterior distributions for key parameters, Team C

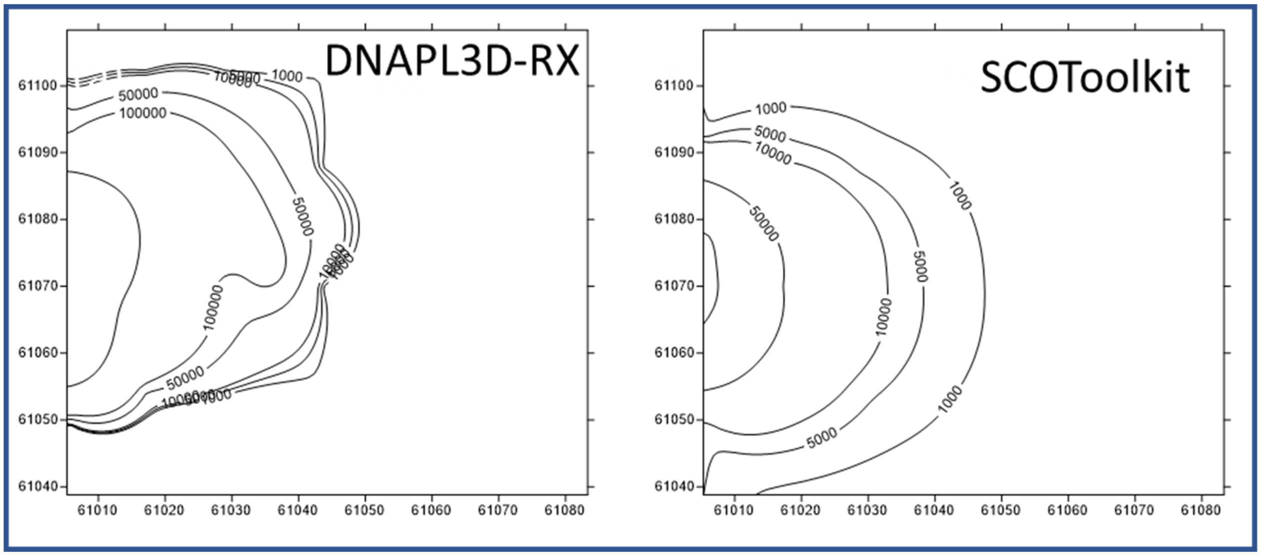


Figure 5-28: Observed vs. Modeled Concentrations for VSD 2 Using Team C Posteriors

EISB was identified as the optimal remedy during Phase 1 under both relative and absolute targets. The optimal remedy to achieve relative percent reductions in TCE plume concentrations, source mass and source mass discharge injected 90,600 kg lactate over 37 months. The optimal remedy to achieve absolute targets in TCE plume concentrations, source mass and source mass discharge injected 1,300 kg lactate over 60 months.

Remedy simulation using the calibrated model (Phase 2 modeling) was found to improve the optimum remedy as compared to remedy simulation with the uncalibrated model. To achieve compliance with the relative percent reduction remedial targets in 71% of calibrated models, the optimal remedy required a marginally lower injection rate (71.6 kg/day) over a shorter timeframe (2.56 years), equating to a 26% reduction in lactate usage. The optimal remedy designed to meet the absolute remedial targets achieved a similarly high level of compliance (72% of calibrated model realizations) for injection of 5,000 kg lactate over 56 months.

The value of considering uncertainty in site characterization and remedy design (through stochastic modeling) is clearly demonstrated by the SCOToolkit's predictions for Team C's CSM of VSD2. The process of calibrating variable parameters made the conceptualization of the source more accurate and permitted optimization of the remedy, achieving cost and time savings (for a successful outcome). Critically, the risk of failure was quantified such that, if greater certainty was required, the part of the CSM driving that risk was known and could be investigated to reduce uncertainty.

Table 5-33: Optimized remedies for VSD2 based on models of DM Team C's CSM report

Parameter	Deterministic, Uncalibrated F&T Model		Stochastic, Calibrated F&T Model	
Remediation Criteria[1]	**Relative**	**Absolute**	**Relative**[4]	**Absolute**
Target Concentration (µg/l)	16,804	231,000	-50%	231,000
Target Source Mass (kg)	13,796	11,192	-25%	11,192
Target Source Mass Discharge (kg/day)	0.152	0.375	-50%	0.375
Optimal remedy	EISB	EISB	EISB	EISB
Injection rate (kg/day)	75.2	0.72	71.6	2.95
Injection duration (years)	3.13	5	2.56	4.65
Compliance[2]	**Pass**	**Pass**	**71%**	**72%**
Concentration	Pass	Pass	71%	99%
Source Mass Discharge	Pass	Pass	100%	100%
Source Mass	Pass	Pass	100%	72%
Remedy Cost ($k)[3]	534	519	2,610	2,520

1 Relative remediation targets calculated for uncalibrated F&T model or for 100 realizations of calibrated F&T model based on Team C CSM report for VSD2. Absolute remediation targets from DNAPL3DRX model for VSD2.

2 Compliance with remediation targets for single realization of uncalibrated F&T model or percent of 100 realizations of calibrated F&T model compliant with remediation targets.

3 Remediation cost including penalty for single realization of uncalibrated F&T model or average of remediation costs for 100 realizations of calibrated F&T model.

4 Actual criteria calculated for each realization.

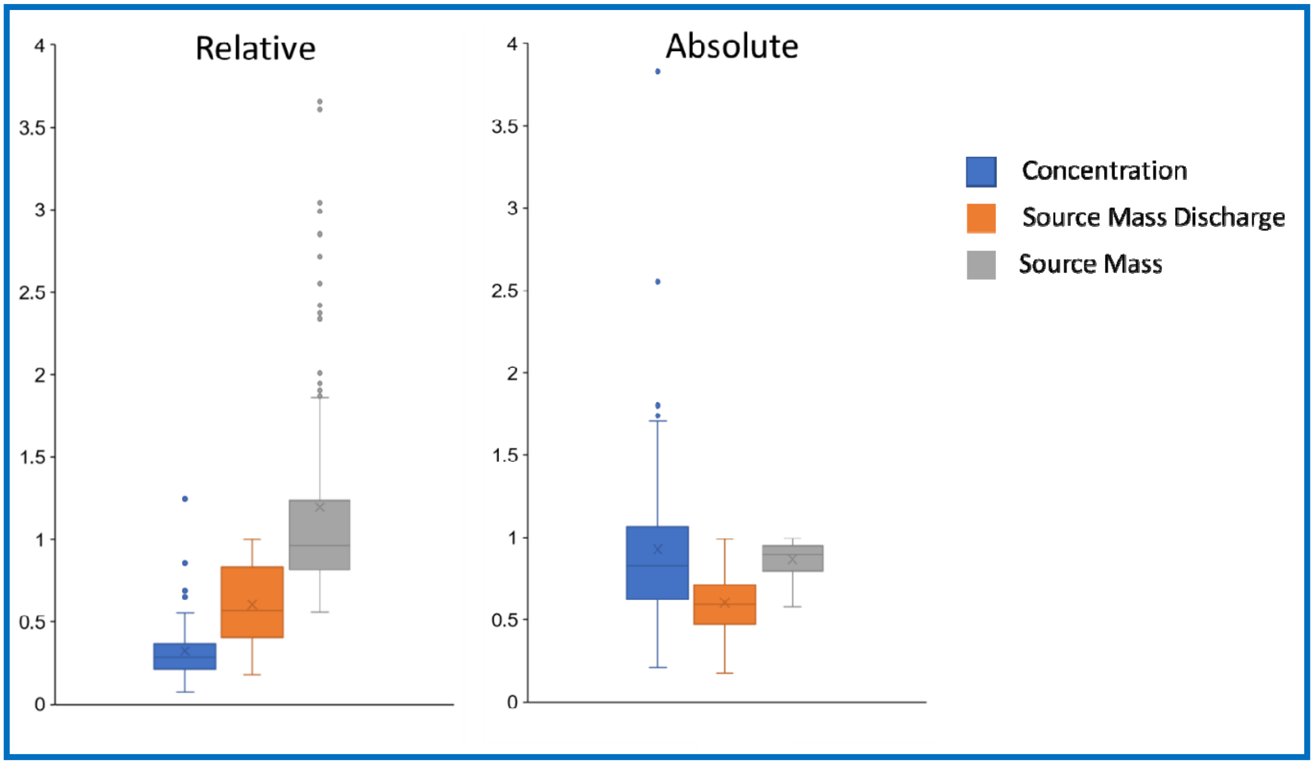


Figure 5-29: VSD2 remedy performance, Phase 2, Team C. Y-axis – simulated value to remediation criterion ratio: > 1 denotes Fail; ≤ 1 denotes Pass. The box represents the 25th to 75th percentiles of the 100 realizations with the line representing the 50th percentile. The "x" represents the arithmetic mean. Whiskers extend to 1.5 times the interquartile range with dots representing simulations that fall outside the whiskers.

5.3.6 Overview of Findings Regarding Stochastic Remediation

Inspection of the approaches and results of the remediation designs of VSD 1 to 3 identified by ScoToolkit shows that:

- Stochastic approaches should not be expected to overcome inadequate or poor site characterization.
- The use of stochastic approaches can quantify the risk of failure such that, if greater certainty was required, the part of the CSM driving that risk was known and could be investigated to reduce uncertainty.
- While analytical models can and should be used to support the development of site conceptual models (provide a holistic check), they may not be suited to remedy design even for low complexity/low heterogeneity sites, such as VSD1.

6 EXPANDING THE RESULTS OF DIVER TO A WIDER VOIA FRAMEWORK

6.1 Data Infilling & Sensitivity Analysis

When creating or refining a CSM, it is reasonable to expect that collecting additional data may lead to a reduction in uncertainty of the overall CSM, or perhaps a certain component of the CSM if the data acquisition is done properly (e.g., correct data, correct location, correct methods, correct interpretation). Many geologic features and geologic-controlled processes (e.g., NAPL migration) are spatially variable and must be evaluated through some averaging process. For example, hydraulic conductivity can vary orders of magnitude within a few centimeters in some unconsolidated alluvial systems. When a component of a CSM (e.g., plume migration rate) requires an estimate of hydraulic conductivity, multiple measurements (local) of hydraulic conductivity are made and averaged (global) to arrive at a value used in the calculation of the estimate. The process may be further refined when there are significant geology changes (units) within the region of interest by calculating different average values for each hydrostratigraphic unit.

In a more simplistic or isotropic system it is expected that each new local measurement results in a better estimate of the global value (reduces uncertainty) and therefore the process of determining the improvement in the global value of each new local measurement is conceptually straightforward. There are formal derivations of this concept collected under the generic heading of "Value of Information" (see Section 3). In the context of site investigation and remediation, however, the systems under consideration are almost always very heterogeneous in most variables of interest and it is extremely difficult to place a value on collecting a single piece of information. The difficulty of the process is often further compounded in site investigation and remediation by the need for interpretation of the new information, bringing the potential for error into the process (the information may have been collected correctly and be of value, however, it is interpreted incorrectly and therefore is of lesser or limited value).

To illustrate this with a common example, let's consider delineating a contaminant plume through the installation of monitoring wells and the acquisition and laboratory analysis of water samples. The process of installing a monitoring well is straightforward as is the process of taking a water sample and getting it analyzed in the laboratory. There are guidance documents for each of these individual steps that can be considered as "effective practice". Effective Practices are methods or techniques that have proven themselves in one or more scenarios to be effective at accomplishing a desired outcome (Jason Santo, Brightspace Community, June 11, 2015) and have been vetted by numerous parties and may also be incorporated into formal guidance documents, such as American Society for Testing of Materials (ASTM) standards. The completion of the monitoring well sampling process under consideration results in a number representing the level of contaminant in water at that point in space and time. If you have followed effective practice for each of the steps you can be reasonably sure that your information (contaminant concentration) is an accurate number, however the challenge can then come in the interpretation of the significance of that accurate number.

In addition to the effective practices followed in acquiring the concentration value (proper well installation, proper sampling procedure, proper analytical procedures) some consideration needs to be given to how the acquired data is interpreted and if it is in fact of value. In addition to the previously identified practices involved in acquiring the data there are additional considerations in the use of the data. Some key questions:

- Was the monitoring well located in the appropriate place?
  - Too far outside the edge of the plume would artificially increase the estimated size of the plume.
  - Did you miss a "hot spot" or is the data point an "outlier"?
- Is the screen of the monitoring well in the appropriate place?
  - In a thin plume the screen may be completely above or below the plume resulting in an estimate of a smaller plume than is present.
- Is the screen of the monitoring well of the appropriate length?
  - A very long screen length can result in lower concentrations due to mixing and "shorten" a plume artificially.

Effective practice approaches to the above bullet points have been developed over time resulting in a method of maximizing the value of each new data point collected for this purpose.

Experience is the intangible that needs to be considered in addition to effective practice. Experience should be able to provide additional value to the process, increasing the value of the data in a way that cannot be captured in an effective practice guidance by reducing the uncertainty in aspects of a decision that require judgement. In the above example, a highly experienced practitioner, with experience in site investigation at hundreds of sites, could be reasonably expected to make decisions that increase the value of the acquired data (e.g., by locating the monitoring well in the most appropriate position).

The DIVER project asked the DM Teams to develop CSMs based on collecting data and interpreting that data to determine specific qualitative and quantitative parameters. Several of those parameters, although commonly evaluated in the industry, have little in the way of published effective practice guidance available. The DIVER team identified three of the required CSM parameters that are not well documented in existing guidance and that were amongst the least accurate across the DM Teams:

- Source zone footprint
- DNAPL mass
- Mass discharge/flux

The highly detailed VSDs produced by the DIVER project provide a unique opportunity to closely investigate these parameters and develop effective practice guidelines for their determination. Developing estimates of the value of information in site investigations in practice is limited by never knowing the "true" answer as well as by the costs of acquiring data. It is unfeasible at most sites to collect hundreds of data points to reduce the uncertainty of an estimate particularly if there is no underlying understanding of the magnitude of that reduction for the cost of the data collected or an understanding of the actual value of the parameter under consideration.

The DIVER VSDs allow for stochastic assessment of each of the above parameters without the high costs of actual field investigation. Each of the above parameters was investigated on VSDs 1 – 3 with the goal of developing an effective practice for quantification as well as indications of the degree of uncertainty in the parameter estimate given a particular level of effort (e.g., how "close" can you expect to be to the actual DNAPL mass present after taking 100 "measurements"). Each of the parameters above are examined in the following sections through presentation of a proposed effective practice approach as well as indications of the uncertainty inherent in each of the approaches. The impacts of the use of the proposed approaches on the parameter estimates of the DM Teams is presented in Section 7.4.

6.1.1 Source Zone Footprint

An estimate of the footprint of a DNAPL source zone is a key component to determining the distribution of contaminants at a site, designing a remediation plan, and performance monitoring following implementation of the remediation. Existing guidance on this subject (ITRC, 2011; ITRC, 2012) is available, however, it does not address the value of information nor quantification of the degree of uncertainty provided by different approaches. The DIVER team (in consultation with numerous other highly experienced practitioners over the course of the project) has developed the following recommendation for effective practice in the determination of the footprint of a DNAPL source zone. It is important to note that this approach has been developed based on the "Outside-in" principle to minimize the risks of creating vertical migration pathways through extensive drilling in a DNAPL source zone.

6.1.2 Step 1: Identify a "Bounding Box"

Determining a box (or other shape) that is thought to completely encompass the source zone can be done based on existing information at most sites.

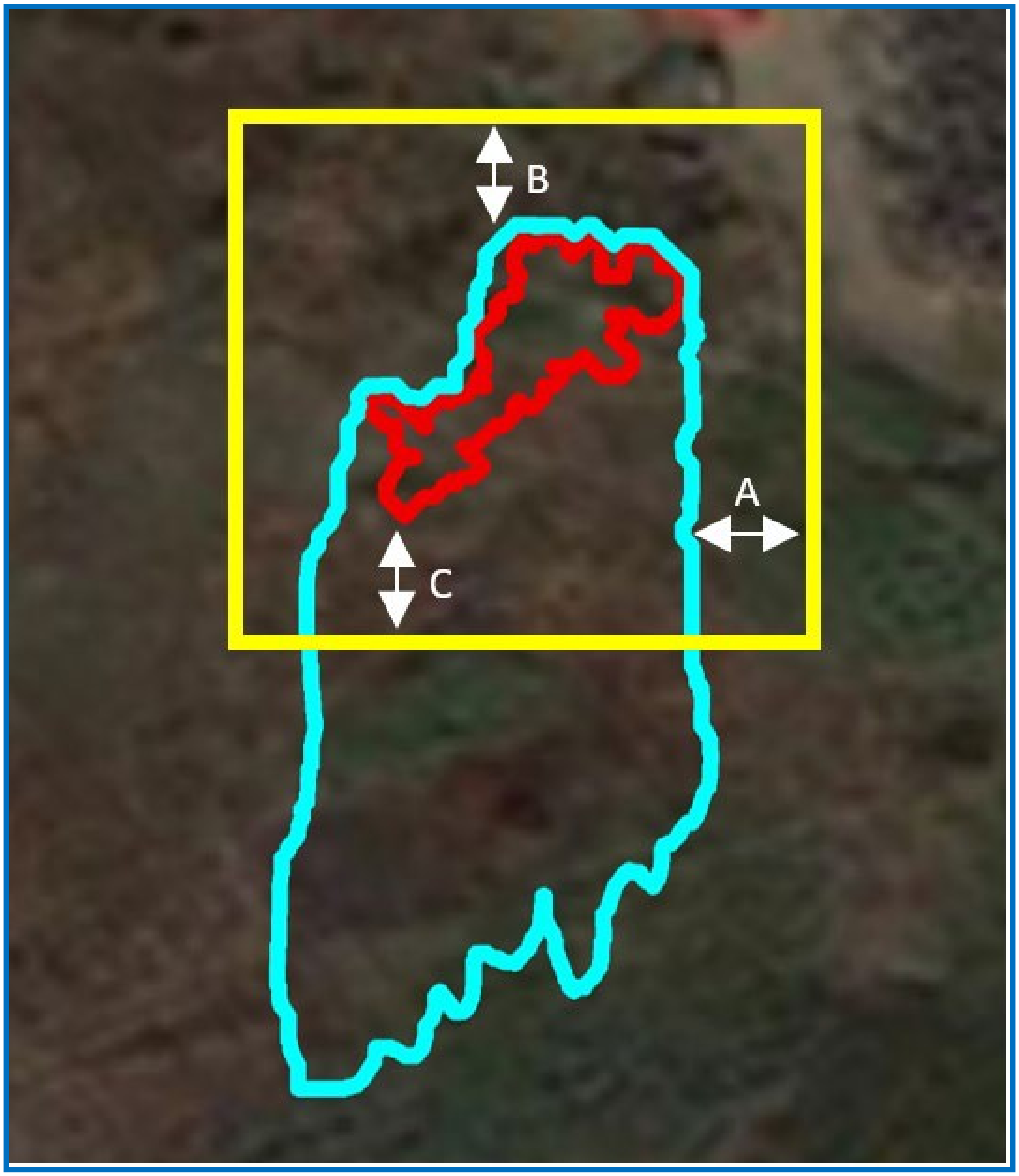


Figure 6-1: Initial determination of a bounding box

The lateral edges of the bounding box (perpendicular to groundwater flow direction) are set such that they are equal to or wider than the lateral edges of the dissolved phase plume in the vicinity of the DNAPL source zone ("A" in Figure 6-1). Plume width near the source is a good approximate indicator of the width of a DNAPL source zone. Choosing lateral edges wider than the measured plume will result in slightly greater investigation costs; however this provides a factor of safety that bounding box will encompass the source zone laterally.

The hydraulically upgradient edge of the bounding box can be located based on the furthest upgradient measurement of contamination in groundwater, soil, or vapor. Increasing the width of the bounding box beyond the mapped width of the dissolved phase plume and extending the hydraulically upgradient edge of the bounding box beyond the furthest upgradient measurement of contamination will result in a greater certainty of not placing the initial borings in the DNAPL source zone, but at increased cost ("B" in Figure 6-1). It is recommended that an appropriate drilling methodology and strategy be adopted to avoid mobilization of pooled DNAPL during drilling if the initial borings encounter DNAPL.

The hydraulically downgradient edge of the bounding box ("C" in Figure 6-1) can be located based on several lines of evidence (geology, concentrations in soil and groundwater, etc.). The location of the hydraulically downgradient edge of the bounding box is typically the most difficult to establish. Special attention should be given to the depositional environment and the associated geologic bedding structure.

The estimate of the vertical extent of the DNAPL source zone ("D") is typically based on the greatest depth of the dissolved phase plume and needs to consider vertical components of the hydraulic gradient in its determination (a downward groundwater flow component will result in a larger estimate of the vertical extent of the DNAPL source zone as the plume is driven downwards).

6.1.3 Step 2: Determine Edge of the DNAPL Source Zone

The proposed effective practice approach for identifying the edge of the DNAPL source zone relies on intrusive investigations to identify the existence of DNAPL in the subsurface. There are many techniques that can be used, and the particular technique is left up to the practitioner, however whatever technique is chosen must: (1) have the ability to positively identify DNAPL (visual observation, dye testing, soil sampling, DYE-LIF) rather than only high aqueous concentrations, (2) not rely on highly variable and site-specific correlations or relationships, (3) distinguish between residual and pooled DNAPL, and (4) not carry a risk of vertically mobilizing pooled DNAPL through capillary barriers. Numerous attempts were made by the DM Teams to correlate MIP response to the presence of DNAPL (see Section 5), however this failed in each instance and is not industry recommended practice.

Starting from all four edges of the bounding box, borings are drilled along parallel lines of investigation at a given spacing to the expected maximum depth of the source zone. If DNAPL is not encountered, then the next boring along the line (at a given spacing) is drilled (Figure 6-2). If DNAPL is encountered, then the edge of the source zone along that line is tagged as midway between the last two holes (Figure 6-3). Increased conservatism can be incorporated into the approach by stepping back a full spacing as compared to a half spacing (identify edge as at hole 2 in Figure 6-3 as opposed to the green circle).

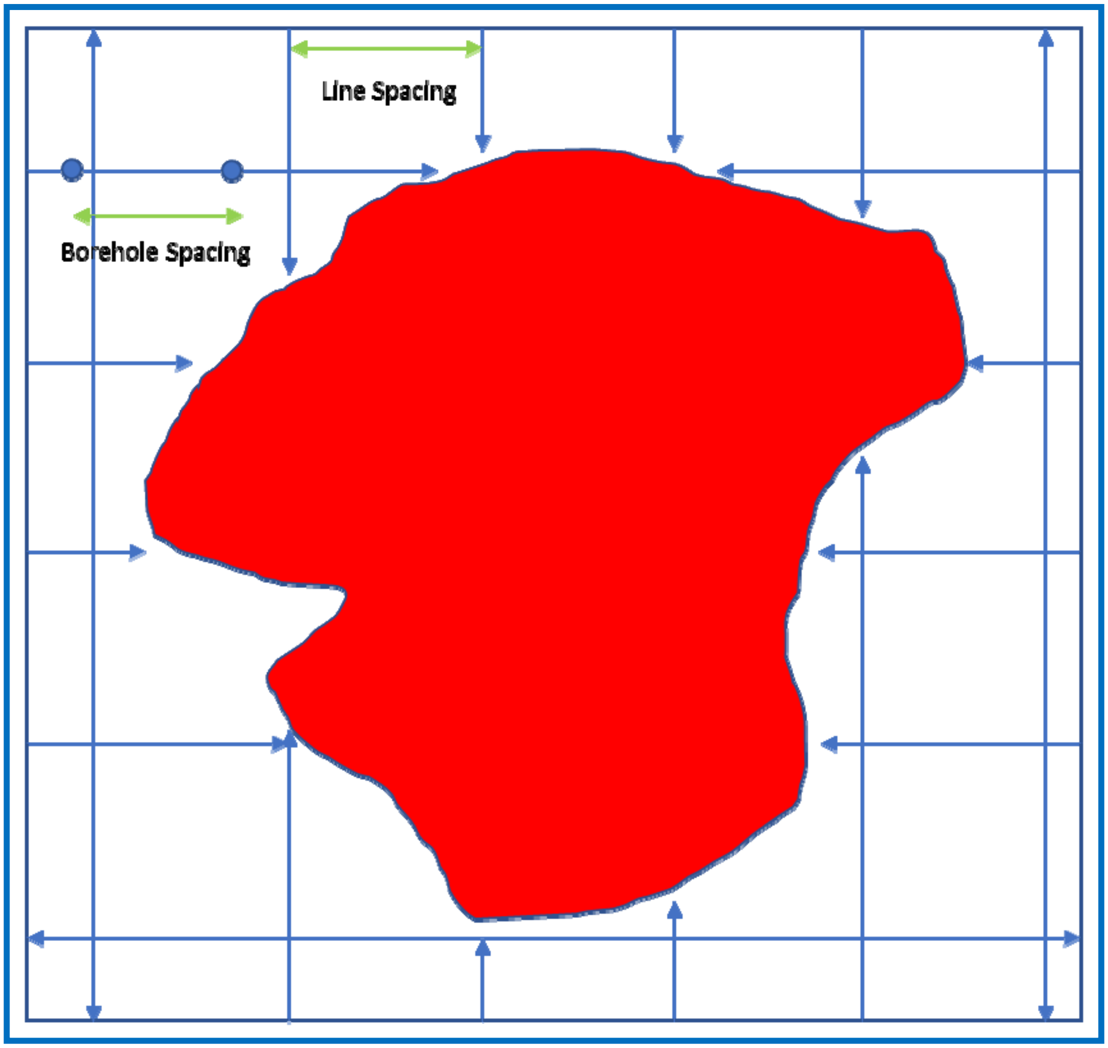


Figure 6-2: Approach to identification of the edges of the source zone

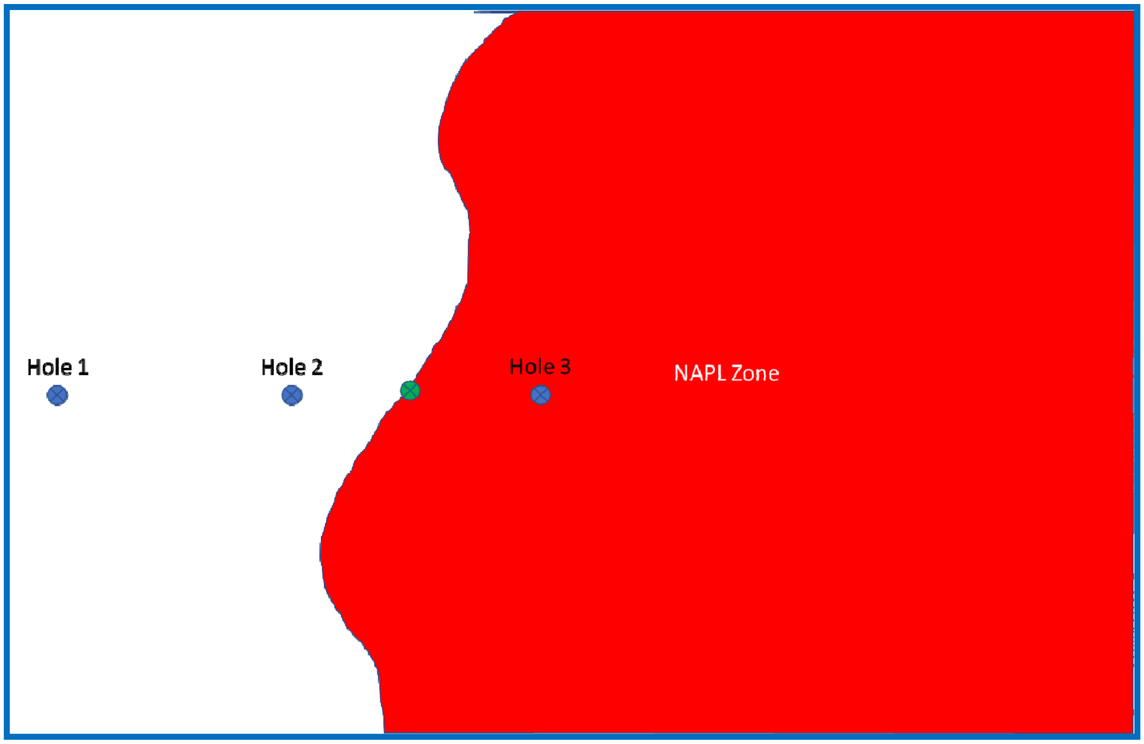


Figure 6-3: Locating the edge of the source zone along a given line. Green marker indicates the estimated location of the edge (midway between Hole 2 [no DNAPL] and Hole 3 [DNAPL]).

6.1.4 Step 3: Calculate the Footprint

The outcome of steps 1 and 2 is a set of points indicating the estimated edge of the DNAPL source zone (confirmed by visual or soil analyses) along each line of investigation. The source zone footprint is then identified by "connecting the dots" in some manner. This can be accomplished in different ways, such as manual interpretation or mathematical approaches to arrive at a bounding polygon. Figure 6-4 presents results from VSD 1 based on two different spacings.

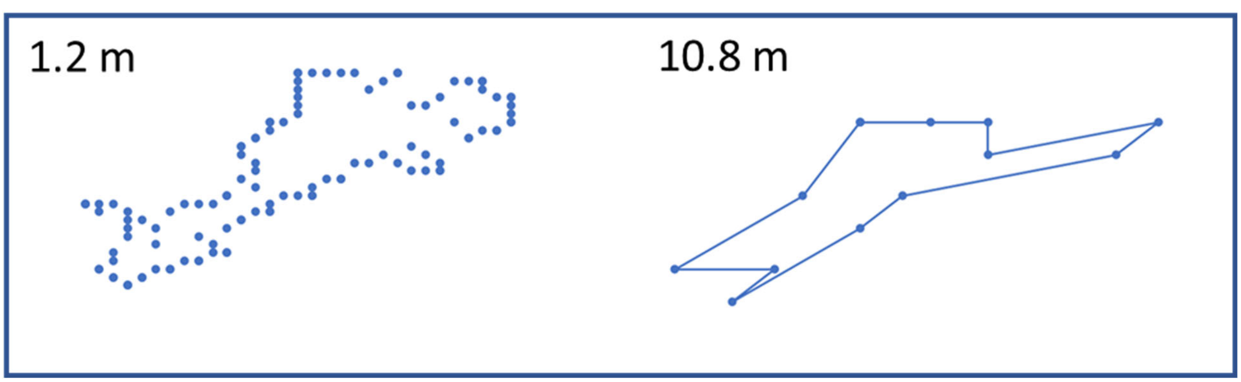


Figure 6-4: Results of source zone footprint effective practice (VSD1) at two different investigation spacings

6.1.5 Step 4: Using the Proposed Effective Practice

To make the proposed effective practice approach attractive there needs to be a way that its use can demonstrably result in precise estimates at reasonable costs or allow for the prediction of decreases in uncertainty as a function of the increased cost of investigation.

The proposed effective practice approach was applied to VSDs 1 – 4 by implementing it at spacings between 1.2 m (model nodal spacing) and 24 m (chosen based on minimum size of DNAPL source) and comparing the predicted (estimated) DNAPL footprint using effective practice to the actual DNAPL footprint for each combination of spacings of boreholes and lines. The bounding box was defined with A=25% of source width, B=10 m, and C=20m. The estimated footprint was calculated by using the bounding polygon approach within the ARCGIS framework. The overall results (across all VSDs) are presented in Figure 6-5 which contains approximately 1,300 individual points. In general, as spacing between boring locations decreases the number of boreholes increases. It is clear that VSD2 is an outlier in this analysis. This is primarily due to the existence of two source zones in VSD2 and the inability of the algorithm to differentiate them.

Figure 6-6 presents an evaluation based on the line and hole spacings and the relative score for the footprint parameter. Each blue dot represents a line and borehole spacing combination that resulted in at least one (out of the 4 VSDs) relative scoring outside the range of 0.8 to 1.2. Again, no definitive pattern is visible, however it was noted that for line spacing less than 15 m and hole spacing less than 10 m, the majority of the relative parameter scores fell between 0.8 and 1.2. Figure 6-7 contains a subset of the total data containing only those pairs of data where the line spacing was less than or equal to 15.6 m and the hole spacing was less than or equal to 12 m. VSD 2 data has also been removed from Figure 6-7.

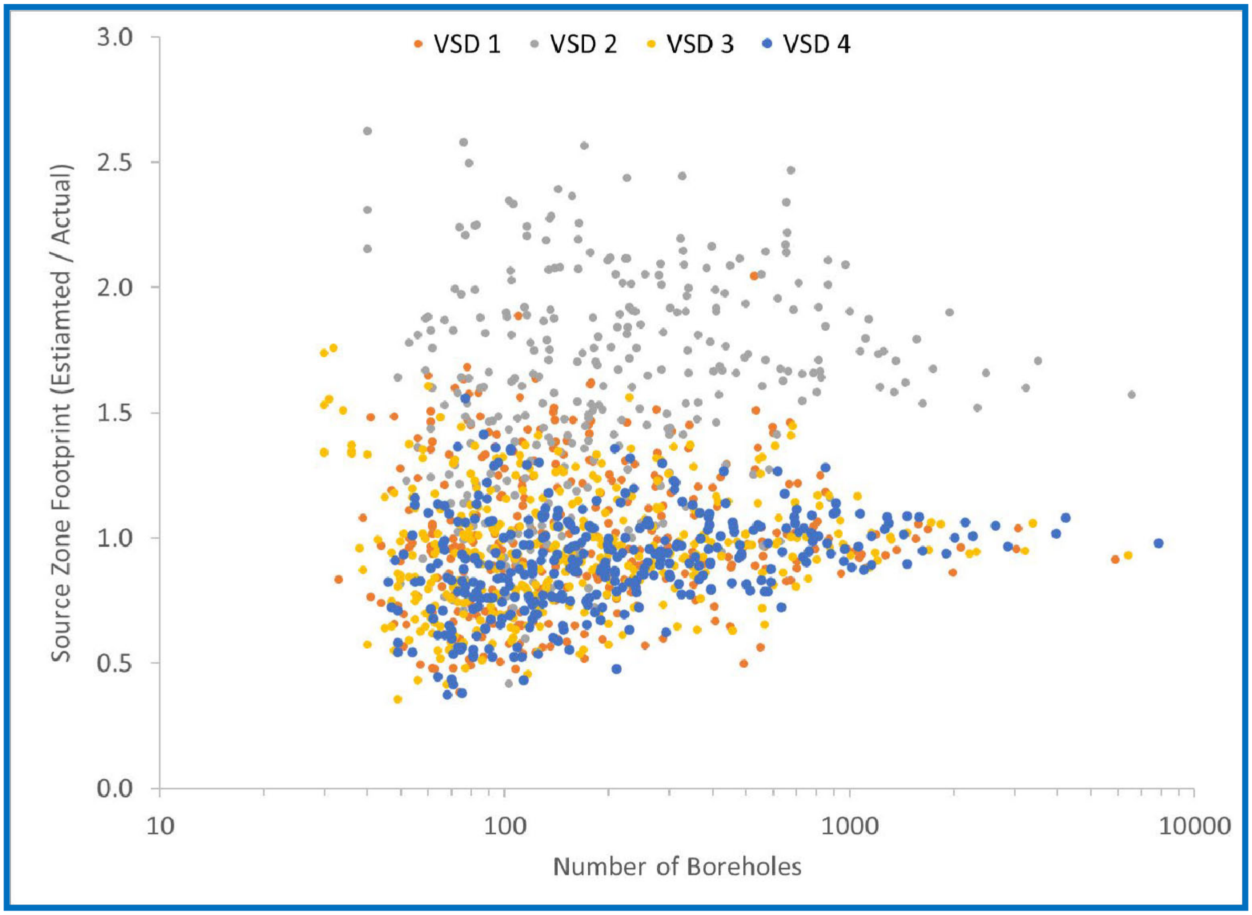


Figure 6-5: Relationship between source zone footprint estimates and number of investigation locations (all data)

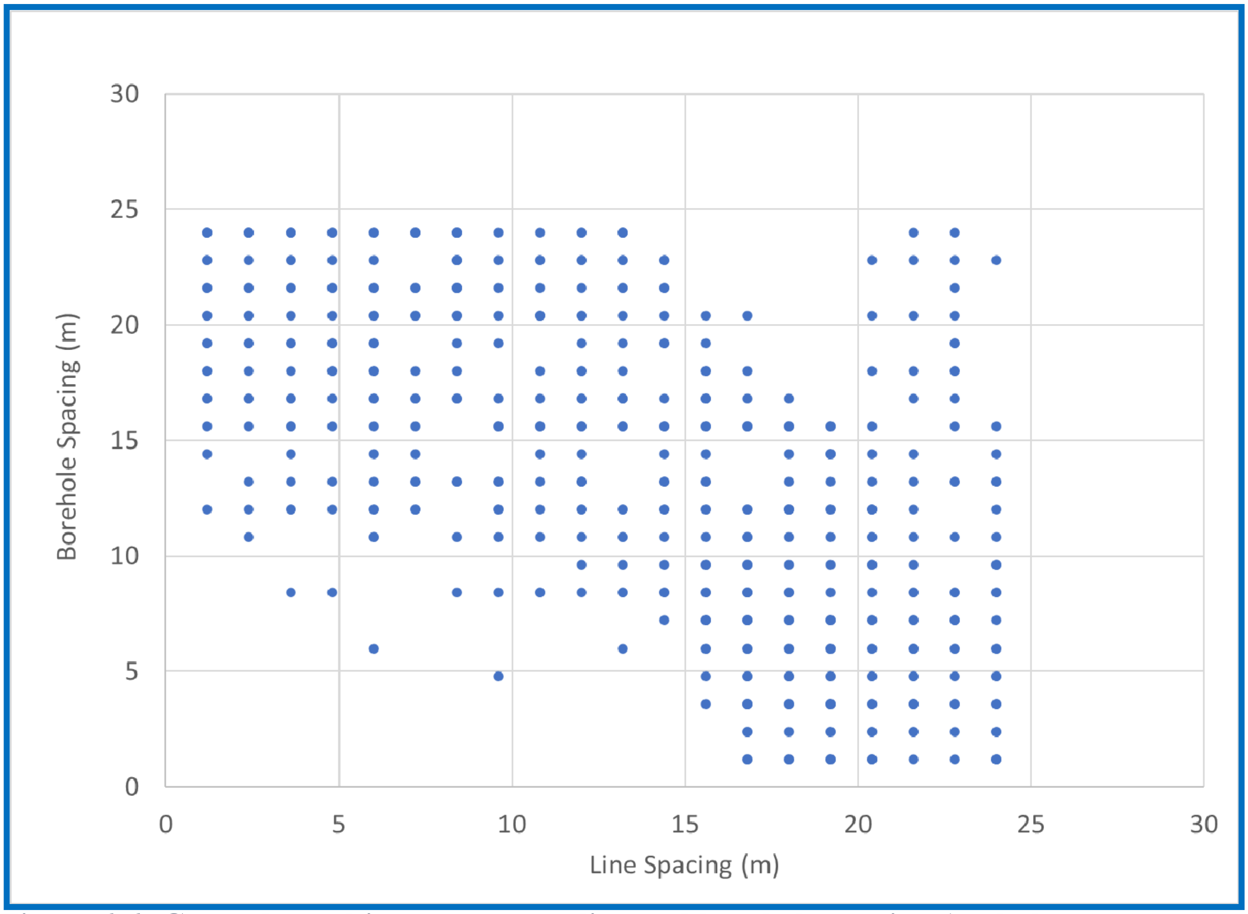


Figure 6-6: General trend in error versus line and borehole spacing (each dot represents a combination where the relative error fell outside the range of 0.8 to 1.2 for at least one VSD).

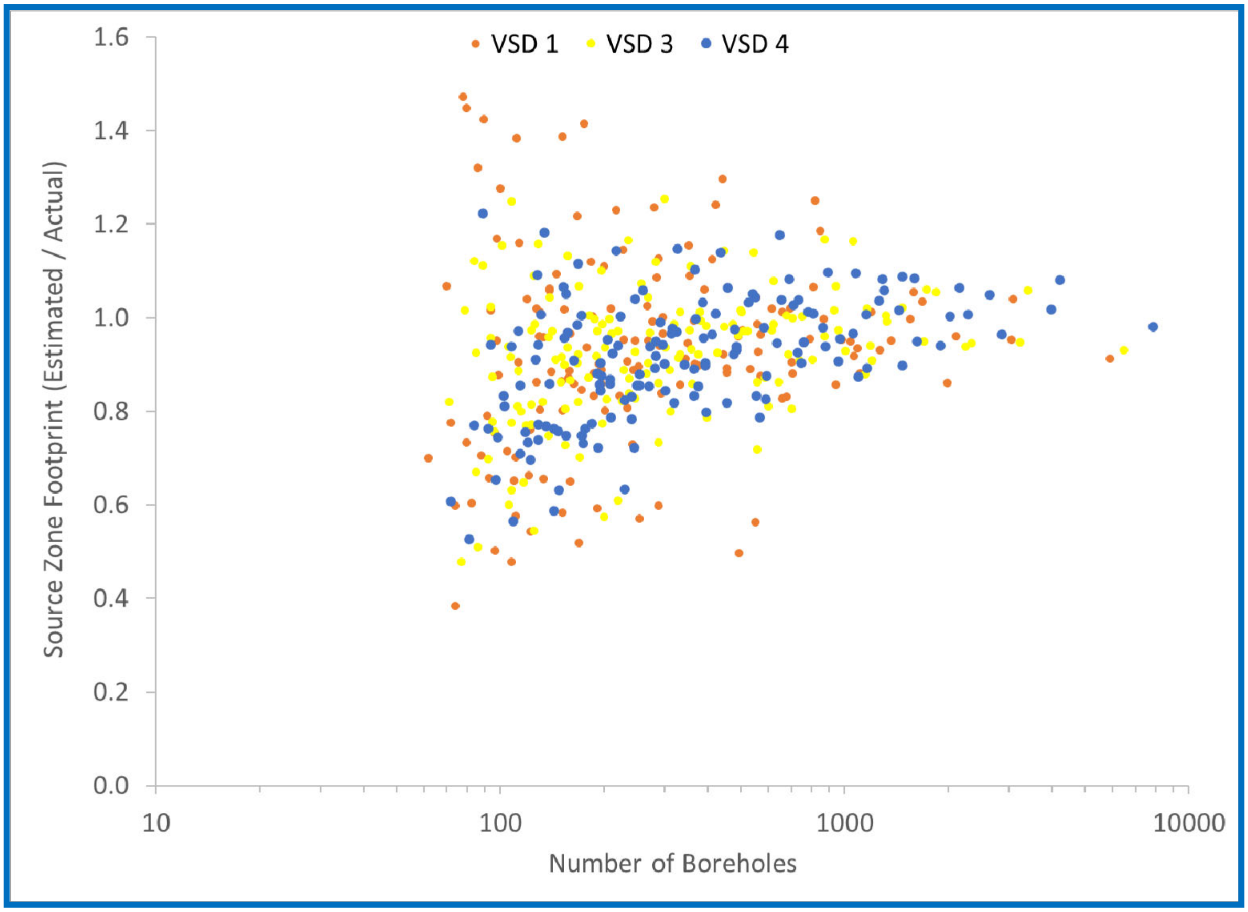


Figure 6-7: Relationship between source zone footprint estimates and number of investigation locations (subset of data)

The intuitive expected pattern of increasing accuracy with increasing boreholes (closer spacings) is now more apparent, and the overall trend is converging to a more accurate answer with large numbers of boreholes. The data can be examined in another way, based on the ratio of the line spacing to the hole spacing. This approach (Figure 6-8) demonstrates that, regardless of the choice of line and hole spacings (provided they are less than 15.6 m and 12 m respectively), it is reasonable to expect less than 20% error (range between 0.8 and 1.2) in the estimate (approximately 85% of the data points lie in this range) using the effective practice approach.

The effective practice approach was tested on VSDs 1, 3, and 4 using a line spacing of 15.6 m and a hole spacing of 12 m (a combination resulting in the fewest number of boreholes and thus the lowest cost). The bounding box was defined as the width of the plume (A), 10 m upgradient of the most upgradient NAPL location (B) and 20 m downgradient of the most downgradient NAPL location (C). The estimates for the three VSDs are shown as the large circles on Figure 6-9 and required 72, 74, and 98 boreholes for VSDs 1, 3, and 4 respectively. For VSDs 1 and 4 the error in the estimate was slightly greater than 20% at the extremes of the recommended spacings. For VSD 3 the error in the estimate was less than 2%.

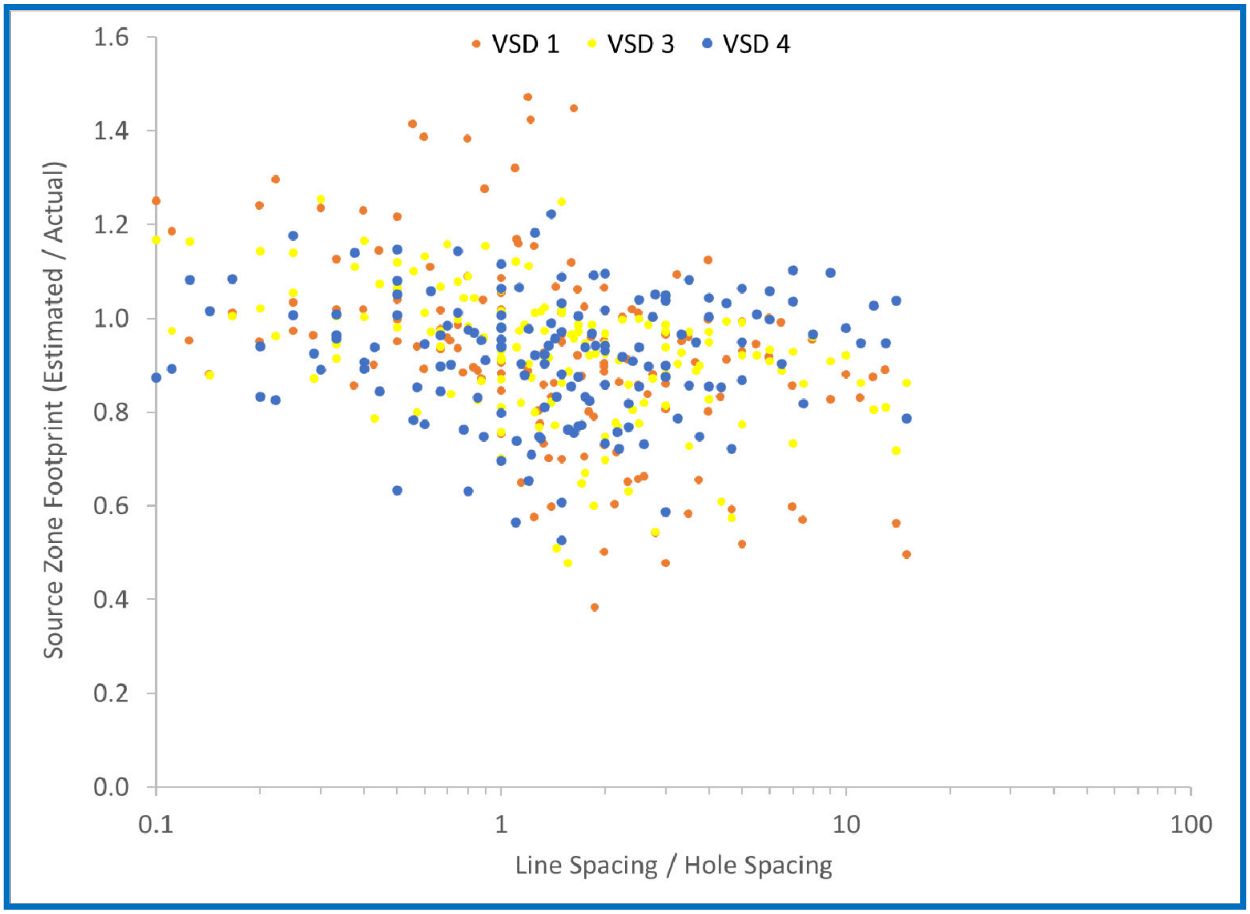


Figure 6-8: Accuracy of source zone footprint effective practice approach based on ratio of line to hole spacings

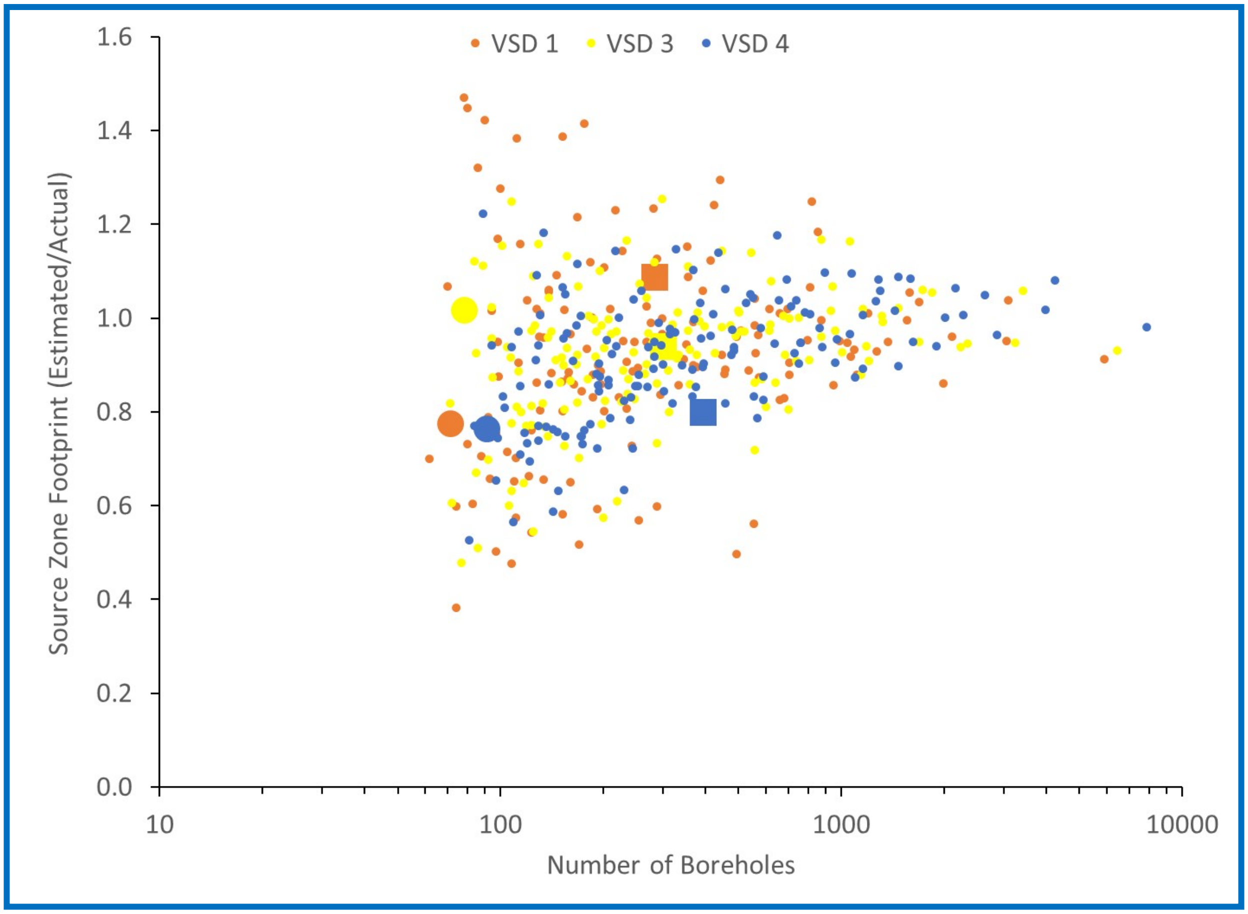


Figure 6-9: Utilization of source zone footprint effective practice on VSDs 1, 3, and 4. Large circles and squares represent the points indicating use of effective practice at the coarsest and finest scales in Table 6.1 (respectively) per VSD.

The final component to examine in the context of effective practice is the overall cost of its implementation. An effective practice whose cost exceeds its value (negative ENV) is not useful as an approach for reducing overall site investigation costs and reducing the cost (and risk of failure) of remedy designs. For example, if the cost of increasing the accuracy of the estimate of the source zone footprint is greater than the cost of additional overdesign in a remedy then the utility of the approach is minimal and the practitioner would better serve their client by including the uncertainty in the design of the remedy (e.g., larger factor of safety). This is examined in more detail in Section 8, however the total costs for three different combinations of hole and line spacings (assuming a drilling cost of $54/m) is provided for information in Table 6-1. Total costs for the coarsest spacing (all of which achieved an expected uncertainty of less than 25%, large dots in Figure 6-9) range from $41,601 for VSD 1 (shallowest source) to $137,592 for VSD 4 (deepest source). Discussion of this in terms of the EVI and ENV is provided in Section 8.

Table 6-1: Total drilling cost of three different line and hole Spacings in VSDs 1, 3, and 4

VSD	Depth (m)	15.6 m by 12 m	9.6 m by 9.6 m	6 m by 6 m
1	10.7	$41,601	$80,314	$154,673
3	18.3	$78,070	$149,218	$298,436
4	26	$137,592	$235,872	$555,984

6.1.6 DNAPL Mass

An estimate of the DNAPL mass contained in a source zone is important in understanding source zone longevity, long term risks presented by the source, and in the design of certain remedial approaches. The accuracy of the mass estimate is less important than the accuracy of the footprint estimate for a remediation approach such as thermal, however for reaction-based approaches such as chemical oxidation/reduction or bioremediation an estimate of the mass present is an important input parameter controlling design effectiveness and overall cost. Existing guidance on this subject (ITRC, 2011; Kueper and Davies, 2009) is available, however it does not address the value of information nor quantification of the degree of uncertainty determining the magnitude of design factors of safety.

The DIVER team (in consultation with numerous other highly experienced practitioners over the course of the project) has developed the following recommendation for effective practice in the determination of the DNAPL mass present in a source zone. It is important to note that this approach requires drilling within a source zone which entails risk of contaminant mobilization. Other approaches exist for estimating source zone mass without drilling within the source zone (e.g., partitioning interwell tracer testing), however they are more interpretive and require application of numerous correlations and extrapolations (ITRC, 2014). The proposed effective practice approach for estimating source zone DNAPL mass is based on the concept of bulk retention. Bulk retention is defined as the volume of DNAPL per volume of soil containing the DNAPL (Kueper et al., 2014). At the full source zone scale the bulk retention is therefore the total DNAPL volume divided by the total source zone volume.

The total DNAPL mass is calculated from the estimate of the total DNAPL volume. The proposed effective practice approach determines core-scale estimates of bulk retention (DNAPL volume in a core relative to total volume of the core) and scales these estimates to the source zone volume. To arrive at a core-scale estimate the top and bottom of the DNAPL-containing portion of the core are determined (Figure 6-10) and the volume of core between those elevations is used as the volume of soil in the core. The volume of DNAPL within the identified portion of the core is then calculated via soil samples, visual identification and estimates of saturation, or some other approach that is capable of positively identifying and quantifying DNAPL volume and mass:

$$V_{DNAPL} = A\sum_{i=1}^{n}(b\theta S_{nw})_i \quad [6\text{-}1]$$

Where A is the cross-sectional area of the core [L^2], b the thickness of a DNAPL impacted section of the core [L], θ the total porosity [-] and S_{nw} the DNAPL saturation in the impacted section [-]. The volume of DNAPL is then divided by the total volume of core to arrive at a local (core-scale) estimate of the bulk retention. Multiple core-scale estimates are required with their arithmetic average being used to estimate the source zone scale DNAPL bulk retention and thus the estimated DNAPL mass in the source zone.

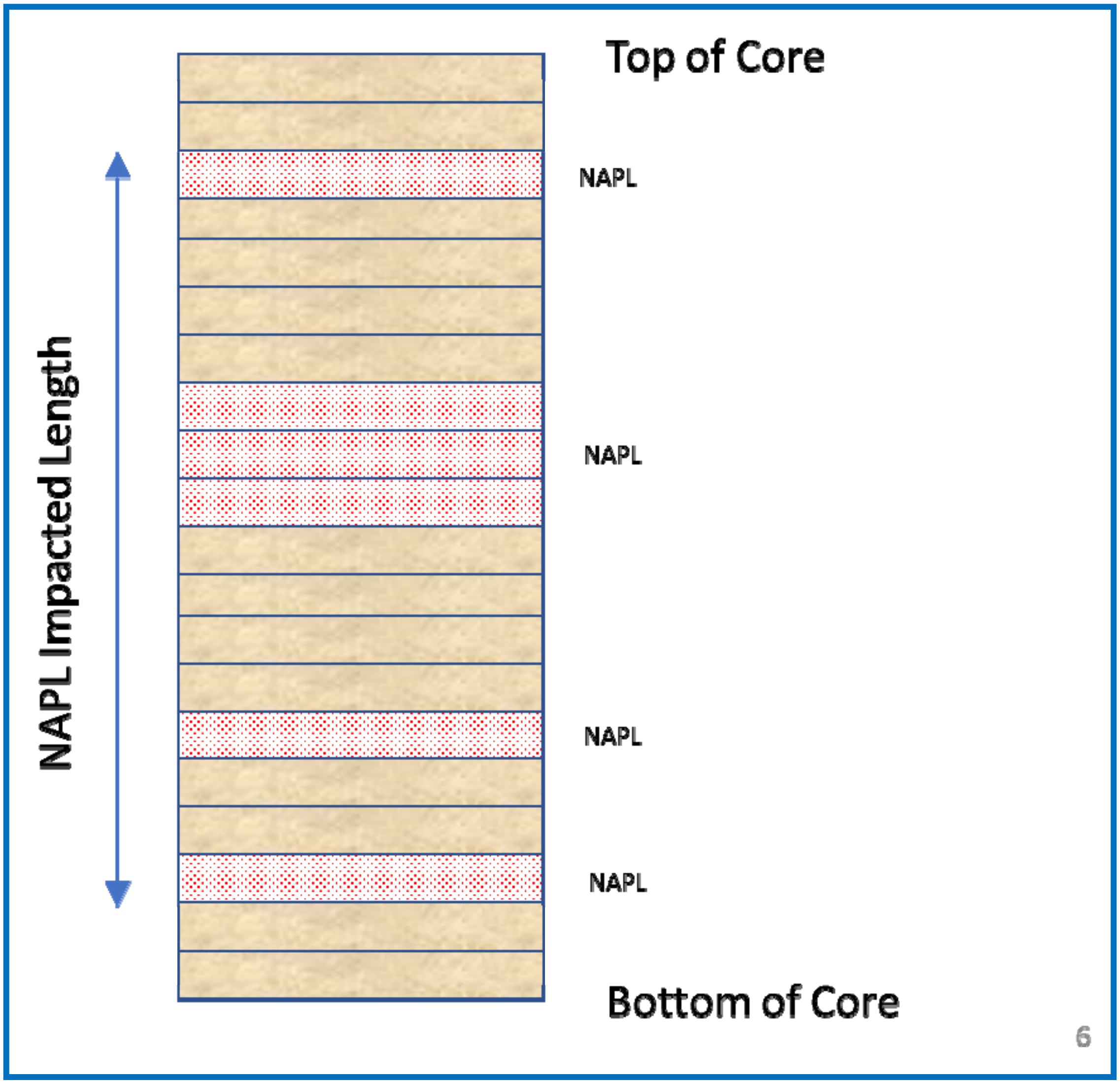


Figure 6-10: Discrete DNAPL zones within a single core

To expand from the core-scale estimates of bulk retention to an estimate of the DNAPL mass at the source zone scale, an estimate of the volume of the source zone is required. There are multiple approaches to arriving at an estimate of the source zone volume (e.g., use the source footprint from Section 6.1.1 and multiply by the estimated vertical thickness of the source, separate the source zone into layers and identify footprints based on the results of the coring performed in this effective practice).

When utilizing the proposed effective practice approach, it is intuitive that the more data (cores) available to estimate the core-scale bulk retention, the more likely the accuracy of the estimate of overall DNAPL mass will be high (calculating the core-scale bulk retention from 100 cores vs. 10 cores should result in a more accurate answer). Cost however is an important constraint on this process as at some point the degree of improvement in the estimate will likely no longer be worth the additional cost of acquiring the data. To examine this in detail and arrive at cost-accuracy relationships that can be used by a practitioner in making this decision, the effective practice approach outlined above was applied to VSDs 1 – 4 through stochastic methods.

In the stochastic approach all possible core locations within the known source zone footprint were identified (one core location per each "column" of model cells). Starting with a single estimate of core-scale bulk retention (calculated from a single core) all possible locations were used to derive source zone mass estimates. For example, if there were 100 possible locations for a single core then 100 estimates of the source zone mass were calculated, each based on a single estimate of core-scale bulk retention at a different location. This process was then repeated with 2 cores, 3 cores, etc. For each "level" (2 cores, 3 cores, etc.) a maximum of 4000 realizations was used to estimate DNAPL mass. Based on the previous example of 100 possible locations this results in 100 mass estimates using 1 core, 4,000 mass estimates using 2 cores, 4,000 mass estimates using 3 cores, decreasing to 1 estimate for 100 cores (using all the data).

The results of the stochastic modelling using VSDs 1-4 are shown in Figure 6-11 based on a normalization of the source zone footprint (boreholes per acre of source zone). All points in the figure were calculated using perfect information; each data point was calculated by coring through the entire thickness of the source zone and knowing the exact distribution of DNAPL to calculate the core-scale bulk retention and the source zone volume was calculated using the exact footprint of the source zone and the exact known thickness.

The stochastic modelling approach allows for the calculation of confidence intervals on the estimated mass, which are highly useful for practitioners balancing the level of uncertainty suitable for the site investigation options with the cost of the proposed investigations. Figure 6-12 presents the 80, 90, 95, and 99% confidence intervals for the estimated DNAPL mass in VSD 1 calculated using perfect information and demonstrates the number of cores required for +/- 20% accuracy at the 80% interval (60 – top graph) and 95% interval (92 – bottom graph).

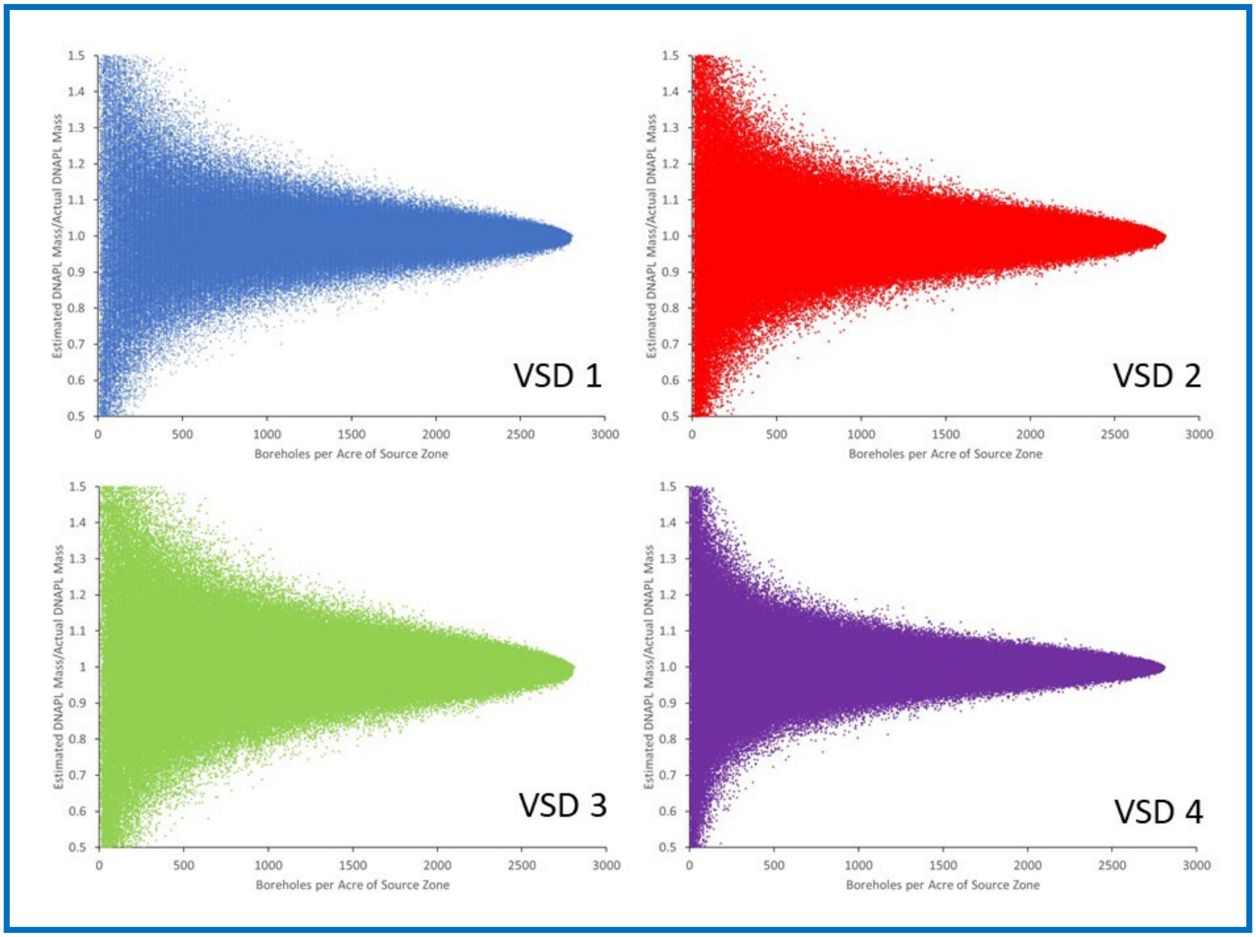


Figure 6-11: NAPL mass estimates based on applying effective practice to VSDs 1 through 4

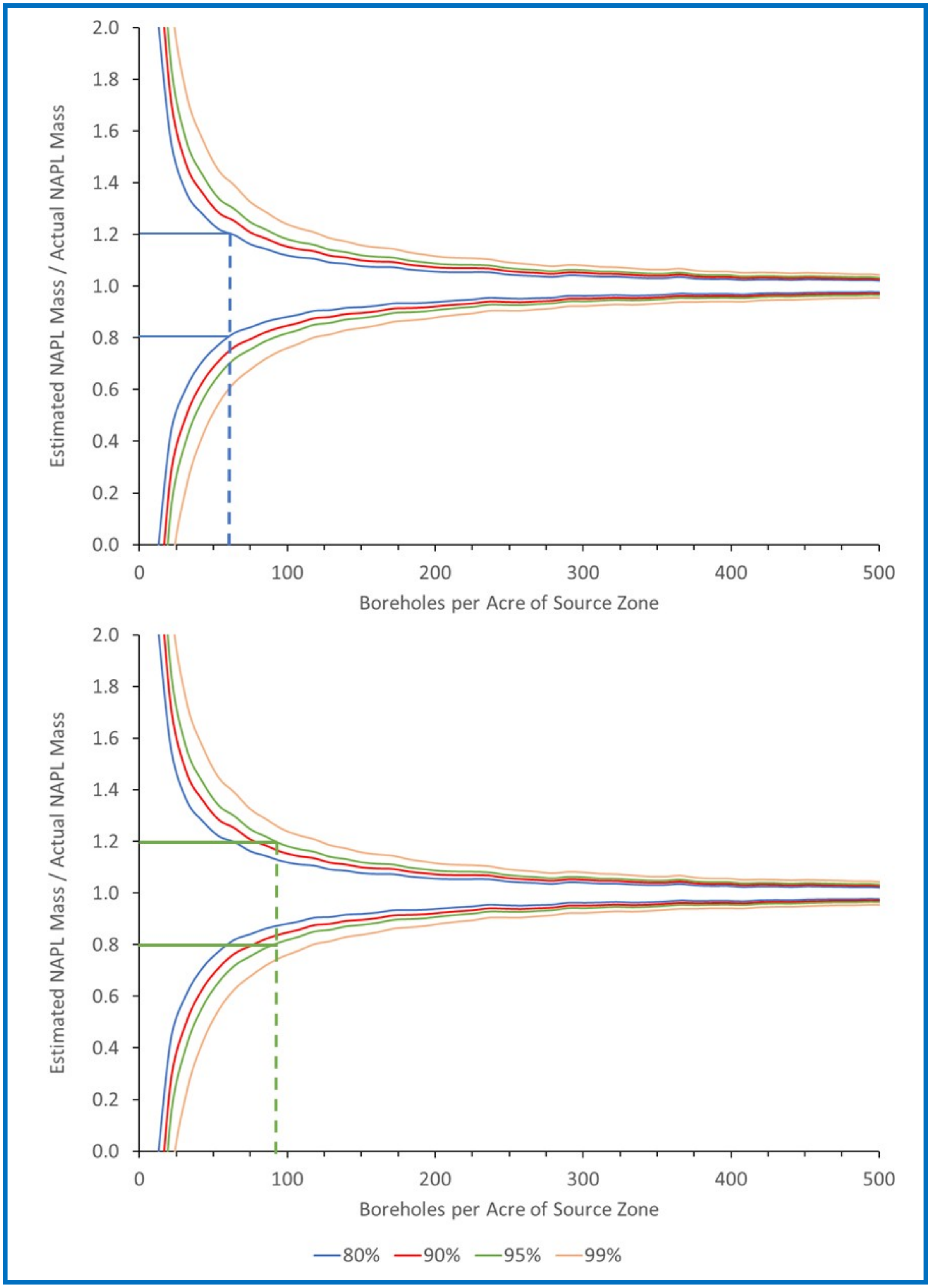


Figure 6-12: Confidence intervals for mass estimates based on perfect information in VSD 1

It is important to note that the results in Figure 6-11 and Figure 6-12 are based on stochastic modelling and do not incorporate the experience of practitioners. The 60 cores required to be 80% confident the estimate is +/- 20% in VSD 1 are based on the assumption of a random selection of core locations. It is reasonable to expect that a practitioner could achieve better results (less cores or greater confidence at a given error interval) by incorporating secondary lines of evidence (such as detailed geology information) and choosing the location of each new core location based on the information gathered from all previous core locations as well as the broader CSM.

The final step in the development of the Effective Practice approach for estimating DNAPL mass in a source zone was a verification step by expert practitioners. A nominated expert was provided with perfect information and asked to order all possible core locations from highest to lowest priority. A DNAPL mass estimate was then calculated in a stepwise manner (first estimate uses the first location, second estimate uses the first and second locations, etc.) using the bulk retention approach. The results of this for two different prioritizations (by the same expert) are shown in Figure 6-13. The inclusion of experience (and perfect information) in the ordering of application of the algorithm reduces the uncertainty for smaller numbers of boreholes, however it is not significantly better as the total number of boreholes increases.

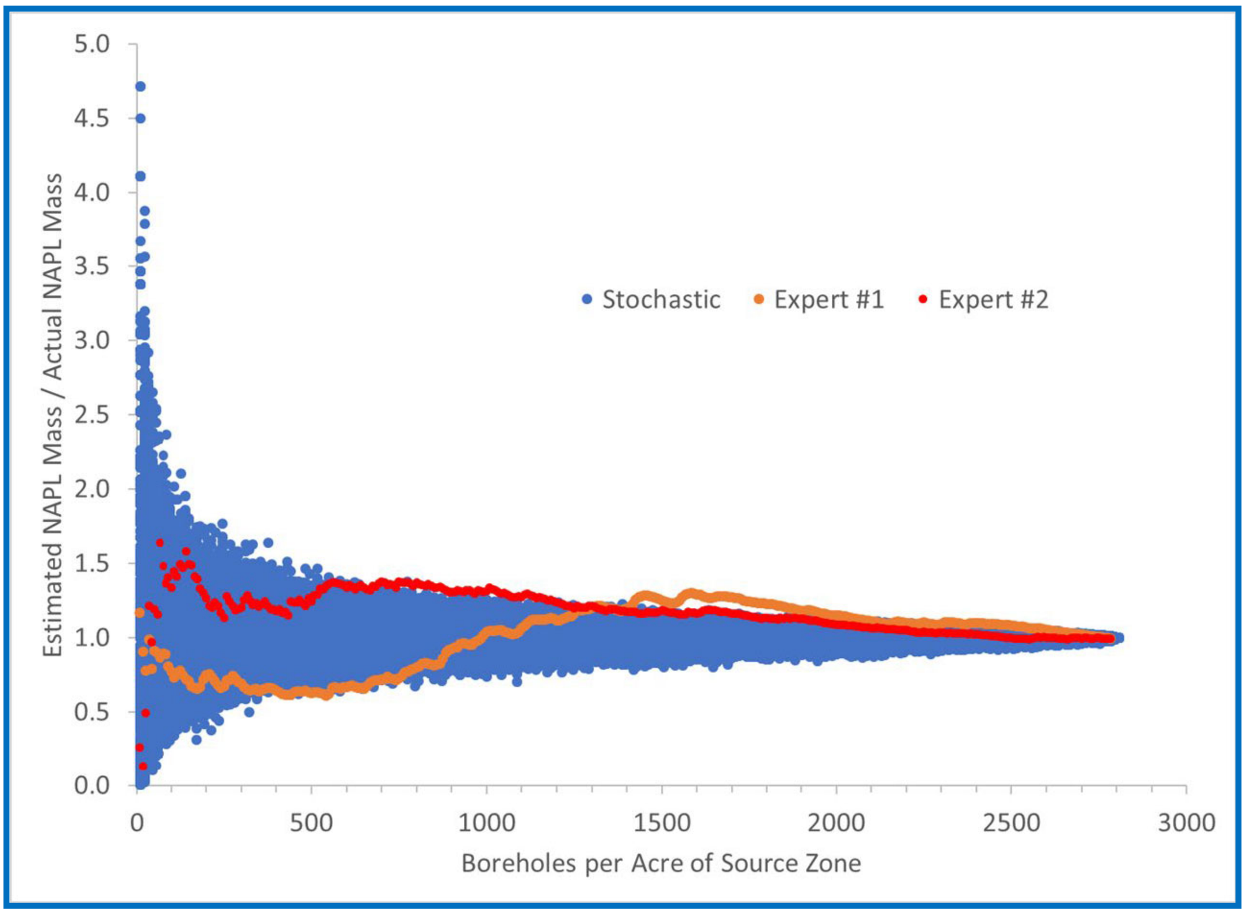


Figure 6-13: Verification of effective practice by comparison with expert analysis

6.1.7 Mass Flux and Discharge

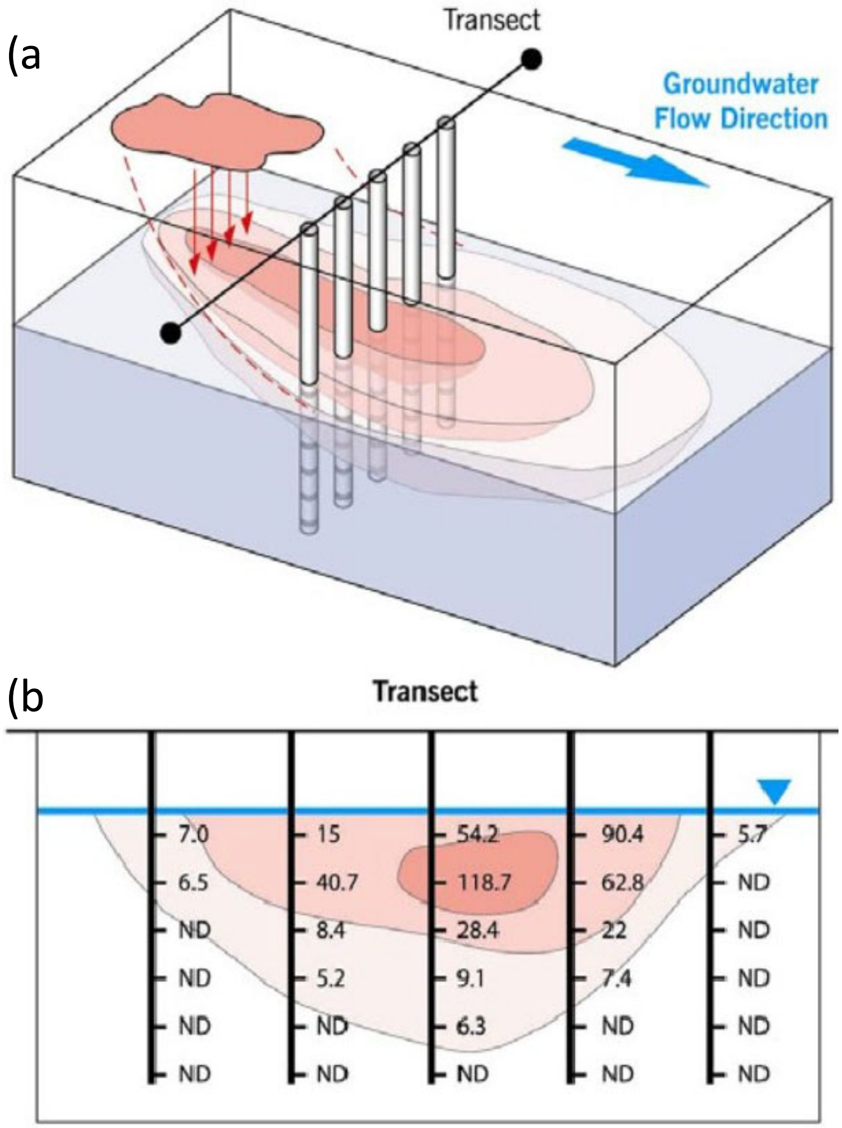
Estimates of mass discharge from source zones and within plumes are important when evaluating the need for or degree of remediation in the context of reducing impacts at downgradient receptors (ITRC, 2014). Measurements of mass flux and mass discharge (mass discharge is mass flux integrated over an area) can also be used to identify the location of upgradient sources using high resolution site characterization as well as evaluating the effectiveness of a source zone remediation effort. Mass flux (J) is calculated as product of the contaminant concentration (C_w) and the groundwater flux (q):

$$J = q * C_w \qquad [6\text{-}2]$$

Mass discharge (Md) is the integration of mass flux across a selected transect (A – often a control plane perpendicular to groundwater flow):

$$M_d = \int_A J\,dA \qquad [6\text{-}3]$$

The most common approach to the estimation of mass flux uses a transect approach, where a vertical plane is defined (most often perpendicular to groundwater flow) that is broken into polygons with estimates of concentration and groundwater flux developed for each polygon (Figure 6-14 from ITRC, 2010).



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7.0	15	54.2	90.4	5.7
6.5	40.7	118.7	62.8	0
0	8.4	28.4	22	0
0	5.2	9.1	7.4	0
0	0	6.3	0	0
0	0	0	0	0

Figure 6-14: Transect approach to estimating mass flux (ITRC, 2010). Panel (a) represents the location of multi-level monitoring wells defining the transect. Panel (b) presents the concentrations measured at each multi-level point in each monitoring well. Panel (c) indicates the polygons assigned to each monitoring point.

Significant theoretical and field-based research has been undertaken on approaches to the measurement of mass flux (e.g., Brooks et al. (2008), Kubert and Finkel (2006), CRCCARE (2016), ITRC (2010)), however little of the published research has examined the value of information concept applied to the use of mass flux in remedial decision analysis. ITRC (2010) identified three common approaches to calculating mass flux across a transect (Table 6-2). The DIVER project used the three developed VSDs to investigate the sensitivity of well spacing on predictions of mass flux using Approaches 1 and 3.

Table 6-2: Details on approaches used for mass flux calculations

Approach	Concentration	Hydraulic Conductivity	Hydraulic Gradient
1	One per polygon	One per polygon	One for entire transect
2	One per polygon	Several for transect	One for entire transect
3	One per polygon	One for entire transect	One for entire transect

The key difference between the approaches is the method of estimating the hydraulic conductivity which is used to calculate Darcy flux. Approach 1 uses hydraulic conductivity results from individual well tests (e.g., slug tests). Approach 2 uses different hydraulic conductivity estimates across the plane (without averaging). Approach 3 uses an averaged hydraulic conductivity across the plane (e.g., obtained through larger scale testing such as pump tests). In this work, given access to perfect data we have only used Approach 1 (hydraulic conductivity calculated as the average along the well screen parallel to flow and applied to the polygon represented by that screen) and Approach 3 (hydraulic conductivity calculated as the average across the transect parallel to flow).

In addition, a Passive flux meter (PFM)-based approach (Approach 4) replicating the physics of passive flux meters where the actual Darcy flux and concentration per model node in the well screen (polygons are 0.15 m in height) was developed. Approach 4 (by definition) must converge to the correct answer with decreasing well spacing (at the smallest horizontal well spacing the approach is using data from all model nodes). Estimating mass discharge from integral pump tests is also a potential effective practice approach (ITRC, 2014) but was not considered in this work.

In this work, using DPT approaches to obtain mass flux estimates (obtaining hydraulic conductivities from HPT testing and concentrations from MIP testing) is not considered as effective practice. Quantitative estimates of hydraulic conductivity from HPT testing are only achievable within the range of 10^{-4} to 10^{-2} cm/s (Curry et al., 2016), and a greater range is expected at many sites. Correlation of MIP results to concentration is qualitative and will vary greatly from site to site. Effective practice relies on accurate quantitative measurement of concentrations (within laboratory range of error) which is not possible with a MIP (https://clu-in.org/characterization/technologies/mip.cfm).

Kubert and Finkel (2006) performed a similar study using a model domain consisting of a spatially correlated hydraulic conductivity field (the same approach as used in DIVER) and a constant concentration "patch" source function on the upgradient side of the domain. The most significant difference between the Kubert and Finkel (2006) model and the DIVER simulations concerns the source. In DIVER the source is based on the DNAPL architecture resulting in spatially variable concentrations (and mass discharges) correlated to the permeability (DNAPL located in higher conductivity lenses creating more spatially variable plume cross sections). Kubert and Finkel

(2006) examined 7 different approaches for calculating mass flux based on a literature review (Table 6-3).

Table 6-3: Approaches of Kubert and Finkel (2006)

Approach	Concentration	Hydraulic Conductivity	Gradient	Equivalent to Approach in Table 6-2
A.1	Measured mass flux from PFM			
A.2	Multi-level	Measured q from PFM		
B.1	Per well screen with multi-level wells[1]	Per well screen with multi-level wells	Average in transect	1
B.2	Per well screen with multi-level wells	Per well screen with multi-level wells	Per well screen with multi-level wells	
C.1	Per well screen fully screened wells[2]	Per well screen fully screened wells	Average in transect	1
C.2	Per well screen fully screened wells	Per well screen fully screened wells	Per well screen fully screened wells	
D	Per well screen with multi-level wells	Average in transect	Average in transect	3

1 – Multiple measurements across height of transect
2 – Single measurement across height of transect

Data from each of VSD 1-3 was used to calculate the predicted mass flux across a flux plane (defined as the distance from the edges of the plume to 0.5 ppb laterally and vertically) located 10 m downgradient of the source zone in each VSD. The number of wells in the plane was varied from a minimum of 2 to a maximum of 39 (VSD 2) and wells were equally spaced in all cases. The number of screens per monitoring well ranged from a single screen (fully screened across the height of the transect) to 0.15 m screens (equal to the model nodal discretization) stacked to cover the entire height of the transect.

Figure 6-15 presents the normalized mass discharge estimates as a function of well spacing for VSD1 for Approach 1. Approach 1 consistently overestimated the mass discharge across the plane (except for the largest well spacing). It should be noted that even at the closest well spacing (equivalent to a well at every column of nodes in the model in the transect) Approach 1 did not converge to the actual mass discharge. This is due to the treatment of gradient within Approach 1, where the gradient is the average across the plane. Groundwater flux in the analysis for Approach 1 is based on the nodal flux outputs from the model, which capture local gradient changes across the transect. It is also important to note that the calculation approaches for C and K in this work are different than those in Kubert and Finkel (2006). Concentrations in well screens in this work are flux-averaged (as would be expected in an actual monitoring well), whereas in the work of Kubert and Finkel (2006) they were arithmetical averages. In addition, hydraulic conductivities at the well screen scale in this work are bulk values calculated based on flow parallel to bedding (Yeh et al., 2005), whereas in Kubert and Finkel (2006) they are geometric averages that are not physically supported. Figure 6-15 also shows the predictions for Approach 1 using the averaging methods of Kubert and Finkel (2006).

The use of flux-weighting and flow parallel averaging results in identical estimates for mass flux regardless of the size of the screens used (e.g., the flux estimate is the same using ten 1 m screens or using one 10 m screen). This is not the case for the arithmetic and geometric averaging approach (Figure 6-16) where the estimate increases with decreasing screen size at any given monitoring well spacing. It should be noted that the estimate using the smallest screen size in Figure 6-16 (top row of dots) converges to that calculated using the flux-weighted and parallel flow averaging approach (Figure 6-15).

Figure 6-15 also presents the results using Approach 4. As expected, the estimate converges to the actual at small well spacings as it is not reliant on an averaged gradient estimate across the transect. Overall variability across different well spacings with Approach 4 is similar to that of all other approaches, indicating that, for VSD1, the relative accuracy of each method is similar across the range of well spacings. However, the absolute accuracy for Approach 4 is greater for all but the largest well spacing.

Figure 6-17 presents the normalized mass discharge estimates as a function of well spacing for each VSD for Approach 4.

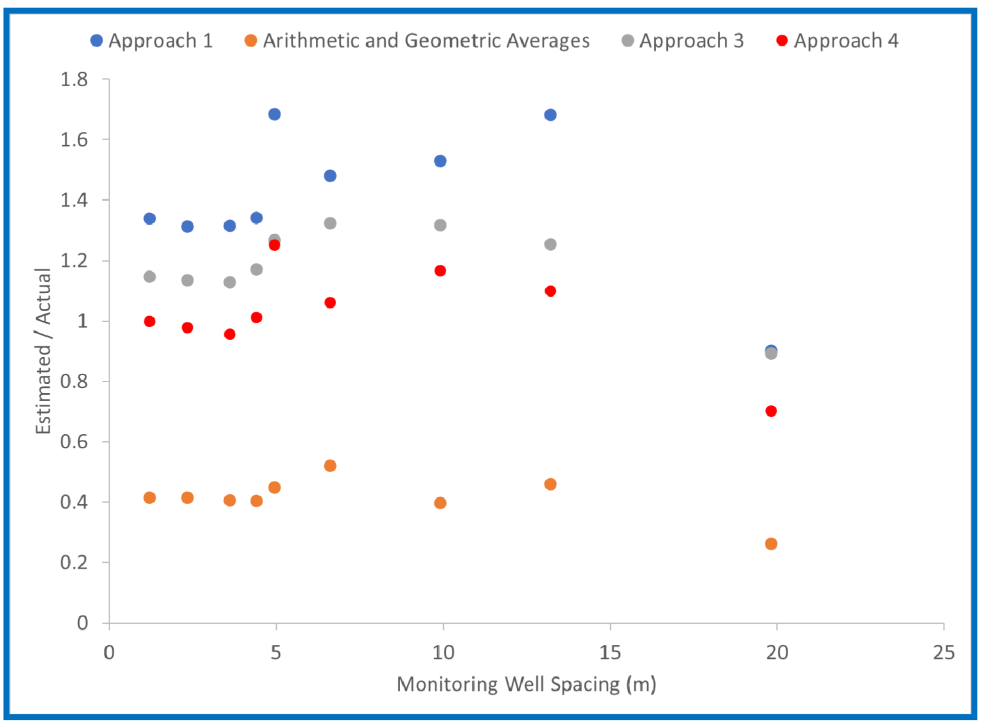

Figure 6-15: Normalized mass discharge estimates for VSD 1 using all approaches as a function of monitoring well spacing

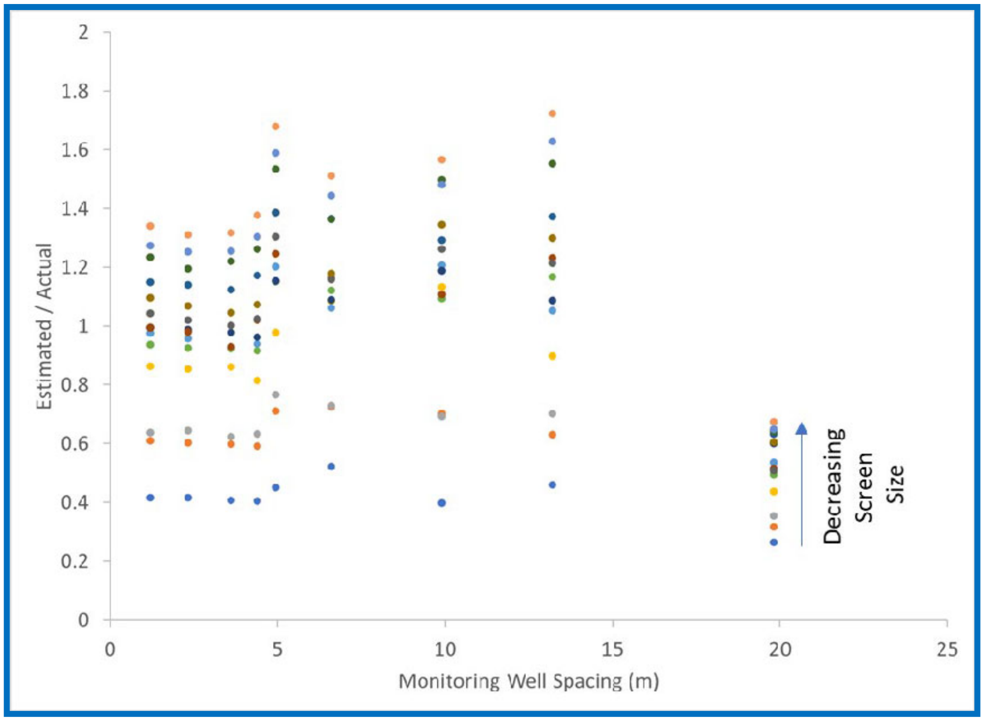

Figure 6-16: Normalized mass discharge estimates for VSD 1 using the averaging method of Kubert and Finkel (2006). Estimates for each monitoring well spacing increase with decreasing screen size (blue through orange).

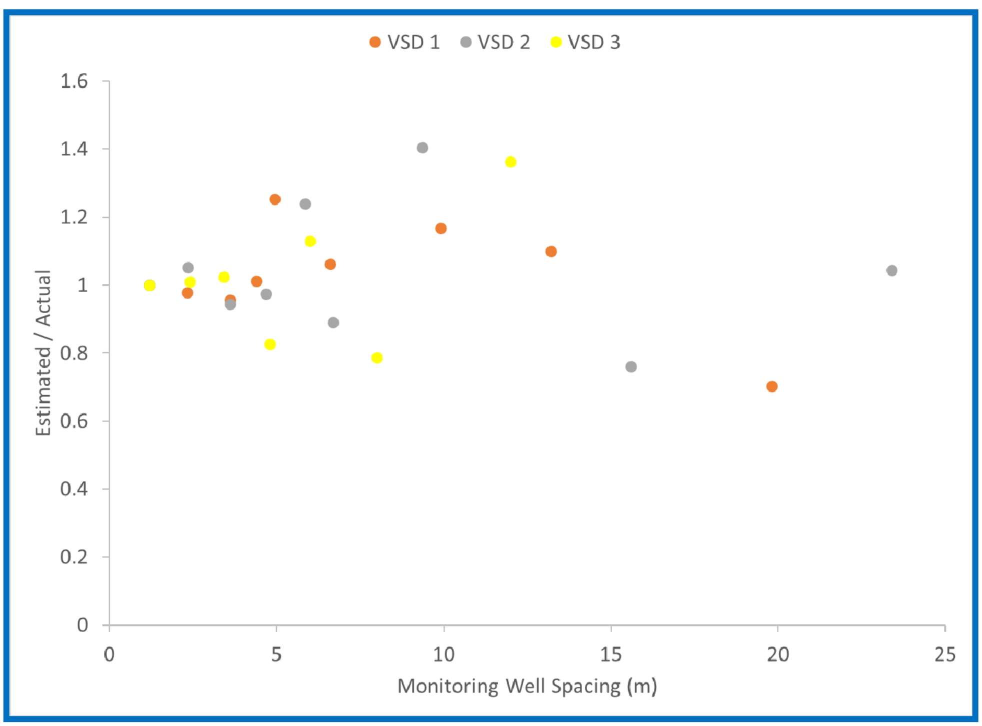

Figure 6-17: Normalized mass discharge estimates for VSD 1 – 3 using approach 4 as a function of monitoring well spacing

Overall, these results support the finding that any of the three approaches to determine mass discharge investigated in this work could be considered effective practice in particular if relative change (e.g., pre- and post-remediation) is the data quality objective. The concept of effective practice is defined by the use of a transect approach and quantitative measurements of concentration, hydraulic conductivity and gradient (or groundwater flux if using PFMs). With the proper design and analysis, other approaches (such as integral pump testing) could be considered effective practice, however they are not likely to provide a more accurate answer than the proposed effective practice approach at a fine monitoring well spacing. For VSDs 1-3 results indicate that estimates using monitoring well spacings greater than 5 – 10 m are equally uncertain within any single approach. However, the three approaches have clear bias where Approach 1 consistently overestimates the mass discharge, Approach 2 consistently underestimates the mass discharge, and Approach 3 can over- or underestimate the mass discharge for a given monitoring well spacing. Approach 4 does converge to the exact answer as monitoring well spacing goes to zero.

6.2 Validation of Effective Practice

The final step in the overall project was an investigation aimed at verifying the outcomes of the project in terms of effective practice. To achieve this, a fourth VSD (of similar nature to the original three) was created to serve as a final "test" for the DM teams. In addition to the original four DM Teams, six new DM Teams (some with less than 5 years' experience) were added for the validation process. The overall validation process was essentially identical to the site investigation and CSM development stage of the project. Both the original and the new DM Teams were asked to develop CSMs with identical parameters to the original VSDs which were then evaluated against the known answers. To determine if the effective practice recommendations developed during the project improved the accuracy of CSMs, six of the ten DM Teams were provided with the effective practice guidance developed for three of the parameters (as described in Section 7):

- Source footprint
- NAPL mass within source footprint
- Mass flux

6.2.1 DNAPL Mass

The DNAPL Mass predictions for each of the original 4 DM Teams for VSD 1 are presented in Figure 6-18 in terms of the expectations based on using effective practice. Following the approach outlined in Section 6.1.6 the lines in Figure 6-18 are the confidence intervals based on a random selection of several borehole locations used to calculate the DNAPL Mass. None of the DM Teams used effective practice in calculating their estimates of DNAPL mass for VSD 1. In 3 of 4 cases using effective practice (for the actual number of boreholes used in the development of the DM Team CSM) for calculating the estimate would have had a high likelihood (>99%) of a more accurate estimate.

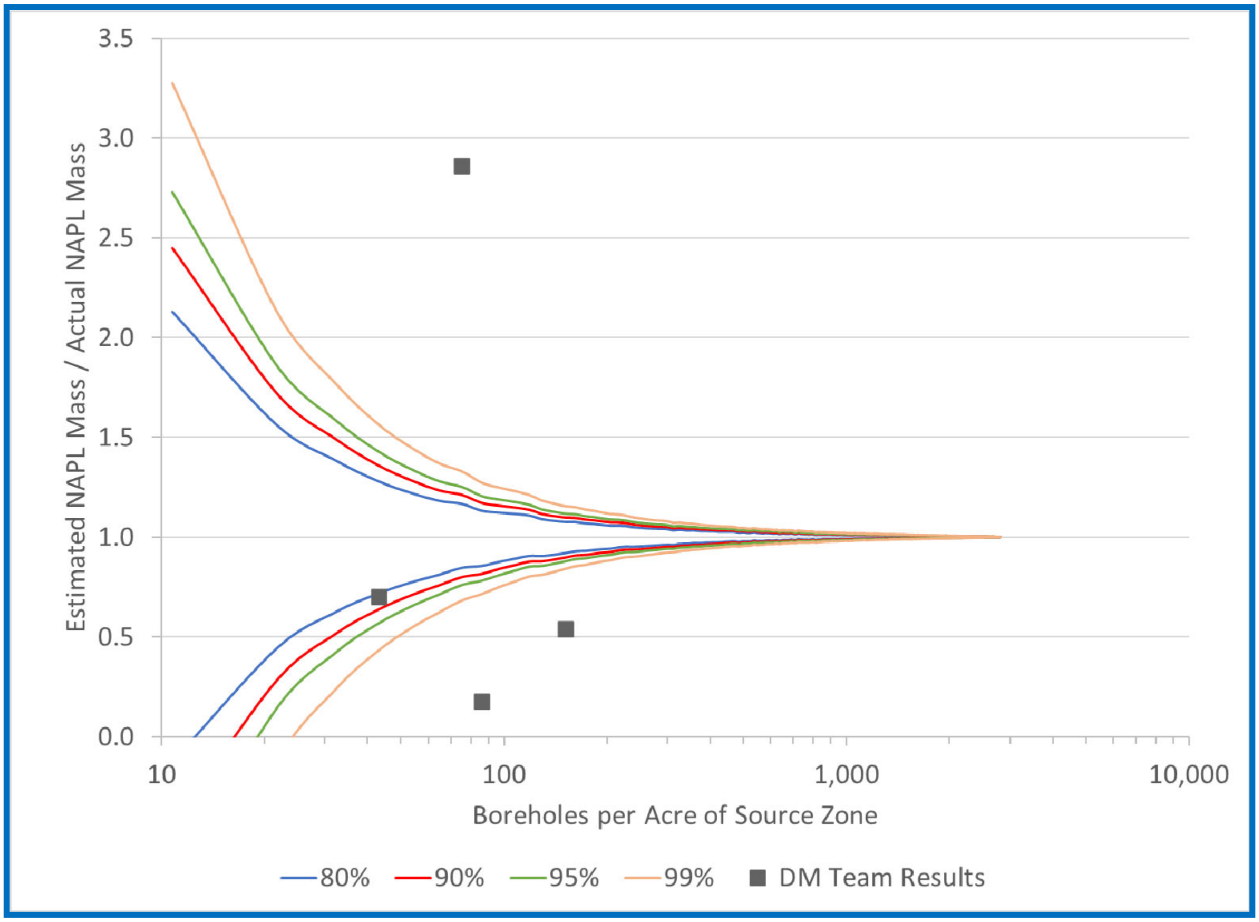

Figure 6-18: DM Team DNAPL mass predictions for VSD 1 compared to the expectations using effective practice

6.2.2 Mass Discharge

Table 6-4 presents an assessment of the approach each DM Team used to predict mass discharge in their CSMs.

Table 6-4: Assessment of DM Team use of effective practice for estimating TCE mass discharge across a transect 10 m downgradient of source zone

VSD	Team A Approach	Score	Team B Approach	Score	Team C Approach	Score	Team D Approach	Score
1	Used average concentrations at 2 wells and calculated Darcy flux	N/A[1]	Used calculated Darcy flux and MIP response	0.35	Used Mass Flux Toolkit, slug tests, measured gradient and average concentration from 2 wells	3.37	Concentrations (wells and MIP) and average Darcy flux from HPT	15.83
2	Used concentration at 1 well and calculated Darcy flux	N/A[1]	Used calculated Darcy flux and average concentrations from 3 wells	0.61	Used Mass Flux Toolkit, slug tests, measured gradient and average concentration from 5 wells	0.26	Concentrations (wells and MIP) and average Darcy flux from HPT	483
3	Used concentration at 1 well and calculated Darcy flux	N/A[1]	Used calculated Darcy flux and average concentration from 4 wells	1.28	Used Mass Flux Toolkit, slug tests, measured gradient and average concentration from 5 wells	1.95	Concentrations (wells and MIP) and average Darcy flux from HPT	1.53

1 – Reported total VOC flux not TCE flux

Figure 6-19 overlays the DM Team scores (squares) for each VSD on the range of expected scores calculated using Approach 4 (circles). Six of nine R_es are overestimates of the true mass discharge for a transect located immediately downgradient of the source zone. The black outlined squares indicate which R_es used only quantitative data in a transect approach (aligned with effective practice). The tendency to overestimate by the DM Teams is partially due to the bias on concentrations towards higher concentration portions of the transect. Team C identified this as a possibility, given the deliberate location of their CMT screens at elevations that were of highest concentration (based on MIP qualitative data obtained prior to the installation of the screens). Three of the four estimates arrived at with MIP data are three of the four least accurate of the nine estimates highlighting the challenges of using qualitative data when estimating mass flux. In general, few DM Teams installed quantitative monitoring infrastructure at small enough (<5 m) spacing (laterally) to expect accuracy within +/- 50% as could be expected to be achieved with a uniform spacing of PFMs or multi-level wells fully screening the aquifer.

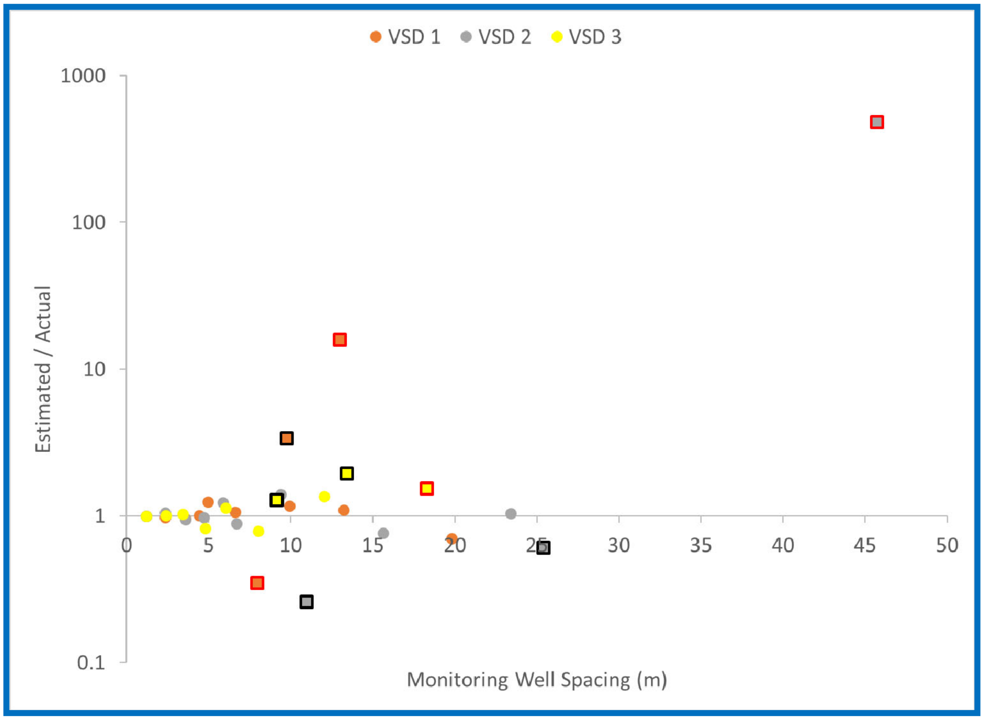

Figure 6-19: Comparison of DM Teams mass discharge estimates (squares) with expectations using a PFM approach (circles). Black outlined squares indicate where DM Teams used quantitative data. Red outlined squares indicate where DM Teams used qualitative data only.

6.2.3 Source Zone Footprint

Based on their CSM submissions, no DM Team used the proposed effective practice to determine their estimate of the source zone footprint. All methods used by the DM Teams are not comparable to the expected results using effective practice and as such no comparisons can be made for this parameter.

6.3 Utilizing Effective Practice in Developing CSMs

The Effective Practice approaches developed during the project were tested by having the DM Teams develop CSMs for VSD 4 in a manner analogous to that used for VSDs 1 – 3. To increase the sample size six additional DM Teams were brought into the project for the verification process. A total of eight CSMs were submitted and were assessed to determine if using effective practice led to improved parameters and lower costs (increased value). In our analysis, we ensured that results associated with using effective practice were based on actions taken by the team, and not simply providing guidance to the teams. One of the DM Teams clearly did not follow the provided guidance as the performed site investigation could not be aligned with the guidance.

As an example, DM Team F did not utilize a grid pattern (or any other pattern) installing boreholes to estimate the source zone footprint and used MIP signals to correlate to the presence of NAPL. In addition, DM Team F used a correlation between MIP signal and DNAPL saturation (and therefore mass) in combination with laboratory analysis of soil samples from boreholes in the source zone. There was minimal information provided on their calculation approach for mass discharge, however the data density was very sparse and parameter testing (such as slug tests for local hydraulic conductivity values and local gradient assessment) was not performed.

In addition to the DM Team that did not follow the provided guidance, four additional DM Teams were assessed to have only partially followed the guidance. For example, DM Team E used the guidance approach in delineating the source zone footprint (albeit at a very low density of locations) but did not use the guidance approach in calculating the DNAPL mass present in the source. DM Team J used the guidance approach to calculate the DNAPL mass present in the source but relied primarily on MIP results to identify the source zone footprint.

To assess the overall improvement of the DM Teams CSM score through use of effective practice, the results were compared to the results from VSD 1-3 (Figure 6-20 and Figure 6-21). The first (left hand side) panel in Figure 6-20 reproduces the results for all parameters for all Teams from VSD 1 – 3. The second (right hand side) panel in Figure 6-20 presents the results for all parameters for all teams from VSD 4. The first (right hand side) panel in Figure 6-21 averages the results for each parameter for VSD1-3 and VSD 4. The second (right hand side) panel in Figure 6-21 breaks the VSD 4 averages out into three groups, teams that did not use the guidance, teams that partially used the guidance, and teams that followed the guidance. Effective Practice guidance was provided (Appendix A) for biodegradation decay coefficient, DNAPL mass, mass discharge, and source zone footprint.

6.3.1 Source Zone Footprint

Overall, the source zone footprint accuracy increased in VSD 4 (as compared to, for example, the plume footprint estimates where guidance was not provided). Partial or complete use of effective practice was clearly demonstrated to increase the average accuracy of the estimate as compared to the estimates for VSD 1-3. There is some variability in this assessment as in some cases Teams not using the guidance scored better than Teams using the guidance.

6.3.2 DNAPL Mass

The results of the estimates for the DNAPL mass parameter in VSD 4 were generally less scattered than for VSD 1-3 and remained centered on the correct answer. The average estimate/truth score decreased from 4 to 3 (all teams) and from 4 to 1.5 when only considering the teams that used effective practice.

6.3.3 Mass Discharge

The average estimate/truth score reduced from 5 to 2 and 7.5 to 3.5 (nearest and farthest transects from source respectively). Given the relatively thin and confined nature of the plume in VSD 4 this improvement could be a function of the hydrostratigraphy (easier to estimate due to less vertical variability), however all estimates for mass discharge from VSD 4 were overestimates as compared to VSD 1 – 3 where one third of the estimates were underestimates.

6.3.4 Decay Coefficient

The increase in accuracy of the estimates of the decay coefficient for VSD4 was very small (< 0.5) and was less accurate for those teams deemed to have used effective practice. Details on the calculation of decay coefficients was scant in most CSM reports so there is greater uncertainty in the assessment of the rigor in which the teams followed effective practice.

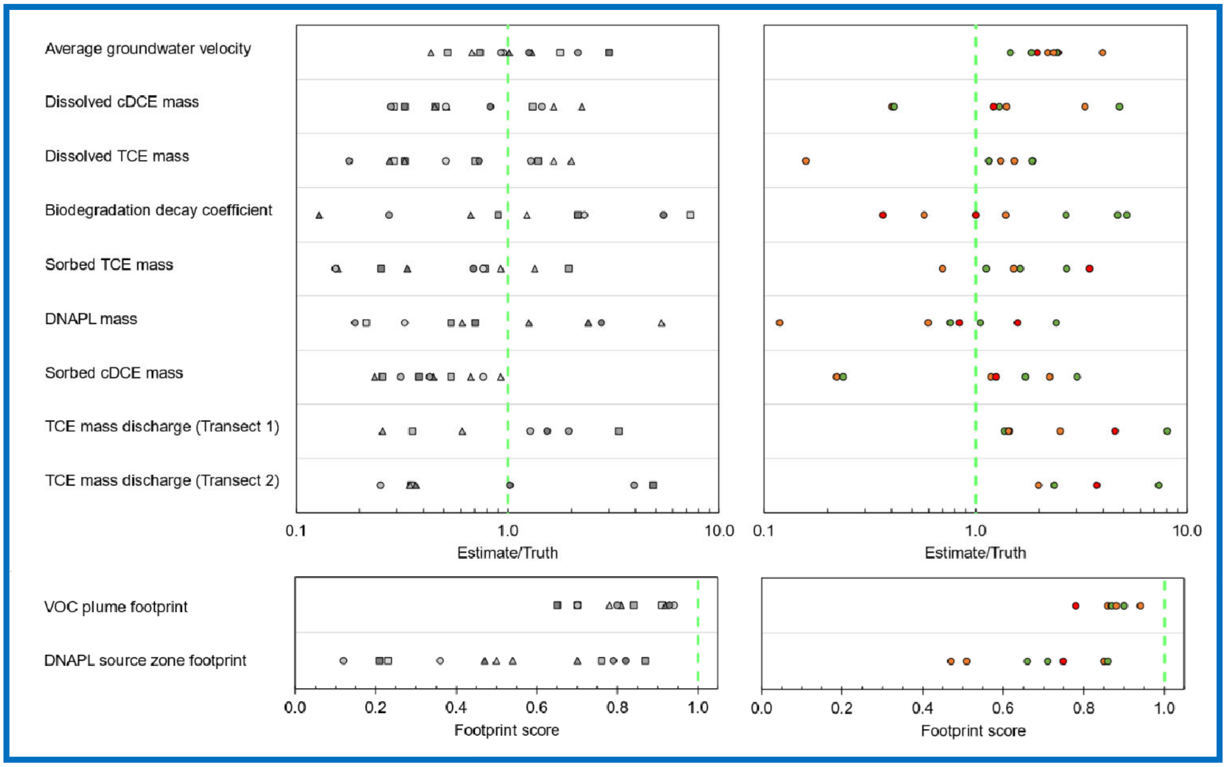

Figure 6-20: Comparison of DM Team performance on VSD 4 to VSDs 1-3

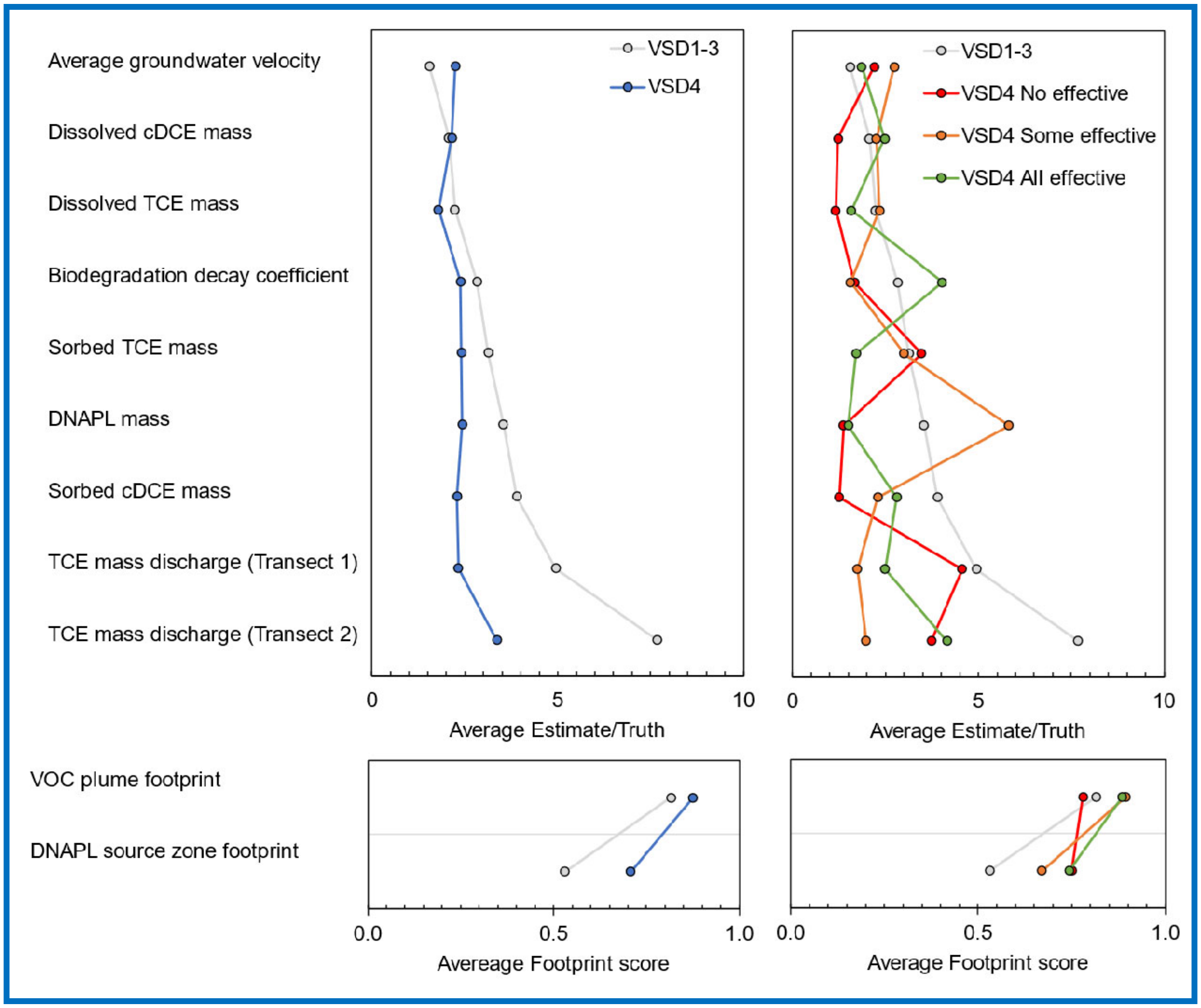

Figure 6-21: Comparison of DM Team performance on VSD 4 to VSDs 1 to 3

The differences in the overall accuracy and cost of the CSMs developed under effective practice are shown in Figure 6-22. Higher values on the vertical axis indicate an overall worse score on the CSM parameters. Combining the overall average parameter score with the total cost creates quadrants that define success and failure, and high and low cost. Note that the definitions of success and failure, and high and low (dashed lines in Figure 6-22) here are relative to the average of all teams over VSD 1-3 and should not be viewed as absolute indicators. Also note that this accuracy is based on a log-transformed absolute value, such that a score of 2 and a score of 0.5 are each treated as a value of 2 (i.e., equal value was assigned to estimates that were over- or underestimated by a factor of 2). Results from VSD 1-3 appeared in all four quadrants.

It is expected that using effective practice should result in a translation down (greater accuracy) and to the left (less cost), particularly for teams that demonstrated lower accuracy in their VSD 1-3 CSMs. The difference between the results from Teams C and D in VSD 1-3 compared to VSD 4 is highlighted in Figure 6-21 Figure 6-22, which demonstrates the expected translation. The differences for Team D can be attributed to their adoption of effective practice (change from their approach in VSD 1-3). Team C elected to use a hybrid of their previous approaches and effective practice where they used DYE-LIF in a grid to estimate source footprint and cores and soil samples to calculate DNAPL mass.

The concept of the benefit of increased accuracy at increased cost, in the context of reduction in remediation cost (and thus overall cost to closure) is examined in greater detail in Section 8.

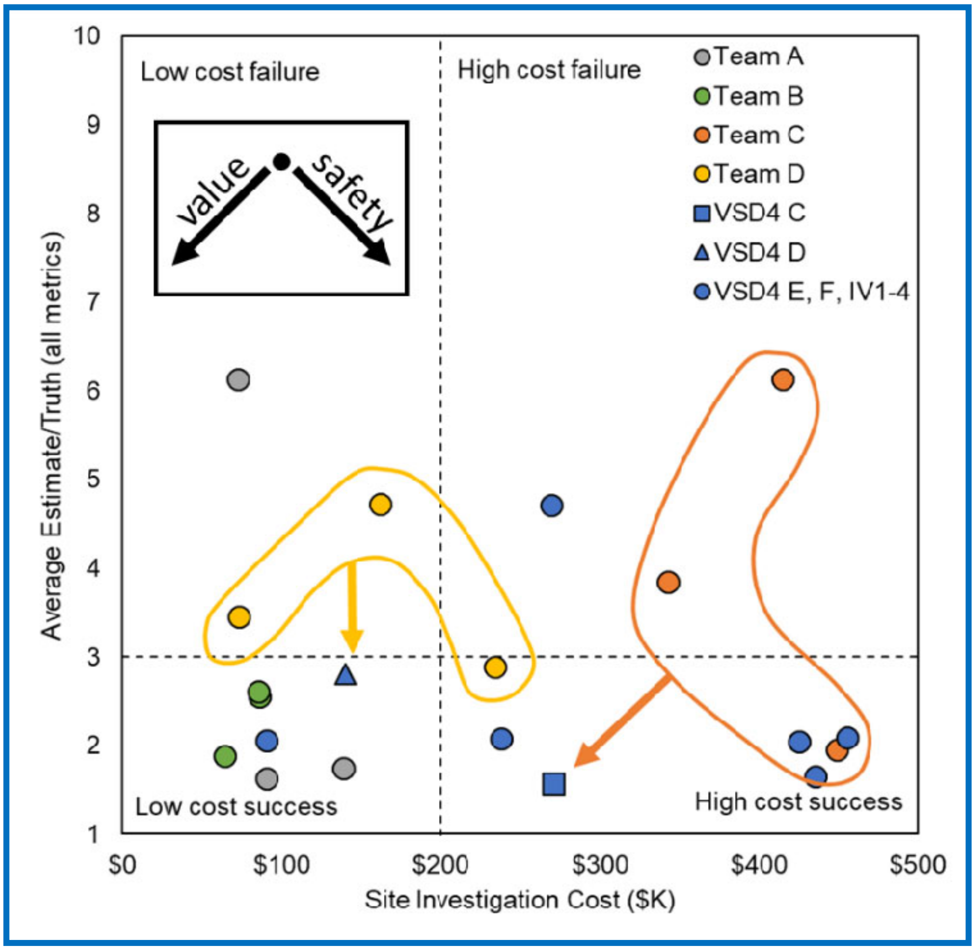

Figure 6-22: Overall improvement under the "quadrants" approach

The horizontal dotted line in Figure 6-22 demarking "failure" and "success" is a relative metric and should only be viewed as such. Using this metric, only one CSM submitted for VSD 4 (Team G – not shown) would be considered a "failure". This failure was driven by very low estimates of DNAPL and plume mass, based on a misunderstanding of the overall Phase 1 CSM for the site.

7 EXPLORING THE RELATIONSHIP BETWEEN SITE INVESTIGATION AND REMEDY DESIGN

It is reasonable to assume that accuracy in site investigations should correlate to improved remediation success and lower remediation cost. The more accurate the CSM developed during site investigation the less uncertainty should be in the remediation design and both the life cycle cost of the design and the likelihood of failure should be reduced.

To investigate this assumption, the DM Teams results on the individual CSM parameters were compared to the DM Teams results on the remediation performance objectives via a correlation comparison. Table 7-1 presents the correlation matrix for scores on individual CSM parameters versus the scores on the remediation performance objectives as well as total site investigation cost and total remediation cost. Green highlighted cells indicate correlations that have Pearson's "r" greater than 0.3 and are significant at the 90% level. Four correlations between CSM parameters and remediation performance objectives were significant:

- DNAPL Mass & Total Remediation Cost
- DNAPL Mass & DNAPL Mass Removal
- TCE Source Discharge & Remediation Mass Discharge Reduction
- TCE Source Discharge & Remediation Concentration Reduction

These four correlations (categorized based on VSD) are presented graphically in Figure 7-1. The correlation between TCE Source Discharge (CSM) and Remediation Mass Discharge Reduction is intuitive (if you understand where the majority of the mass discharge is you can focus the remediation) as is the correlation (not as strong) between TCE Source Discharge (CSM) and Remediation Concentration Reduction.

The correlation between DNAPL Mass estimate in the CSM and DNAPL Mass removal in remediation is also strong and intuitive, however it is interesting that in six cases (across all 3 VSDs) the remediation objective was achieved despite a (sometimes large) underestimate of DNAPL mass present. This is due to very significant factors of safety applied to the remediation designs (see section 5.2.1), specifically the injection of 140% to 370% greater lactate mass than the stoichiometric amount. The correlation between DNAPL Mass estimate (CSM) and Total Remediation cost is also intuitive in that, generally, DNAPL mass underestimates resulted in lower remediation costs because the design is based on a smaller treatment requirement. The implications of this in the context of remediation failure and using probability distributions developed for decision analysis is further explored in Section 7.1.

It is also interesting to explore in more detail the correlation between DNAPL Mass reduction and Mass Discharge reduction (Figure 7-2). Various forms have been hypothesized for this relationship in the past (Fure et al., 2006; Johnston et al., 2014; Brooks et al. 2018) based on source zone architecture, underlying geology, age of the source, and other factors. With the exception of the cases where Mass Discharge after remediation increased (All VSDs for DM Team B, and VSD 3 of DM Team D) in all but two cases (Team A VSD2 and VSD3) the relative reduction in mass discharge was less than the relative reduction in DNAPL mass (i.e., most points appear below the 1:1 line in Figure 7-2).

The exploration of the correlations and relationships between CSM accuracy and remediation success demonstrates there is no relationship across Teams and VSDs, and conclusions are obscured by large factors of safety applied by some Teams used to implement their remediation design (that overcome CSM limitations) as well as critical flaws in the development of the CSMs (fundamental errors arrived at through application of investigation or analysis approaches that are not considered best practices).

Figure 7-3 compares site investigation cost and remediation cost across all VSDs and DM Teams and identifies individual data pairs based on the success or failure of the remediation design. Team B consistently spent the least for site investigation and remediation and in all cases failed to achieve the remediation goals (i.e., POs). Team A on the other hand spent similar amounts as Team B on site investigation, significantly more on remediation, and achieved success in all VSDs. Team C consistently spent the most for site investigation and significantly less than Team A on remediation yet achieved success in only 2 of 3 VSDs.

Table 7-1:Correlations between investigation parameters and remediation performance objectives. Green highlights indicate a Pearson's "r" > 0.3 and are significant at the 90% level.

Significance "p"	*Average Groundwater Velocity*	*Dissolved cDCE Mass*	*Dissolved TCE Mass*	*Biodegradation Decay Coefficient*	*DNAPL Mass*	*Sorbed TCE Mass*	*Sorbed cDCE Mass*	*TCE Mass Discharge (Transect 1)*	*TCE Mass Discharge (Transect 2)*	*DNAPL Footprint*	*Plume Footprint*	*Total Site Investigation Cost*	*Total Remediation Cost*	*DNAPL Mass Removal*	*Mass Discharge Reduction*	*Concentration Reduction*
Average Groundwater Velocity																
Dissolved cDCE Mass	0.001															
Dissolved TCE Mass	0.003	0.0008														
Biodegradation Decay Coefficient	0.72	0.85	0.48													
DNAPL Mass	0.87	0.71	0.69	0.74												
Sorbed TCE Mass	0.009	0.06	0.008	0.99	0.25											
Sorbed cDCE Mass	0.317	0.52	0.68	0.1	0.61	0.53										
TCE Mass Discharge (Transect 1)	0.41	0.28	0.32	0.44	0.25	0.86	0.8									
TCE Mass Discharge (Transect 2)	0.61	0.91	0.99	0.69	0.63	0.78	0.93	0.34								
DNAPL Footprint	0.46	0.72	0.58	0.63	0.25	0.4	0.99	0.52	0.82							
Plume Footprint	0.94	0.57	0.64	0.74	0.56	0.79	0.4	0.36	0.81	0.52						
Total Site Investigation Cost	0.64	0.15	0.52	0.29	0.7	0.94	0.6	0.71	0.18	0.84	0.93					
Total Remediation Cost	0.88	0.95	0.97	0.33	0.06	0.7	0.99	0.26	0.94	0.81	0.46	0.47				
DNAPL Mass Removal	0.436	0.54	0.52	0.52	0.01	0.92	0.24	0.15	0.7	0.33	0.6	0.63	0.14			
Mass Discharge Reduction	0.4	0.15	0.27	0.67	0.14	0.79	0.4	0.06	0.54	0.94	0.4	0.87	0.005	0.12		
Concentration Reduction	0.37	0.31	0.44	0.47	0.15	0.73	0.75	0.07	0.65	0.39	0.49	0.68	0.004	0.03	0.0008	

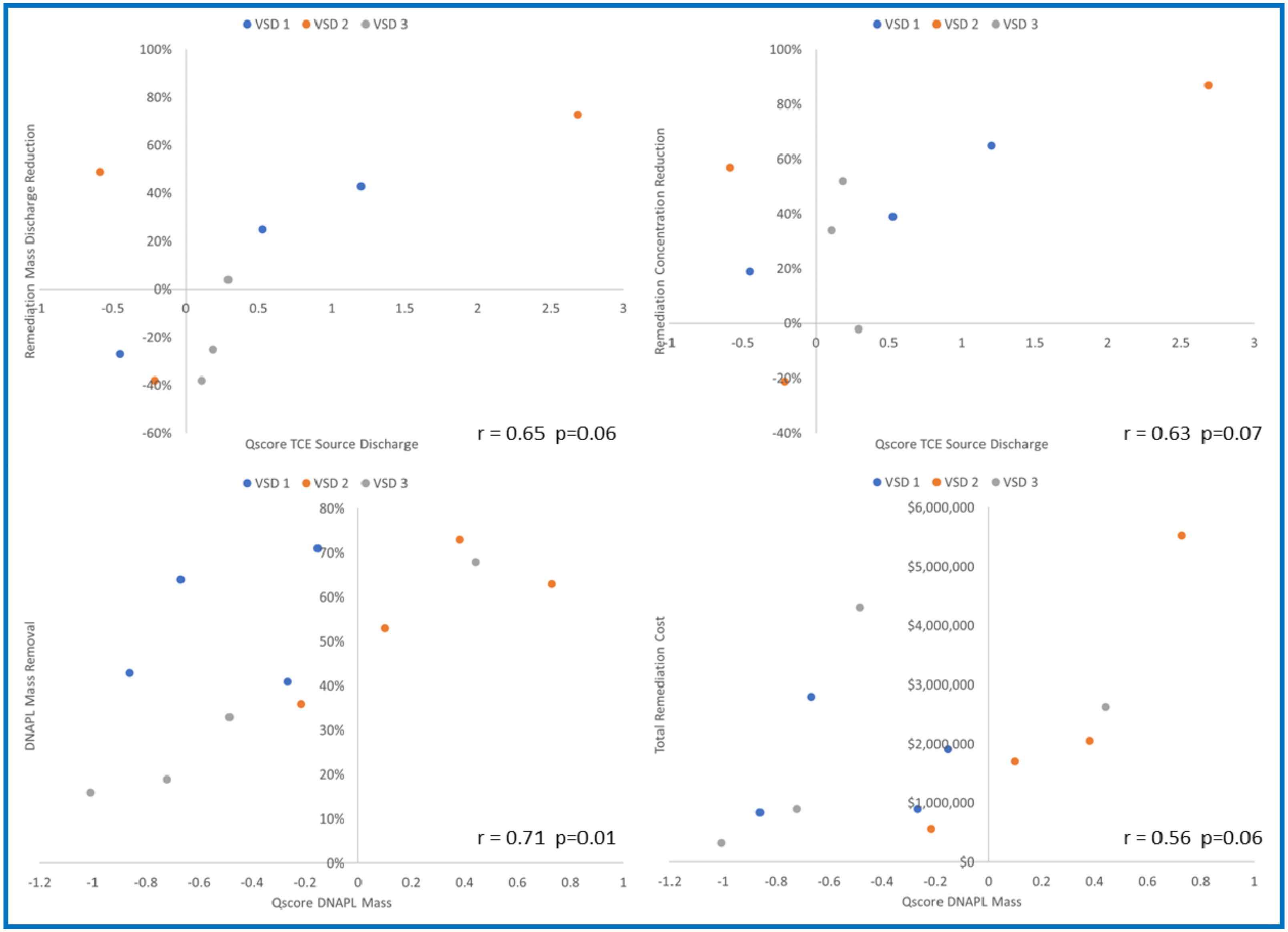

Figure 7-1: Relationships (across VSDs 1 – 3 and all DM Teams) between CSM parameters (based on QScore) and remediation performance objectives.

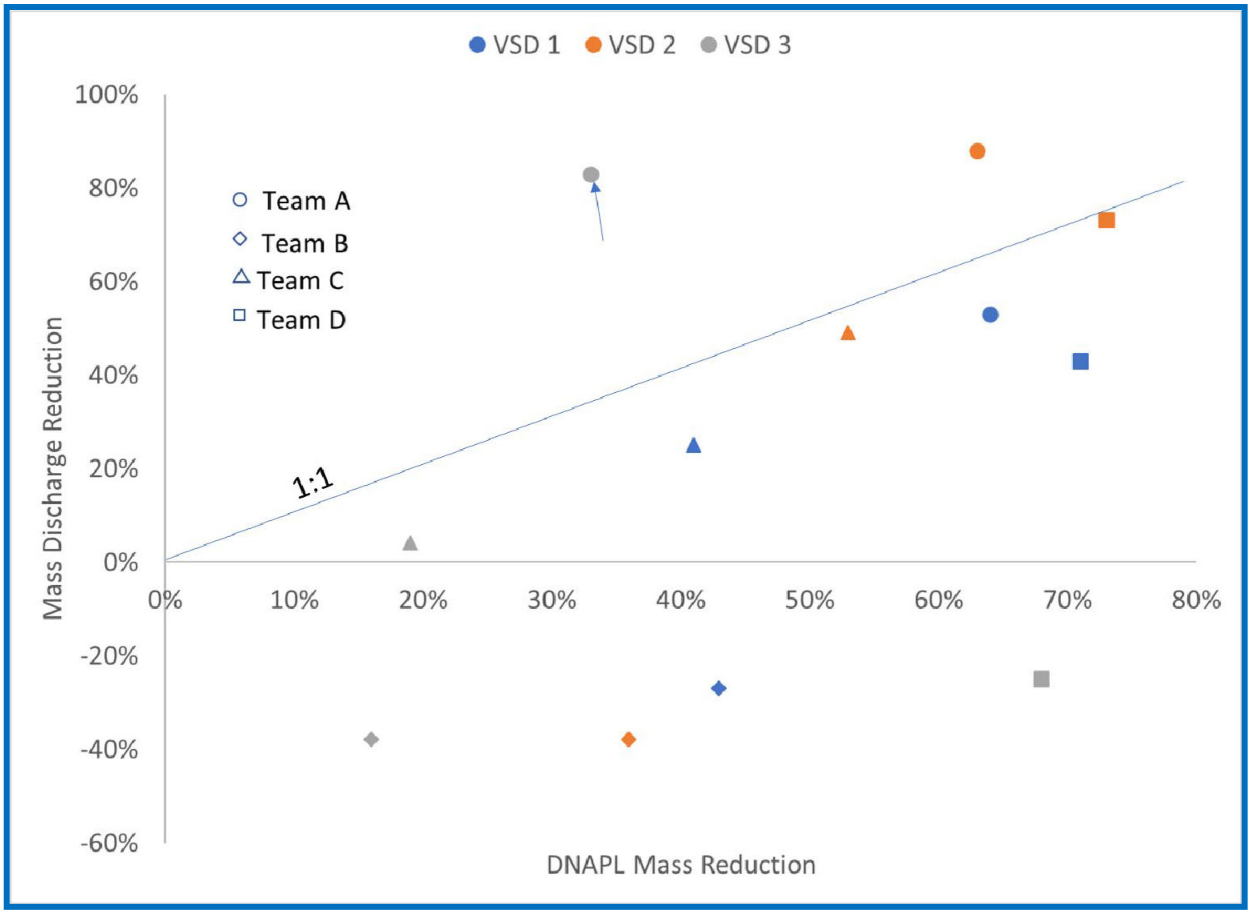

Figure 7-2: Relationship Between DNAPL Mass Reduction During Remediation and Mass Discharge Reduction Following Remediation (Negative Mass Discharge Reduction indicates Mass Discharge Following Remediation was Larger than Prior to Remediation).

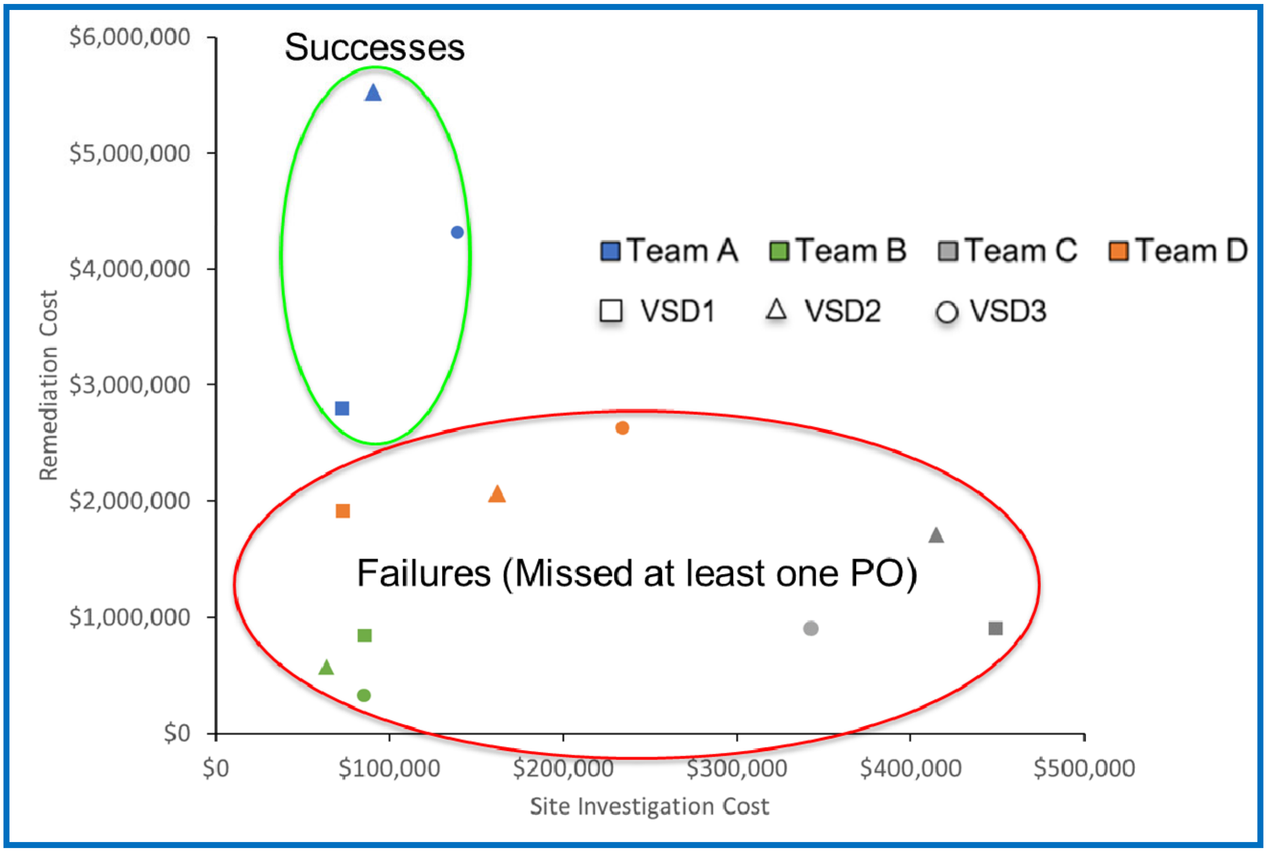

Figure 7-3: Site investigation cost vs. remediation cost correlated to remediation success and failure

The final segment of the DIVER project looked closely at each DM Team remedy in terms of its reason for failure, its overdesign to achieve success in some scenarios, and the benefit that could have been achieved through use of the effective practice derived for the key parameters (DNAPL Mass, Source Zone footprint, Mass flux) in terms of successful outcomes.

7.1 Detailed Exploration of the Failure Mechanisms and Potential for Optimization of DM Team Remediation Designs

A common approach in engineering design is the incorporation of a factor of safety. This approach is well understood in traditional engineering (e.g., bridge building) and is also used in remediation design (see for example, "Reliability and Statistics in Geotechnical Engineering, Baecher, G & Christian, J. Wiley, 2013). The factor of safety in remediation design can be incorporated in multiple ways, such as overestimating treatment zone volumes, overestimating the quantity of reactant to add to a system, a larger number of injection or extraction wells with smaller separation distances for in-situ injection technologies, or overestimating the required heating time or number of thermal units applied in a thermal remedy.

7.2 Factors of Safety Used in Remedy Designs

A focus of the examination of the reasons for failure of the DM Teams to meet achievable POs was to understand if application of a high factor of safety (at significant additional cost) compensated for the lower accuracy of the CSM parameters. The examination of safety factors such as overestimation of treatment zone volume is straightforward and can be qualitatively assessed by comparing the CSM source footprint parameter to the injection zone footprint in the remediation design. In a similar manner the selected dose of lactate can be compared to the theoretical dose based on generic stoichiometry to determine the excess lactate injected for the estimated NAPL, dissolved, and sorbed mass and therefore derive a factor of safety for this component of the design. The factor of safety estimate for each remedy was calculated based on the estimated DNAPL mass reported by the DM Teams as a CSM parameter (Table 7-2). It is common practice to apply a safety factor greater than one (i.e., equal to the stoichiometric dose) to the lactate mass, but that factor is typically less than 50 based on DIVER team experience. Application of a factor of safety above theoretical requirements is required for remediation design purposes, even with access to perfect information as not all injected lactate reacts with contaminant mass (e.g., due to by-passing, travel through zones of little or no contamination, hydraulically displaced outside the source zone).

Table 7-2: Lactate factor of safety based on DNAPL mass estimates

Team	VSD	Mass of DNAPL Estimate fr)om CSM (kg)	Theoretical Lactate Mass Based on CSM Mass Estimate (kg)[1]	Lactate Mass Applied in Remedy (kg)	Factor of Safety
A	1	2176	663	246,634	372
A	2	79,720	20,249	580,575	29
A	3	7003	1779	253,215	142
B	1	390	119	7598	64
B	2	9070	2304	16,534	7
B	3	2105	535	5518	10
C	1	5500	1676	60,085	36
C	2	18,791	4773	189,840	40
C	3	4080	1036	50,108	48
D	1	7118	2170	70,622	33
D	2	35,800	9093	142,238	16
D	3	59,368	15,079	103,218	7
QU	1	10,160	3097	193,591	63
QU	2	14,923	3790	55,292	15
QU	3	21,440	5446	213,584	39

1 – Calculated based on the theoretical stoichiometric H_2 electron donor mass needed to meet the VSD-specific DNAPL mass removal objective for the DM Team's DNAPL mass

Nonetheless, the factor of safety applied by the DM teams far exceeded optimum practice and lead to excessive costs. In general terms, overcoming uncertainty in performance of any remediation technology by exaggerated safety factors is undesirable and in some cases during a feasibility study, may lead to incorrect decisions for remedy selection. In contrast, as shown in Table 7-2, the safety factors used by the QU team with access to perfect information resulted in safety factors within reasonable limits.

7.3 Assessing the DM Team Designs

Each of the DM Team's remediation designs and performance was assessed considering both design success and failure and CSM accuracy. A success/failure analysis flowchart was developed to indicate which of the 12 DM Team designs should be investigated for potential optimization of the remedy design using effective practice developed in the project (Figure 7-4). Five possible endpoints were identified:

- Success at reasonable cost
- Success at excessive cost
- Failure based on bad interpretation of good data
- Failure due to poor CSM (bad/limited data)
- Design failure

A summary of each of the remedy/CSM pair and the endpoint of each on the flowchart is presented in Table 7-3. Each pair in the table is color-coded to its respective endpoint in the flowchart.

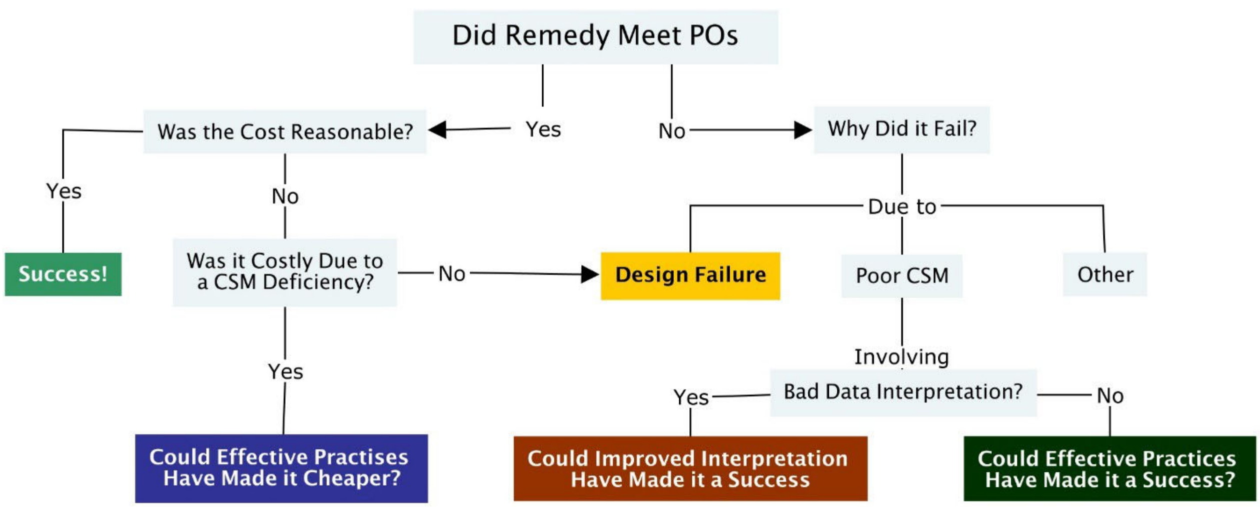

Figure 7-4: Flowchart assessment process for DM Team remedies

Table 7-3: Evaluation of failure mechanisms of DM Team remedies on VSD 1

DM Team (POs Met)	PO Assessment	CSM Assessment	Remedy Assessment	End-Point in Figure 7-4
A (3 of 3)	Mass = Y Dis = Y Conc = Y	Overestimated source footprint (Figure 5-9). Underestimated DNAPL mass by 79%.	Remedy design was logical based on their CSM, however installed 80% of injection wells downgradient of true source zone.	Could effective practice have made it cheaper?
B (1 of 3)	Mass = Y Dis = N Conc = N	Underestimated DNAPL mass by 96%. Used MIP correlations.	Very low number of injection wells and very low mass of lactate injected.	Could improved interpretation have made it a success?
C (1 of 3)	Mass = Y Dis = N Conc = N	Underestimated DNAPL mass by 46%. Used correlation to DYE-LIF.	Remedy design was adequate to reach POs	Could improved interpretation have made it a success?
D (1 of 3)	Mass = Y Dis = N Conc = N	Missed majority of source zone footprint (Figure 5-9). Underestimated DNAPL mass by 30%. Very low data density (2 samples) used to calculate mass.	Remedy design was logical based on their CSM, however did not install injection wells in downgradient half of source zone.	Could effective practice have made it a success?

Table 7-4: Evaluation of failure mechanisms of DM Team remedies on VSD 2

DM Team (POs Met)	PO Assessment	CSM Assessment	Remedy Assessment	End-Point in Figure 7-4
A (3 of 3)	Mass = Y Dis = Y Conc = Y	Overestimated DNAPL mass by 434%. Overestimated source zone footprint (Figure 5-10).	Remedy design was logical based on their CSM, however resulted in many unnecessary injection wells and excessive lactate mass.	Could effective practice have made it cheaper?
B (1 of 3)	Mass = Y Dis = N Conc = N	Underestimated DNAPL mass by 39%. Used dissolved phase concentrations to estimate DNAPL mass and MIP to estimate source footprint. Overestimated source footprint (Figure 5-10)	Remedy design was logical based on their CSM however small factor of safety on lactate mass and did not treat upgradient portion of source zone.	Could improved interpretation have made it a success?
C (1 of 3)	Mass = Y Dis = N Conc = N	Overestimated DNAPL mass by 26%. Missed smaller source zone.	Remedy design did not address second source zone and was therefore unable to meet POs.	Could effective practice have made it a success?
D (2 of 3)	Mass = Y Dis = Y Conc = N	Overestimated DNAPL mass by 140%. Missed smaller source zone.	Remedy design did not address second source zone and was therefore unable to meet POs.	Could effective practice have made it a success?

Table 7-5: Evaluation of failure mechanisms of DM Team remedies on VSD 3

DM Team (POs Met)	PO Assessment	CSM Assessment	Remedy Assessment	End-Point in Figure 7-4
A (3 of 3)	Mass = Y Dis = Y Conc = Y	Underestimated source footprint (Figure 5-11). Underestimated DNAPL mass by 67%	Significant overdesign not linked to CSM.	Could effective practice have made it cheaper?
B (0 of 3)	Mass = N Dis = N Conc = N	Underestimated source footprint (Figure 5-11). Used dissolved phase concentrations to estimate DNAPL mass and MIP to estimate source footprint. Underestimated DNAPL mass by 90%.	Remedy design was logical based on CSM.	Could improved interpretation have made it a success?
C (0 of 3)	Mass = N Dis = N Conc = N	Estimated DNAPL volumes based on DYE-LIF and assumed saturation calibration. Underestimated DNAPL mass by 81%.	Remedy design was logical based on CSM.	Could effective practice have made it a success?
D (2 of 3)	Mass = Y Dis = N Conc = N	Overestimated DNAPL mass by 177%. Used assumed DNAPL saturations (residual or pooled) rather than soil concentration data.	Remedy design was logical based on CSM.	Could effective practice have made it a success?

7.4 Application of Effective Practice for Optimization

Each of the remedies proposed by Team A was examined in detail as examples of the "Could effective practices have made it cheaper?" endpoint given that POs were met in all cases. Table 7-6 summarizes the cost and achievement of each of the remedies compared to the optimal (achieves the three POs at lowest cost) design.

Table 7-6: Comparison of Team A remedies to optimal remedies

VSD	Team	Cost	DNAPL Mass Reduction	Total VOC Dissolved Phase Mass Discharge Reduction	Average Maximum TCE Groundwater Concentration Reduction
VSD 1	Team A	$3.36M	64%	53%	68%
	Optimal	$1.75M	84%	75%	62%
VSD 2	Team A	$6.34M	63%	88%	91%
	Optimal	$1.49M	58%	53%	64%
VSD 3	Team A	$5.07M	33%	83%	90%
	Optimal	$2.64M	48%	59%	64%

7.4.1 Team A VSD 1

The overall CSM score for DM Team A on VSD 1 was 6.13. The analysis summarized in Table 7-3 indicated that the team had a significant error in the placement of the source zone (Figure 7-5) and underestimated the DNAPL mass present by 79%. The Team spent $72,493 on its CSM and $3.36M on its remediation (which achieved all three POs). Figure 7-5 also displays the locations of the injection wells used in their remedy.

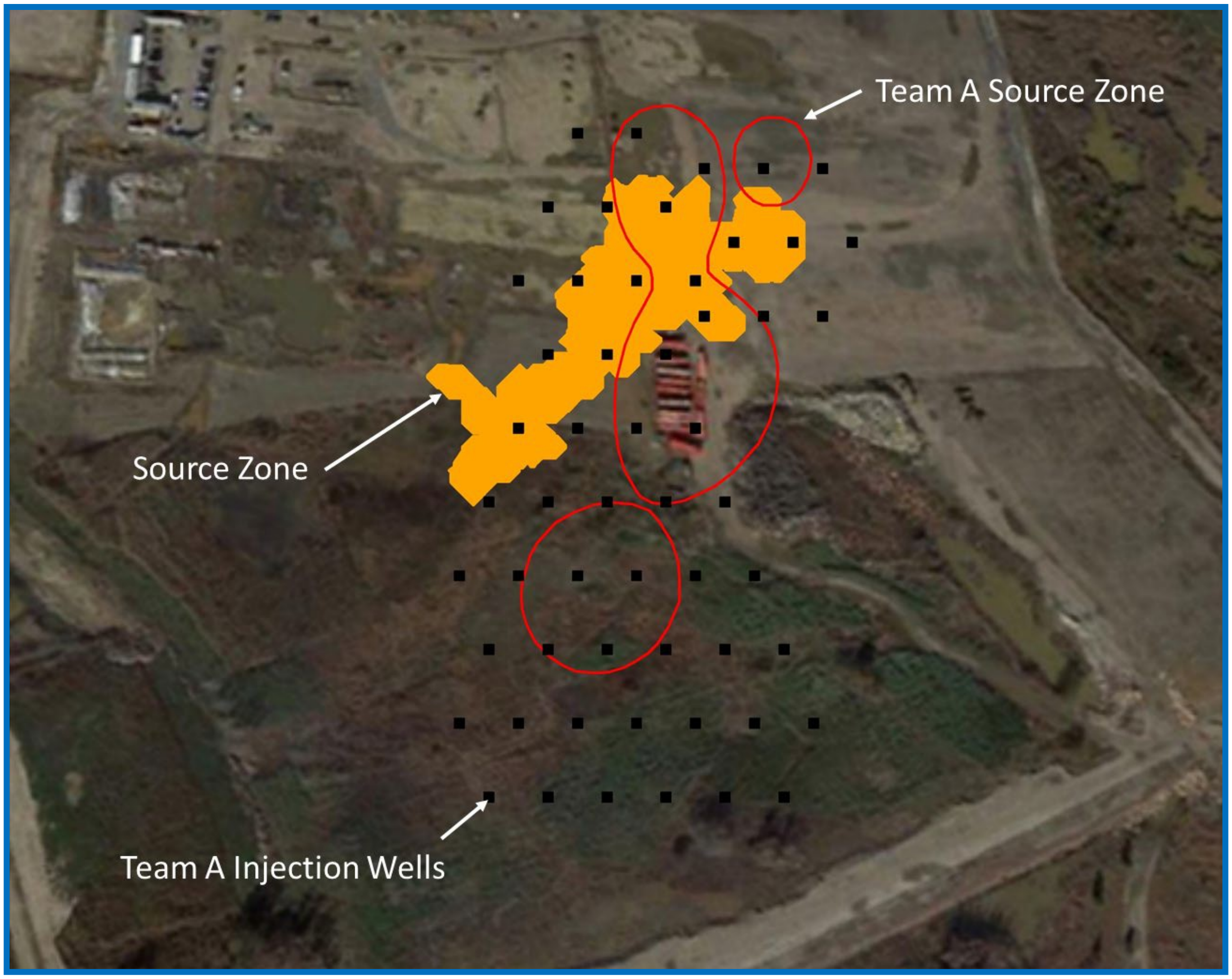

Figure 7-5: Team A VSD 1 source zone estimation and injection well locations

The cost of Team A's design implementation was $1.61M more than the remediation cost for the optimal remedy developed with perfect information. The majority of the additional cost was spent installing a large number of unnecessary injection wells and injecting lactate into those wells. This additional cost can be directly attributed to the errors in their source zone footprint estimate.

The Team A VSD 1 remedy was used to determine if the effective practice approach developed in the DIVER project for source zone footprint could achieve cost reduction while still meeting the POs and to link conclusively the excessive cost to the error in the CSM parameter.

In its most simple form, the objective function presented in Section 3.1.3 (Equation 3.3) is simply equal to the cost of the remedy (assuming you must remediate, and the risk/failure cost is not considered). We know the VPI is the cost of the optimized remedy ($1.75M). The VCI is the cost of the DM Team remedy ($3.36M). The difference between VCI and VPI provides the upper bound on the value of any additional data gathered through site investigation (Figure 7-6), however it is unlikely that VPI would ever be reached even at very extensive levels of site investigation as demonstrated in Section 6. We can use the developed effective practice approaches to assess the ENV of additional information to improve the Team's design.

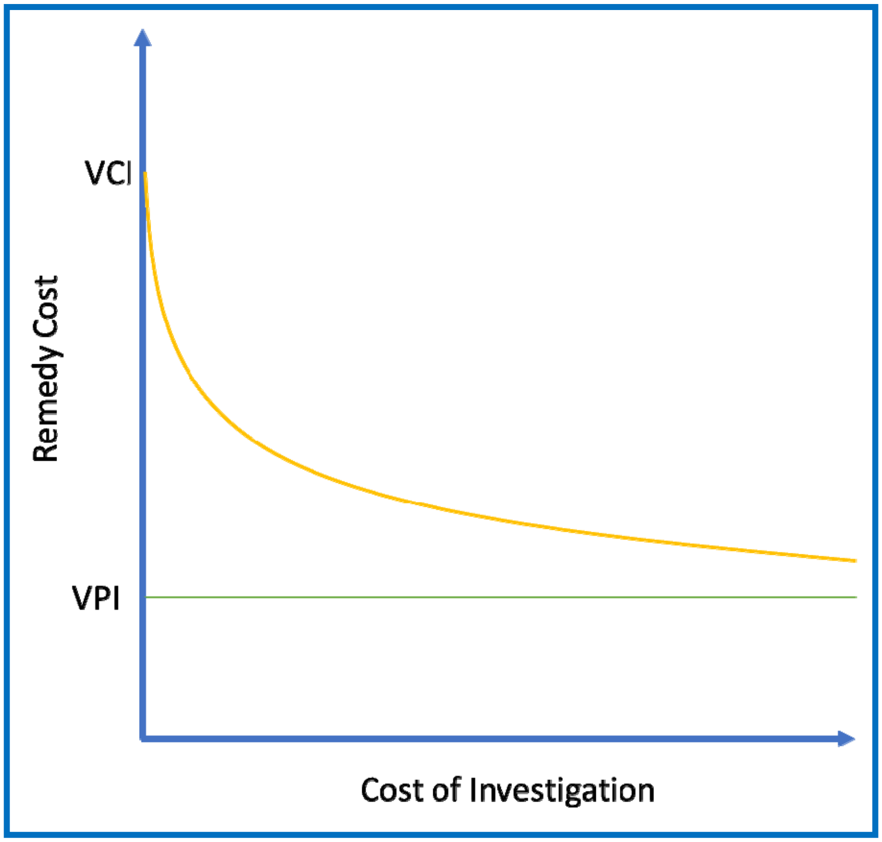

Figure 7-6: Conceptualization of limit on value of additional information: the diminishing return problem for optimization of any remedy.

Based on the results of the stochastic modeling performed in the development of effective practice for source zone footprint, equal line and hole spacing are appropriate, and with a 12.5 m spacing the expected uncertainty is +/- 30% (Section 6.1.1). The cost of this drilling to increase the accuracy of the location of the source zone for VSD 1 is approximately $450,000. Utilizing this approach, the source zone estimated footprint and the redesigned injection well field are presented in Figure 7-7. Three additional injection wells were added (highlighted in the yellow circle) where the source zone was identified, and no injection wells were added outside of the identified source zone footprint in the additional design.

The revised Team A VSD 1 remedy design was simulated using DNAPL3D-RX with injection rates maintained based on the average value from the original design (no attempt to correct for errors in the estimate of DNAPL mass). The total remediation cost was reduced by $1.05M. The revised design still met all remediation POs. The net value of the additional information gained by the drilling was $600,000. Additional savings could have been realized by increasing the spacing between the injection wells, however that would be adding interpretation to the original design that would likely be biased by knowledge of perfect information.

It is important to note that the revised design still incorporates a significant factor of safety for the lactate injection which is what leads to meeting POs despite the significant remaining error in the DNAPL mass estimate. If Team A had used effective practice to arrive at a more accurate DNAPL mass estimate and continued to use the large factor of safety the overall remedy cost would have been significantly higher. However, if Team A had used effective practice to estimate DNAPL mass and had adjusted their factor of safety, the remedy cost would have been far lower and likely similar to the cost of the optimum remediation design using perfect information.

Figure 7-7: Redesign of Team A VSD 1 remedy based on updated source footprint

7.4.2 Team A VSD 2

The overall CSM score for DM Team A on VSD 2 was 1.6. The analysis summarized in

Table 7-4 indicated that the team had a significant error in the placement of the source zone (Figure 7-8), shown outlined in red, and overestimated the DNAPL mass present by 434%. The Team spent $90,614 on its CSM and at a cost of $5.53M for remediation (which achieved all three POs). Figure 7-8 also displays the locations of the injection wells used in their original remedy.

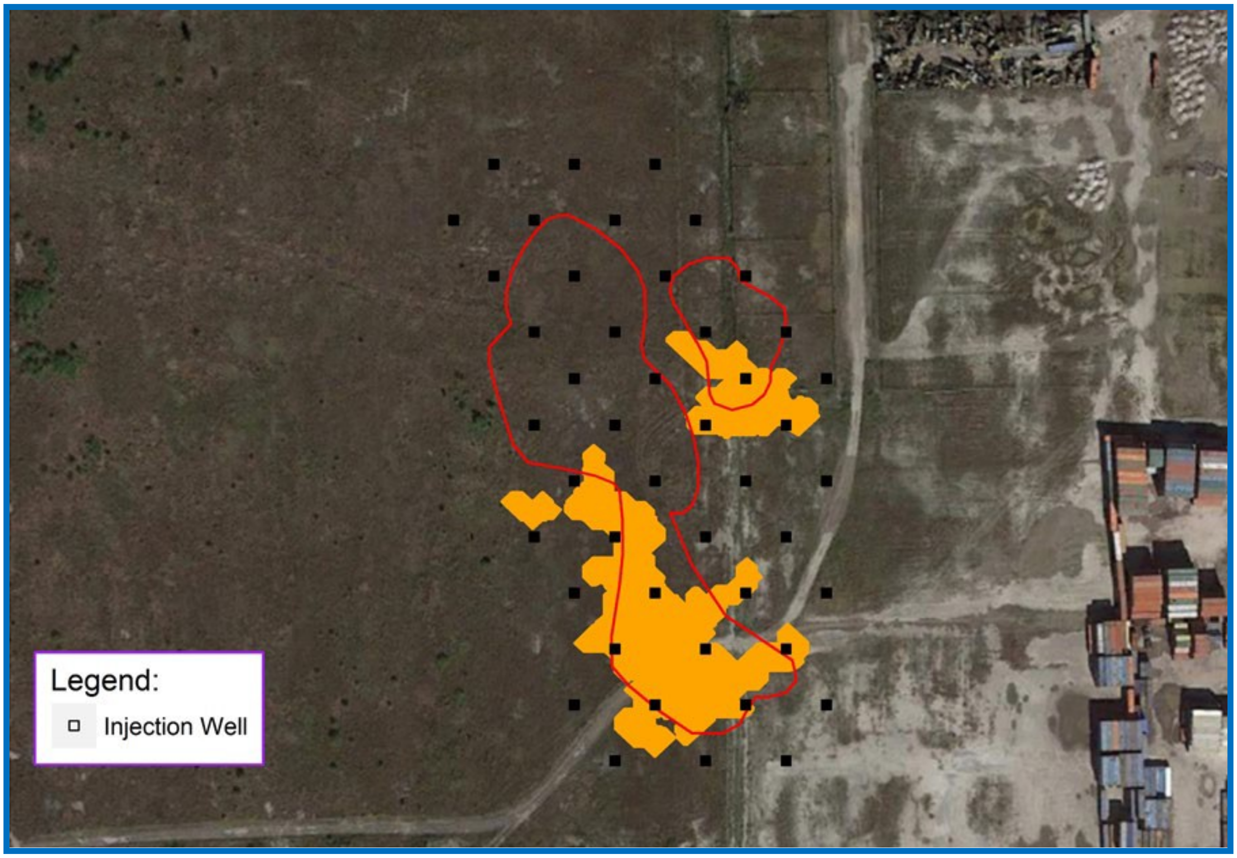

Figure 7-8: Team A VSD 2 source zone estimation and injection well locations

Building on the results presented for VSD 1, the potential benefit gained (reduction in remedy cost) by using the effective practice approaches for both source zone footprint and DNAPL mass was calculated by determining the additional cost required for investigation versus the reduction in remedy cost. Using a 12.5 m spacing of boreholes, the source zone footprint estimate is shown in Figure 7-9 (blue line). The cost of this additional investigation was $173,004. Based on the estimated footprint and using 200 boreholes per acre (inside the footprint) the 95% confidence interval on the DNAPL mass is 13,430 kg to 16,415 kg. The cost of investigation to achieve this estimate was $28,500.

Based on the conservative assumption that investigations returned an upper limit of 16,415 kg and using a factor of safety of 30 and the theoretical stoichiometry, an estimated lactate mass of 67,000 kg would be required. The Team A remedy was redesigned considering the revised source zone footprint and the updated lactate estimate. Total cost of the revised remedy was $2.53 M, resulting in a net cost savings of $2.80 M. The revised remedy achieved all POs but was still $1.04M more than the optimum remedy designed based on perfect information.

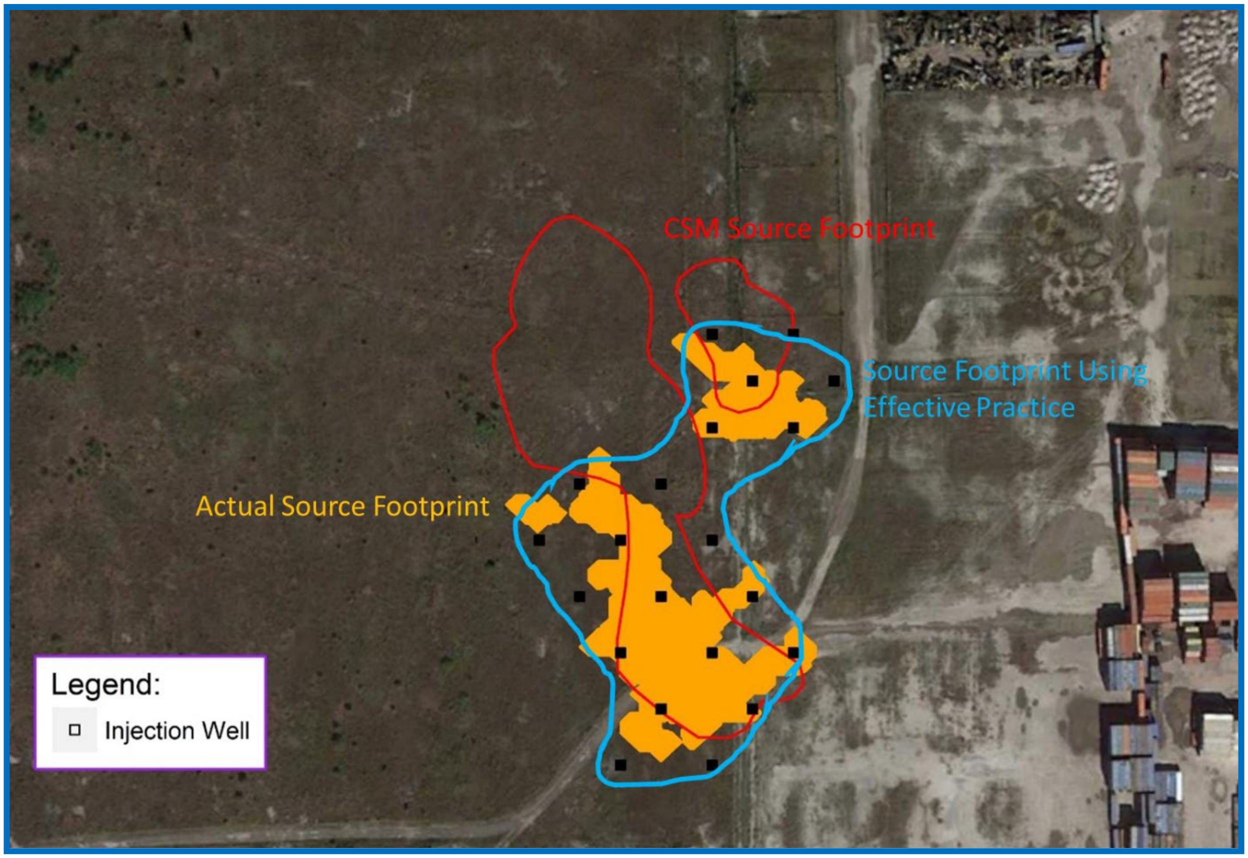

Figure 7-9: Redesign of Team A VSD 2 remedy based on updated source footprint and DNAPL mass estimate

7.4.3 Team A VSD 3

The process adopted for VSD 2 was repeated for VSD 3, using effective practice to estimate source zone footprint and DNAPL mass. The additional investigation costs were $221,540 for footprint investigations and $23,126 for DNAPL mass estimates. Team A underestimated the source zone footprint (Figure 7-10) and underestimated the DNAPL mass by 67%. It is unclear why Team A focused so much of their injection infrastructure on the plume downgradient of the source; this was removed in the redesign (Figure 7-11) and its removal did not affect the performance of the remedy.

The revised remedy achieved all three POs at a net cost reduction of $609,693. The revised remedy cost was still $820,000 more than the optimum remedy designed using perfect information.

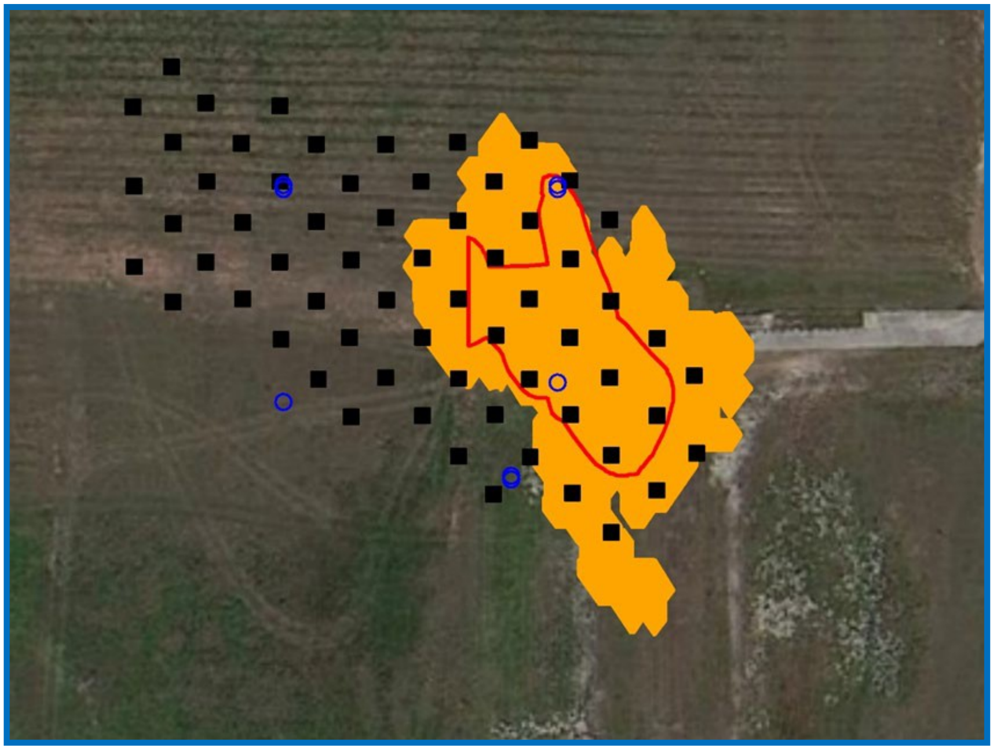

Figure 7-10: Team A VSD 3 source zone estimation and injection well locations

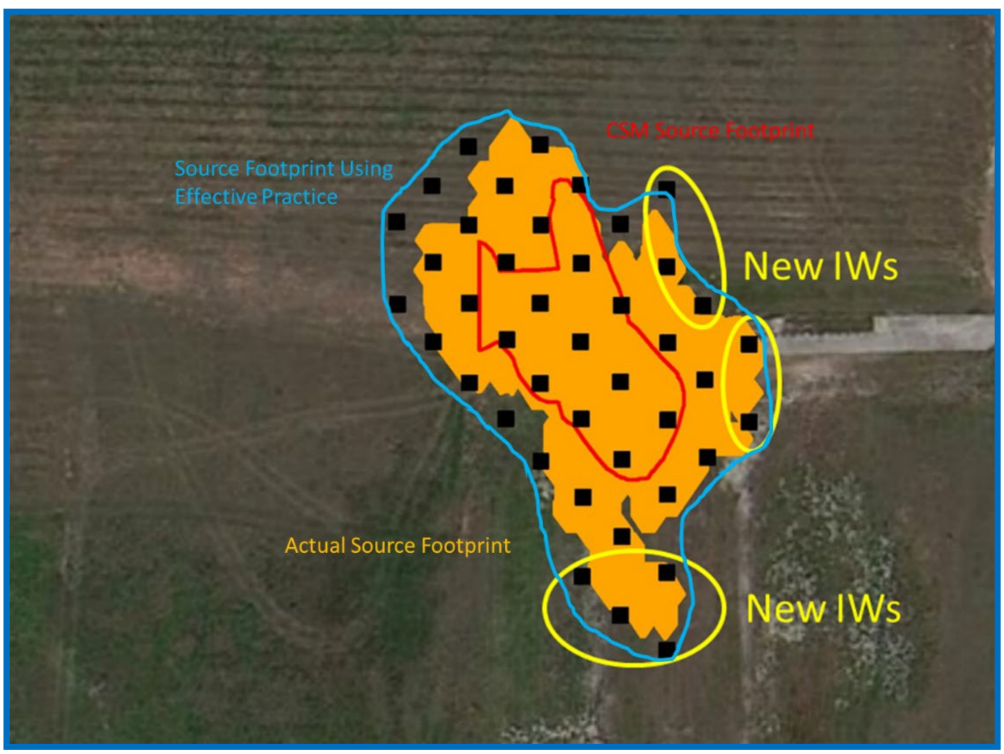

Figure 7-11: Redesign of Team A VSD 3 remedy based on updated source footprint and DNAPL mass

8 SUMMARY OF FINDINGS, CONCLUSIONS AND IMPLICATIONS FOR FUTURE RESEARCH/IMPLEMENTATION

The DIVER project has resulted in some significant insights into current practices being used to investigate and remediate contaminated sites. In addition, the project has revealed that (amongst the participants) poor interpretation of data was as widespread as limitations (e.g., acquired in the wrong place, not enough data collected, acquired in the wrong way) in the data itself when developing CSMs and translating those CSMs into remedial designs. The following sections synthesize the various findings of the DIVER project in a detailed assessment of the project objectives.

8.1 Summary of Findings and Achievement of Project Objectives

Objective #1: Evaluate the use of various site investigation tools and approaches as chosen and applied by experienced practitioners in the industry to generate more accurate CSMs through the lens of VOI considerations.

The original four DM Teams engaged in the DIVER project used a wide variety of site investigation tools and approaches to gather data for the generation of their CSMs. The DM Teams tended to follow similar approaches and use similar tools across the three VSDs. Even when presented with alternate approaches for estimating a parameter of a CSM (effective practice) the DM Teams did not uniformly adopt the practice, but rather attempted to incorporate some aspects of effective practice into their existing approaches. This suggests that a certain degree of "momentum of practice" is occurring, whereby practitioners continue to do what they were trained to do or what has worked for them in the past. The concept of what has worked in the past is somewhat uncertain in the environmental field as the ultimate goal post, no further action (NFA) is rarely achieved at groundwater contaminated sites (NRC, 2013; Clayton, 2017) and many sites continue through multiple investigation phases and five-year reviews of the remedy.

DM Teams (both the original four who investigated VSDs 1-3 and those added for VSD 4) made data analysis and interpretation errors that were unexpected given the senior nature of the practitioners. The most common error was the use of qualitative tools in a quantitative manner, e.g., attempting to correlate MIP readings to dissolved concentrations, as an indicator of the presence of NAPL, or to estimate CVOC soil concentrations. The most common consequences of attempting to use such correlations were inaccurate delineation of source zones and the subsequent inaccurate estimate of source mass. The use of MIP to delineate plumes, however, was appropriately done by the DM Teams. Other analysis errors included extrapolating DNAPL saturations (pooled versus residual) over large soil volumes based on borelog notations. In many cases the DM Teams acquired data in relevant locations but did not use the data in an effective manner, reducing the accuracy of the key parameters in the CSMs.

The majority of the DM Teams (with the exception of DM Team C) did not collect what experience and effective practice indicates would be a sufficient amount of data to develop accurate interpretations and estimations of key parameters (e.g., the average number of soil samples per DM Team per VSD was less than 30 and in 9 of 12 cases, 3 or fewer monitoring wells were used to estimate mass discharge). This may be due to a focus on keeping costs down (Team C's site investigation programs which were data dense were consistently the most expensive), however the low sampling density resulted in significant inaccuracies and uncertainty and coupled with data analysis errors resulted in large errors in aspects of their CSMs that translated to failed remedies or excessively costly remedies due to the large factors of safety required to achieve POs. In five of the 12 cases, even the use of a factor of safety over thirty could not overcome CSM limitations, especially for inaccurate estimates of source mass and mass discharge parameters.

No evidence was found that the DM Teams used the concepts of value of information in planning their investigation approaches. This is not surprising given the limited adoption of this concept amongst practitioners and the perceived difficulty of the concepts when applied to actual sites. Some form of decision-making was in evidence based on strategies employed following the initial mobilizations (each DM Team used an iterative approach with multiple mobilizations to collect data); however it was not possible to conclusively determine if this was entirely intuitive, based on the momentum of practice concept (e.g. either a confirmation bias or an anchoring bias) , or if some form of value of information assessment was performed (and not reported).

Objective #2: Develop effective practices for characterization of complex sites (including DNAPL sites) that increase accuracy and decrease uncertainty in CSMs in scenarios common to challenging DoD sites.

The wide-ranging approaches (and relatively poor outcomes) taken by the DM Teams to developing estimates for key parameters of the CSMs indicates there is no widely accepted standardized approach or effective practice in the industry for many facets of a CSM. This is despite a number of guidance documents specifically focused on DNAPL sites, mass flux estimation, and complex site investigation (EPA, 2010; EPA, 2018; ITRC, 2003). The DIVER project team used stochastic methods on the highly detailed data sets developed for the project to develop effective practice approaches combined with their collective experience at hundreds of sites for quantifying both magnitude and uncertainty of source zone footprint, DNAPL mass present in source zones, and mass discharge from source zones (Section 6 and Appendix A).

The proposed effective practice approach for source zone footprint involves an outside-in intrusive approach (DPT or drilling) starting on a bounding box known to be outside the source zone. The distance between grid lines and the spacing of investigation locations along grid lines are inversely proportional to the accuracy and cost and proportional to uncertainty. The approach progresses locations inwards from the bounding box until the source zone is found. Identification of the source zone must be through a primary method (visual confirmation, soil concentrations, DYE-LIF response, etc.) and not through a secondary method or correlation to a relative strength signal (i.e., MIP).

The proposed effective practice approach for estimating NAPL mass uses the source zone footprint approach as an input parameter but builds on that approach through intrusive investigations and quantitative measurements of DNAPL mass in soil. The approach uses the concept of bulk retention, whereby the DNAPL mass per individual soil core mass is found at a number of locations and then averaged across the estimated volume of the source zone. The proposed approach requires drilling within the source zone, which if not properly performed, can lead to short-circuiting of contamination and a worsening of the overall environmental impacts.

Appropriate techniques are available for drilling in suspected source zones; however, the risk must be carefully evaluated, and experienced drillers and investigation personnel utilized. All DM Teams in the DIVER project undertook drilling within the suspected source zones.

An effective practice approach was also developed for estimating source zone mass discharge, based on concentration measurements in a flux plane perpendicular to the direction of groundwater flow and estimates of groundwater flux (either via PFMs or measurements of hydraulic conductivity and hydraulic gradient). The general approach to the estimation of mass discharge using the flux plane concept is well documented in the literature and was incorporated into the proposed effective practice. Similar to literature approaches, in the proposed effective practice estimates of concentrations and groundwater flux at discrete locations are averaged across representative areas of the flux plane (i.e., transect) to arrive at a mass discharge estimate that encompasses the presumed spatial distribution of the source zone. Commercial tools exist to assist in the data analysis based on the fundamental approach (e.g., Mass Flux Toolkit).

Despite the volume of guidance in the peer-reviewed literature and in guidance documents, and the availability of free commercial packages to perform the analysis, in 50% of cases the DM Teams used qualitative data in their estimate of mass discharge and in only 25% of the cases did the DM Teams use a commercial software package. The DIVER team acknowledges that other methods for estimating mass discharge, such as integral pump tests, may be as accurate as the flux plane approach. However, these methods tend to be more complex and contain a greater window for errors than the flux plane approach. The effective practice approach developed from the DIVER project extends the existing approaches (see Objective #3) by examining the degree of uncertainty reduction with increasing data density (both lateral spacing in the flux plane and vertical spacing of measurements (screen length) within a monitoring location).

Objective #3: Quantify the value of additional information gathering for the estimate of some key parameters (source footprint and mass, source discharge, degradation rate) in Conceptual Site Models.

The highly detailed VSDs produced by the DIVER project provided a unique opportunity to develop effective practice guidelines for some key parameters. The DIVER VSDs allowed for stochastic assessment of each parameter with the goal of developing an effective practice for quantification as well as indications of the degree of uncertainty in the parameter estimate given a particular level of effort (e.g., how “close” can you expect to be to the actual DNAPL mass present after taking 100 “measurements”).

The return on investment when determining a source zone footprint using effective practice decreased rapidly as investigation spacing was reduced when applied to the VSDs in the DIVER project. In general, the expected accuracy of the estimate did not change significantly between borehole spacings of 6 m and 12 m. However, the average cost of investigation increased by almost a factor of four between 12 m and 6 m spacings (indicating little additional value for the additional cost). The most critical finding in terms of source zone footprint is that using effective practice provides a primary line of evidence-based estimate at reasonable cost which was superior (in terms of cost and/or accuracy) to that of the DM Teams.

The value of additional information (gathered using effective practice) in terms of quantifying the DNAPL mass present at a site did not show as distinct a threshold as source zone footprint. Expected accuracy (based on random sample locations) increases rapidly with additional investigation locations such that the 95% confidence interval for a +/-20% estimate is reached at less than 100 sample locations per acre in all VSDs. Use of effective practice by an experienced practitioner (selection of locations as opposed to random locations) demonstrated that +/- 20% could initially be achieved in fewer boreholes, however the accuracy decreased (compared to random location selection) with increasing numbers of boreholes before converging to the correct answer at a very large number of boreholes. This implies that, provided effective practice has been used to identify the source zone footprint, random sample locations (or sampling on a grid) using effective practice is likely to be as accurate as locations chosen by an experienced practitioner with access to sequential sample results.

Significant theoretical and field-based research has been undertaken on approaches to the measurement of mass flux (e.g., Brooks et al. (2008), Kubert and Finkel (2006), CRCCARE (2016), ITRC (2010)), however little of the published research has examined the value of information concept applied to the use of mass flux in remedial decision analysis. The DIVER project applied the methodology of Kubert and Finkel (2006) to the VSDs generated as part of the project. When applied to the sites in the DIVER project, the accuracy of estimates of mass discharge were highly accurate (+/- 10%) at a lateral well spacing of approximately 5 m. All estimates across all VSDs and all well spacings were within +/- 50% of the actual value. The use of effective practice is more important than the quantity of data collected provided measurement locations along the flux plane are on the order of 10 m or less.

Objective #4: Compare and evaluate stochastic and deterministic approaches to remediation design based on a common CSM.

Overall, except for DM Team A, the performance of the DM Teams at meeting remedy POs was poor. DM Teams B, C, and D met only nine of 27 POs across the three VSDs. Not meeting the POs was clearly linked to deficiencies in the CSMs developed by the teams. DM Team A achieved their success at meeting the POs not through more accurate CSMs, but rather by using a very significant factor of safety in design (with associated high cost compared to optimum remedy) of the EISB remedy.

A significant portion of the work performed on the DIVER project involved examining the performance of a stochastic approach (SCOToolkit) to remediation design. Stochastic modeling approaches can make a key contribution to decision making for groundwater remediation, especially given the limitations of more traditional deterministic approaches identified in this project. Stochastic modeling offers enhanced capacity to identify the most influential parameters on the calibration and predictive simulations, informing potential priority areas of improvement for the model and site characterization. Stochastic modeling is not limited to applications in the most complex systems, rather it is expected that these approaches should be applied where enhanced understanding to determine the most important parameters for the predictions of interest is required, whether model calibration is highly dependent on these parameters and whether those parameters are adequately characterized.

Stochastic approaches should not be expected to overcome inadequate or poor site characterization. The DIVER project clearly demonstrated the garbage in garbage out (GIGO) principal in this regard, whereby history-matching calibration, multiple realizations, and optimization using SCOToolkit could not overcome the inherent errors in the CSM provided as the basis for remediation design. During model calibration with SCOToolkit, significant changes from priors to posteriors were observed for many parameters (Section 5.3.2), indicating the inadequate nature of the priors, that is, inaccurate estimates of key CSM parameters. In addition, the parameter changes during calibration were, in most cases, still not enough to allow SCOToolkit to find a realistic optimized remedial design.

DM Team A and VSD 1 provide an illustrative example. The actual, prior, and posterior values for key parameters are provided in Table 8-1. In all cases calibration pushed the parameters in the direction of the actual values (overcorrecting for source mass and velocity) implying a better CSM than the one used by DM Team A in their remedy design. However, SCOToolkit could find a solution that achieved all POs in only 2% of the realizations, compared to DM Team A that achieved all POs. The optimum SCOToolkit remedy (limited data set given that a remedy was found in only 2% of the cases) injected 42,173 kg of lactate over 2.27 years as compared to the 246,634 kg of lactate injected by DM Team A over 5 years.

Table 8-1: Priors, posteriors, and actuals for DM Team A VSD1 CSM

Parameter	Prior	Posterior	Actual
Source Discharge (kg/day)	2.62	0.59	0.38
Source Mass (kg)	6,060	16,167	10,160
Degradation Coefficient (day^{-1})	0.001	0.015	0.14
Velocity (m/yr)	7.3	4.0	6.2

The stochastic approach using the SCOToolkit also struggled to find remedies to meet POs (achieved POs in 52% of realizations) even when given an accurate CSM based on access to perfect information. The performance of the optimal remedy as identified by SCOToolkit was challenged by the source mass reduction objective due to uncertainty in the source mass (high standard deviation in the posterior value), rather than source mass discharge and plume concentration objectives that were met in a high proportion of model realizations. While parameter variability is considered by SCOToolkit, the spatial distribution of variable parameters, that likely contributed to the differences between the SCOToolkit and DIVER Team optimal solutions, is not. SCOToolkit is a powerful tool for optimization of remedy design at sites with long temporal datasets for many observation points. It is desirable for linear regression to have at least 5 times the number of calibration data points as calibration parameters. Given that SCOToolkit has up to 17 calibration parameters a minimum of 85 calibration points would be required (Parker et al., 2018).

SCOToolkit allows the use of uniform fully screened upgradient injection galleries for EISB remedy design. This potentially limited the comparison of experienced-based and stochastic remedy design given the multiple different approaches (single time direct injection, injection into the source itself, cyclical injection through wells at different elevations) used by the DM Teams. This potential limitation was not tested however, given the lack of success of the DM Teams at reaching POs in cases where remedy designs not available in SCOToolkit were used.

Objective #5: Investigate the relationship between CSM deficiencies, remediation designs and remediation outcomes.

Assessment of the twelve CSMs from the original DM Teams found that 64% of the individual CSM parameters were within a factor of 3, and 92% were within a factor of 10. It is difficult to determine the importance of a factor of 3 error versus a factor of 10 error in an absolute sense. It is likely the importance will be different for each parameter, for the end use of each parameter (e.g., remedy design versus risk assessment) and at individual sites.

Correlating CSM deficiencies and remedy deficiencies illustrated the key linkages between the two factors. For the EISB remedy implemented in this project, poor estimates of DNAPL mass and source zone footprint were directly linked to failure to meet POs following remedy implementation. Other CSM deficiencies such as inaccurate values of groundwater velocity, plume age, and source zone mass discharge were also linked to failures of the remedy. DM Team D used the performance monitoring period to revisit their CSM and optimize their remedy design, which led to better performance (in terms of meeting the POs) but did not achieve all three POs. Modifying a remedy design during implementation of the remedy (as compared to achieving a more accurate CSM prior to remedy design) is challenging given the changes imparted to the system by the remedy itself and can result in significant additional cost and time penalties.

The CSM deficiencies that led to not meeting remediation outcomes were identifiable from the data collected by each DM Team during their site investigations. In many cases the DM Team's estimates for key flow and transport parameters were inconsistent with the data (e.g., source discharge vs. groundwater velocity vs. plume length). Simple analytical modeling would have provided screening-level evaluations of key flow and transport processes that would have identified inconsistencies between the CSM parameters, and the data collected. Improved descriptions of the distributions of inherently variable or uncertain parameters could have been obtained through integration of modelling approaches with CSM development, a path that would have required additional resources to support the Teams efforts. Working under a fixed price contract may have limited the options for application of even simple modeling tools.

Modeling, and in particular model calibration, is not an antidote to inadequate or poor site characterization. Where a model demonstrates that best available estimates of key flow and transport parameters are inconsistent with observation data (concentrations, mass discharges etc.), the conceptual model should be re-evaluated before progressing to more advanced modeling and/or remedy design. There was no indication this step was performed by any of the DM Teams in this work.

Objective #6: Assess remedial design optimization based on life cycle costs under conditions of inaccurate CSMs using a value of information approach.

The exploration of the correlations and relationships between CSM costs/accuracy and remediation costs/success (in the context of life cycle costs) demonstrated there was no relationship across Teams and VSDs, and any general conclusions are limited by large factors of safety applied by some Teams to the EISB remediation design (that overcome CSM limitations) as well fundamental errors arrived at through application of investigation or analysis approaches that are not considered effective practice leading to inaccurate CSMs. .

Each of the DM Team's remediation designs and performance were assessed considering both remediation design success and failure and CSM accuracy. Five possible endpoints were identified:

- Success at reasonable cost (0 of 12 designs)
- Success at excessive cost (3 of 12 designs)
- Failure based on bad interpretation of good data (4 of 12 designs)
- Failure due to poor CSM (5 of 12 designs)
- Design failure (0 of 12 designs)

Each of the three "success at excessive cost" end points (DM Team A for all VSDs) was analyzed in detail by revising the CSMs based on use of effective practice on the source footprint and DNAPL mass parameters. The remedy designs were modified by adding additional injections wells to newly "discovered" areas of the source zone and scaling the lactate mass to the new DNAPL mass estimate. In all cases POs were achieved at lower remedy costs, and the savings in remedy cost offset the additional site investigation costs (Table 8-2).

Table 8-2: Remediation return on investment of site investigation costs

VSD	Team A Designed Remedy Cost	Additional Investigation Cost Using Effective Practice	Revised Remedy Cost Considering Effective Practice Information	Remedy Cost Savings	Return on Site Investigation Investment
1	\$3.36M	\$0.45M	\$2.31M	\$1.05M	1.3x
2	\$6.34M	\$0.20M	\$2.53M	\$3.81M	18.0x
3	\$5.07M	\$0.25M	\$3.46M	\$1.61M	5.4x

9 CONCLUSIONS

As discussed in the introduction and in Chapter 3, VOIA has not been widely used by remediation practitioners for a variety of reasons. However, VOIA is a very powerful conceptual framework for decision making, even though the underlying statistical principles may be well beyond most practitioners. In an ideal hypothetical future, it may be possible to predict more precisely the exact value of any additional site characterization data on the final outcome of a remedial pathway of a complex decision tree model. This would require accurate models at an appropriate scale of the underlying geology and hydrogeology, the rate of all biogeochemical processes controlling the fate of the chemicals of concern, distribution and speciation of those same chemicals, and the rates of transformations achieved by all applicable physical, chemical or microbially -mediated processes in the subsurface. This scenario is beyond current technical capabilities and requires such a massive amount of data that the likelihood of success is low. Alternatively, artificial intelligence and machine learning using large data sets of performance data for remedial technologies applied at many thousands of sites with similar chemicals could provide algorithms that would allow for computer simulations to make the VOIA component of decision tree models a common tool for remedial decision making. We consider the DIVER project as a very early-stage entry towards a more accurate basis for applying VOIA to the overall remedial decision framework.

Returning then to the conclusions from the results of the DIVER project, we provide the following observations, conclusions and recommendations for future research.

1. **The DIVER Project successfully created a virtual infrastructure that provided a digital environment capable of virtual investigations of hypothetical but realistic geological and contaminant distribution models.**

2. **The mixed outcomes by experienced practitioners of creating accurate CSMs for key parameters influencing design of in-situ technologies such as EISB reflected subsurface heterogeneity, insufficient density of subsurface testing, and some poor data interpretation.**

3. **Value of Information analyses showed that application of the effective practices developed in part from virtual interrogation of "perfect data" created for the project resulted in significant improvements in CSM accuracy for the parameter, DNAPL source mass, DNAPL footprint and source mass discharge.**

4. **VOIA has not been widely used by remediation practitioners for a variety of reasons. However, VOIA is a very powerful conceptual framework for decision making, even though the underlying statistical principles may be well beyond most practitioners.**

5. Remedial decisions to address groundwater contamination fall in the category of "noisy" problems (Kahneman, et al, 2020).

We found surprisingly little agreement between the various expert teams investigating four different "case studies", namely the four VSDs that formed the basis of the virtual investigations and the subsequent performance of the EISB technology. While the DM teams made some reasonable estimates of CSM parameters, only one of the DM teams succeeded in meeting all remediation POs in all three of the VSDs. This result is due in part to the heterogeneous nature of subsurface environments, and the non-random distribution of system properties. The same experts with similar levels of experience all arrived at very different outcomes analyzing the same problem, a characteristic of "noisy" decision, analogous to medical diagnoses. This clearly highlights the difficulties in developing correlations for algorithms that can be generalized using a small data set.

6. The assumption that a higher investment in site investigations would result in lower remediation costs proved unfounded.

It is generally perceived intuitively that more data will lead to a better outcome for remedial decisions. DIVER has shown clearly that more data will only lead to this outcome if the right tools are applied, and the data are properly evaluated with a focus on those parameters in a CSM that have the largest impact on remedial outcomes.

7. For DNAPL impacted sites, applying effective practice for estimating DNAPL mass, source zone footprint, and mass flux from source areas will reduce life cycle costs and increase probability of meeting POs.

The primary error made by most DM teams was an inaccurate estimate of these parameters, leading to either unsuccessful implementation of the EISB remedy, or an overly costly remedy with excessive amounts of electron donor, that is, an excessive safety factor in design, as well as unnecessary injection wells. The effective practice method proposed here should lead to reduced life cycle costs at DNAPL sites.

8. A small data set was the main constraint on developing the types of correlations that would be the fundamental basis of a general methodology for applying VOIA to remedial decision making.

While the DIVER project generated a very large amount of data considered as "perfect information" for four DNAPL release sites, the variability in the virtual investigation results did not provide sufficiently robust correlations between the level of data acquisition and the performance outcome of applying EISB to the problem. The VSD data sets, however, have significant value for generation of a larger set of correlations through use as a training tool, as presented in the related TEMPO project (ER-201566-T2).

9. Application of the SCO Toolkit proved problematic due to inherent limitations of using analytical models to simulate complex subsurface environments.

The stochastic approach using the SCOToolkit also struggled to find remedies to meet POs (achieved POs in 52% of realizations) even when given an accurate CSM based on access to perfect information. While parameter variability is considered by SCOToolkit, the spatial distribution of variable parameters, that likely contributed to the differences between the SCOToolkit and DIVER Team optimal solutions, is not. SCOToolkit is a powerful tool for optimization of remedy design at sites with long temporal datasets for many observation points. It is desirable for linear regression to have at least 5 times the number of calibration data points as calibration parameters. Given that SCOToolkit has up to 17 calibration parameters a minimum of 85 calibration points would be required (Parker et al., 2018). Furthermore, the usefulness of stochastic approaches cannot be expected to overcome inadequate or poor site characterization which usually results in inaccurate estimates of key CSM parameters and selection of inappropriate remedial actions.

10 FUTURE RESEARCH

While the goal of a universal set of algorithms to predict the performance of in-situ technologies at DNAPL impacted sites is still elusive, the DIVER project has shown that future research should focus on building more extensive data bases from real world sites combined with application of machine learning tools to develop the appropriate algorithms for better decision making in site remediation. The limits of modeling such complex systems were illustrated by the testing of the SCOToolkit to compare theoretical tools to experienced based rules of thumb.

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Appendix A

Effective Practice Guides

The following are effective practice guidance documents containing recommendations for approaches to obtaining and analyzing data, based in part on the results of the virtual site assessments, and in part, based on industry experience and team knowledge on best practices for CSM development at DNAPL impacted sites.

Attenuation Rate Constants

Attenuation rate constants for contaminants dissolved in groundwater.

Importance for EISB Remediation and Decision Making

- Attenuation rates provide information on the existing contaminant attenuation as either a function of time or distance as well as an estimate for potential lag times for EISB treatment programs and remediation timeframes.
- This information is required for system design to support microbial efficiency such as injection well spacing, amendment requirements, total volume of bioaugmentation culture (if needed) and injection frequency.

Tool Selection

Different tools and methods exist to estimate attenuation rate constants. Depending on available data and project timelines, Effective Practice can include multiple tools/methods:

- Long-term groundwater concentration data from single wells;
- Groundwater concentration data along the centerline of plume;
- Solute transport models;
- Microcosm studies (laboratory);
- Field pilot studies;
- Compound specific isotope analysis (CSIA) using Rayleigh model, where applicable.

Strategy

Methods for evaluating attenuation rate constants are well described elsewhere, as presented in the key references. In addition, there are several emerging tools and methods that have the ability to more accurately estimate *biodegradation* rates exclusive of physical processes. While different methods provide useful information on attenuation, at minimum, Effective Practice should involve calculating degradation rate constants via Method #1 or #2 (below) to understand plume duration (i.e., source strength over time) and remediation timeframes for EISB design and Method #3 (below) to provide biodegradation rates more conclusively.

- Method #1: Point Attenuation Rates – Natural logarithm concentration vs. time plots;
- Method #2: Bulk Attenuation Rates – Natural logarithm concentration vs. distance along plume centerline;
- Method #3: Biodegradation rates (exclusive of physical processes such as advection, dispersion, etc.).

Data Analysis

Method #1: Point Attenuation Rates

- Calculate rate constants derived for a single well over time using a linear best-fit regression and determining the slope of the line. At minimum 6 time-points should be used for statistical relevance.
- Calculate these rate constants from multiple wells over the entire plume and evaluate range of attenuation rates.
- Assess general trends of multiple wells over the entire plume to understand overall plume attenuation and plume trends (steady, regressing, etc.).
- Compare these rate constants against those calculated via another method and/or those reported in the literature to provide context for the results.

Method #2: Bulk Attenuation Rate (following Newell et al. (2002) methods)

- Perform a linear regression and then multiply the slope by the groundwater velocity divided by the retardation factor to get the rate constant, or
- Perform tracer studies – adjust contaminant concentration comparison to existing tracer data and then calculate a bulk attenuation rate.

Method #3: Biodegradation rates

- Calibrate a solute transport model by adjusting the rate constant; or
- Use CSIA data incorporated in the Rayleigh model for a single well over time or between two wells at multiple locations along a hydraulically connected transect in the direction of groundwater flow.

Limitations and Sources of Uncertainty

- Methods #1 and #2 provide attenuation rates that include both physical and chemical/biological processes such as dispersion, sorption/desorption, advection and degradation/transformation processes;
- Tools and methods to obtain attenuation rates and/or determine biodegradation rates specifically often require multiple sampling rounds and potentially longer periods of time for assessment;
- Laboratory methods such as microcosm studies need to be conducted carefully to ensure conditions applicable to those in the field;
- Specialized analytical methods, such as CSIA, provide degradation rates more specifically but may not be an available dataset for the site (and are currently not available in DIVER).

Key References

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Source Delineation

The spatial extent (laterally and vertically) of the Confirmed/Probable and Potential DNAPL source zone

Importance for EISB Remediation Design and Decision Making

- Delineating the DNAPL footprint is required to understand the boundaries of the DNAPL source zone and develop the target area and volume for treatment, and forms the basis for the DNAPL mass estimate.
- Treatment zone volume affects capital investment for injection and monitoring well installation and volume of substrate to be injected.
    - Underestimation leads to underestimation of costs and poor performance of the program.
    - Overestimation leads to over-design and greater than required costs.

Tool Selection

Effective Practice involves the use of multiple lines of evidence to delineate the source zone volume within an acceptable degree of accuracy. The following information and tools could be included in the lines of evidence approach:

- Visual screening of all soil cores for observations of DNAPL and sampling monitoring wells for DNAPL;
- Compare measured concentrations in soil obtained from core to calculated thresholds (both 5% DNAPL saturation threshold and partitioning threshold);
- Historical evidence of DNAPL use, storage, handling and disposal;
- Hydrophobic dye testing of soil samples at locations informed by PID readings;
- Groundwater sampling and chemical concentration analyses;
- DYE-LIF optical screening tool (in conjunction with evidence from above tools);
- MIP screening tool (in conjunction with evidence from above tools).

Strategy

The following strategy is recommended:

- Once DNAPL presence has been established, lateral and vertical delineation should be performed.
- An initial estimate of source zone width can be obtained by determining the width of the dissolved phase plume downgradient of the suspected source.
    - Warning: Determination of the width (e.g. using a flux plane) at a location that is not downgradient of the source zone may result in an underestimation of the source zone width if additional lateral migration of DNAPL has occurred downgradient of that plane.
- The upgradient extent of the DNAPL source zone can be initially estimated by low concentrations of the dissolved phase in groundwater samples.
    - Warning: Given the nature of DNAPL migration it is possible that a narrow "finger" of DNAPL exists that is not captured in a coarse resolution of sampling points.
- The upper and lower extent of the DNAPL source zone can be estimated by determining the upper and lower extent of the dissolved phase plume downgradient of the suspected source.
    - Warning: Geologic controls on groundwater flow must be considered (e.g., a diving plume may result in a deeper estimate of DNAPL source extent).
- Initial delineation via plume dimensions will tend to produce a "box" shape which is not realistic – however is a useful first estimate. Depending on the density of the data collected, it is appropriate to place a factor of safety on the size of the bounding box.
- Following the above steps, employ various tools within the estimated source zone (see Tool Selection above).
- The process of determining a DNAPL mass estimate should be performed in conjunction with the delineation of the source zone. Locations of cores for DNAPL mass calculation should be based

on the current understanding of the extents of the DNAPL source zone, and the results of the analysis of the cores should be used to refine the extents of the DNAPL source zone.

Data Analysis

Kueper and Davies (2009) recommend delineating the DNAPL source zone into Confirmed/Probable and Potential regions. For the purposes of the DIVER project, it is recommended that a single region be determined, based on the best estimate of the actual DNAPL source extents (Confirmed/Probable). Note that not all 'Tools' need necessarily be employed at any particular site. Some tools may be more effective than others depending on budget, contractor availability and geologic conditions.

Limitations and Sources of Uncertainty

Given the nature of DNAPL migration, it is not feasible to determine the exact location and extent of individual DNAPL migration pathways within the overall confines of the source zone. Because data collection efforts typically involve a finite number of local-scale measurements taken at discrete locations, some uncertainty will exist regarding the delineated spatial extent of the source zone (Kueper and Davies, 2009). An expectation of the uncertainty, based on the DIVER project, is shown in Figure 1.

Identification of the downgradient edge of the DNAPL source zone is often the most difficult, given the existence of a high concentration plume. It is recommended that a significant portion of the effort of additional delineation be spent on this region.

Identification of closely spaced but separate DNAPL source zones is also often difficult, particularly if the plume from an upgradient source overlaps with the plume from a downgradient source. If historical records indicate the potential for multiple release locations, effort should be made to delineate the "clean-space" between sources. Note this may not be required in all situations, and the need should be evaluated based on the remediation goals for the site. For some remedies, significant cost savings are possible if separate DNAPL source zones are identified and adequately delineated.

Key References

Kueper, B.H. and Davies, K.L., 2009. Assessment and Delineation of DNAPL Source Zones at Hazardous Waste Sites. United States Environmental Protection Agency, EPA/600/R-09/119.

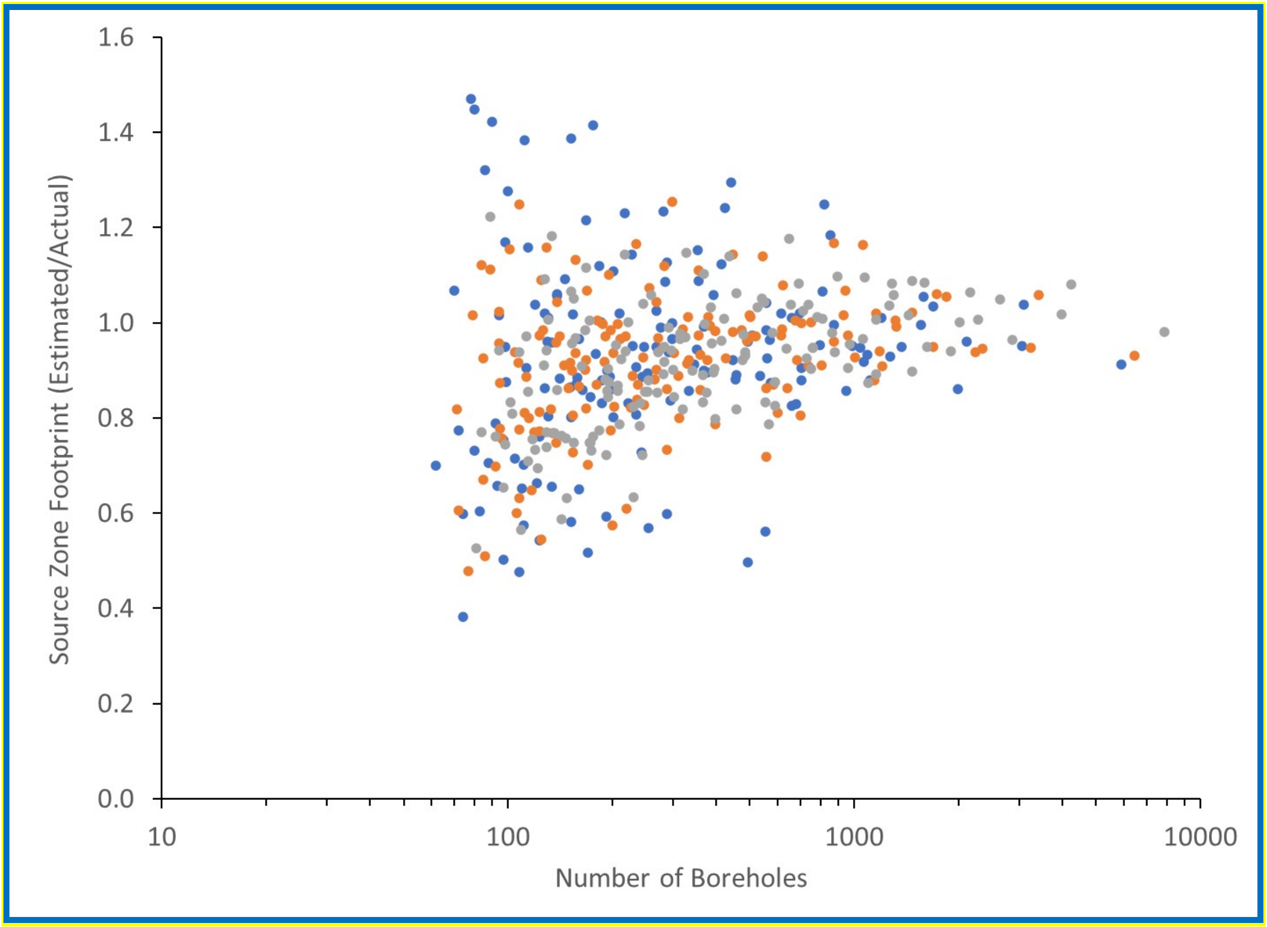

Figure 1: Expectation of Source Footprint Uncertainty Based on Sites in the DIVER Project

DNAPL Mass

Source zone DNAPL mass estimate.

Importance for EISB Remediation Design and Decision Making

Contaminant mass reduction during EISB within DNAPL source zones works via enhanced dissolution of the DNAPL and desorption of the DNAPL/sorbed phase mass, and biodegradation in the water phase.

- DNAPL mass estimates are critical for estimating nutrient and electron donor mass required to reduce DNAPL mass, and estimate longevity of source treatment.

Strategy

A bulk retention capacity approach is recommended, informed by multiple soil cores. The preferred approach should:

- Obtain full length undisturbed cores within the Confirmed/Probable and Potential DNAPL source zone footprint;
- For each core, screen for visual observations of DNAPL, high PID readings and positive dye tests;
- Obtain laboratory soil concentrations for intervals of suspected DNAPL;
- Calculate DNAPL saturations from laboratory soil concentrations;
- Calculate bulk retention capacity for the full-length core using DNAPL saturations assuming no DNAPL is present in regions where no indicators were present;
- Obtain multiple cores and average the bulk retention capacity;
- Apply the calculated average bulk retention capacity to the determined source volume to estimate DNAPL mass.

Correlations of MIP data to DNAPL saturations results in large and unpredictable errors, do not constitute Effective Practice, and are **<u>not recommended</u>**.

Figure 1 depicts the accuracy of the DNAPL mass estimate using Effective Practice as a function of number of core locations for one investigation of one of the sites in the DIVER project. It should be noted that this accuracy/performance is not guaranteed with the implementation of Effective Practice.

Tool Selection

A combination of high resolution tools and sampling methods is required.
Recommended tools include:

- Soil borings, undisturbed soil sampling, chemical analysis of soil and subsequent calculation of DNAPL saturation from concentrations in soil (or, alternatively, laboratory measurement of saturations);
- Soil screening tools (PID, dye testing);
- Measurement/ knowledge or estimate of site-specific parameters (porosity, foc);
- Historical release records, if available.

Data Analysis

The approach requires an estimate of the overall volume of the DNAPL source zone, which is obtained via approaches outlined for DNAPL delineation. The source zone volume should be updated based on information collected during coring to estimate DNAPL mass. The Uncertainty Relationship figure (Figure 2) presents the "estimate bound envelopes" based on the results of the DIVER project to assign likely error bars to the estimate.

Limitations and Sources of Uncertainty

Given the nature of DNAPL migration, estimates using Effective Practice will always contain a significant degree of uncertainty due to (for example):

- Identification of DNAPL presence in a soil core – most approaches likely introduce bias (e.g. visual observation misses regions of core with low DNAPL saturations);
- Method is dependent on estimate of DNAPL source zone volume;
- Variable DNAPL composition within source zone introduces uncertainty when averaged across the source zone;

Key References

Kueper, B.H. and Davies, K.L., 2009. Assessment and Delineation of DNAPL Source Zones at Hazardous Waste Sites. United States Environmental Protection Agency, EPA/600/R-09/119.

Kueper, B.H., Stroo, H.F., Vogel, C.M., and C.H. Ward. Chlorinated Solvent Source Zone Remediation, SERDP-ESTCP.

Pankow, J.F., and J.A. Cherry. 1996. Dense Chlorinated Solvents and other DNAPLs in Groundwater, Waterloo Press, Portland, Oregon, USA.

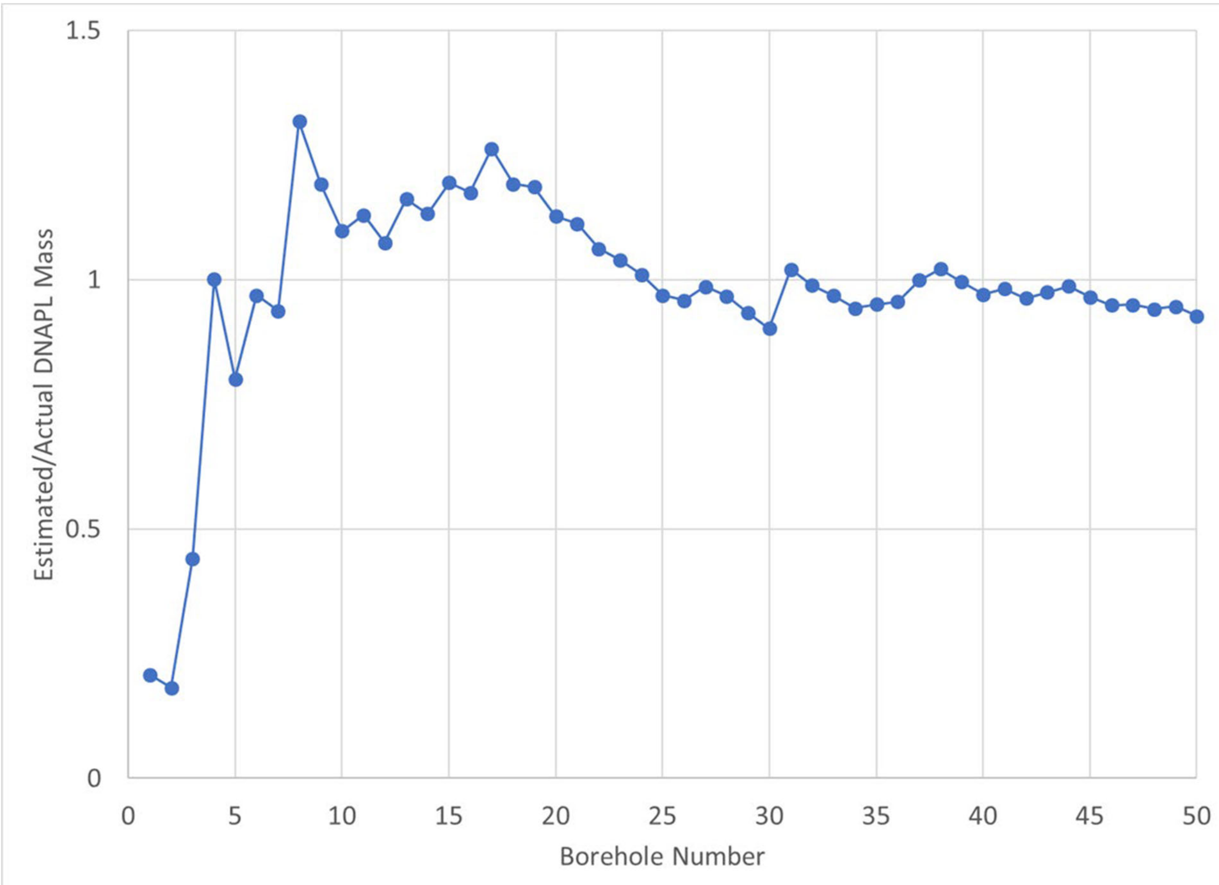

Figure 1: DNAPL Mass Estimate Accuracy Using Effective Practice as a Function of Number of Core Locations – Expert User

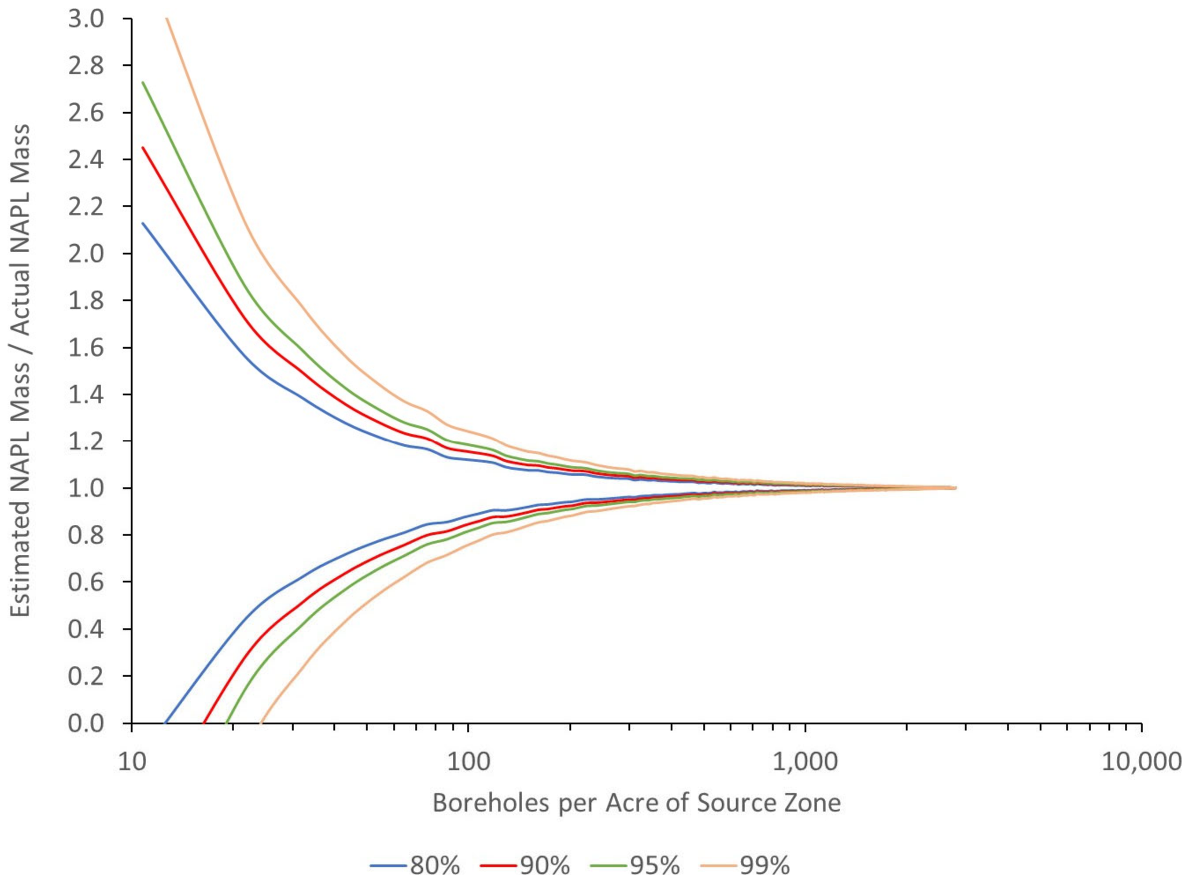

Figure 2: Estimate of Uncertainty Using Effective Practice Approach as a Function of Number of Core Locations

Source Mass Discharge

Total mass of dissolved chemical of concern per time discharging from the source zone

Importance for EISB Remediation Design and Decision Making

- Source mass discharge provides an understanding of the strength of the mass moving through the groundwater per unit time in the direction of groundwater flow.
- This information dictates optimal well placement for performance monitoring and provides baseline data for reduction targets, expected remedial efficiency and timeframes to achieve goals.
- The source mass discharge and required reduction to achieve remediation goals impacts estimated doses of electron donor and nutrients.

Tool Selection

Effective Practice for mass discharge involves estimation through vertical "planes" (discharge planes) or transects located some appropriate distance downgradient of the source zone. A discussion of alternate approaches (and their limitations) to estimating mass discharge can be found in ITRC (2010) and CRC Care (2016). Mass discharge estimates through the discharge plane approach are dependent on estimates of groundwater flux (based on hydraulic conductivity and hydraulic gradient measurements) and spatial density of concentration measurements.
Different methods are possible for data collection within the discharge plane approach:

- Approach #1 - Multilevel wells (short screen, nested wells) with estimates of hydraulic conductivity for each screen and an estimate of hydraulic gradient across the plane;
- Approach #2 - Passive flux meters (PFMs);
- Approach #3 - Hydraulic Profiling Tool and Groundwater Sampler

Strategy

The following strategy is recommended:

- Determine the discharge plane location based on the downgradient extent of the DNAPL source. The plane should be located close enough to the downgradient of edge of the source zone such that biodegradation is not significantly impacting estimates, but not intersect the source zone itself;
- Determine the width and vertical thickness of the plume to bound the discharge plane;
- Monitoring points should extend vertically and horizontally to the edges of the discharge plane;
- If using Approach #1 or #3:
  - Determine the hydraulic gradient across the plane via up- and downgradient monitoring wells. Uncertainty can be reduced by obtaining multiple local values of hydraulic gradient and applying them to the appropriate location in the plane;
  - Determine hydraulic conductivity for each point where a concentration measurement is made.
  - An estimate of statistical variance of the hydraulic conductivity in the plane (both laterally and vertically) should be developed to guide the spacing of measurements.

Data Analysis

Lateral spacing of measurement points influences the accuracy of the mass discharge estimate. The impact of lateral spacing developed during the DIVER project for the recommended approaches is depicted in Figure 1. For detailed explanation of calculations and data analysis please consult the key references provided in the references section.

Limitations and Sources of Uncertainty

Some considerations when collecting data and implementing Effective Practice:

- Data from HPT is semi-quantitative; therefore, measurements should be calibrated to site-specific measurements conditions using slug or packer testing in a subset of monitoring wells to estimate hydraulic conductivity.
- Results from PFM deployments include assumptions on the deviation of the local flow-field due to the presence of the PFM that results in a degree of uncertainty in each data point that should be considered.
- Results from the uncertainty relationships derived in the DIVER project indicate no difference in mass discharge predictions based on vertical screen length, as long as the entire plane (in the vertical direction) is screened. This may be due to the geology, source distribution, and flow fields in the sites used to develop the relationships.
- Correlations of concentration to MIP data are highly inaccurate as inputs to an estimate of mass discharge and do not constitute Effective Practice.

Key References

ITRC, 2010. Use and Measurement of Mass Flux and Mass Discharge.

CRC Care, 2016. CRC CARE Technical Report 37: Flux-based Groundwater Assessment and Management.

Guibeault, M.A., Parker, B.L., and J.A. Cherry, 2005. Mass and Flux Distributions from DNAPL Zones in Sandy Aquifers, Ground Water, Vol 43, pgs. 70-86.

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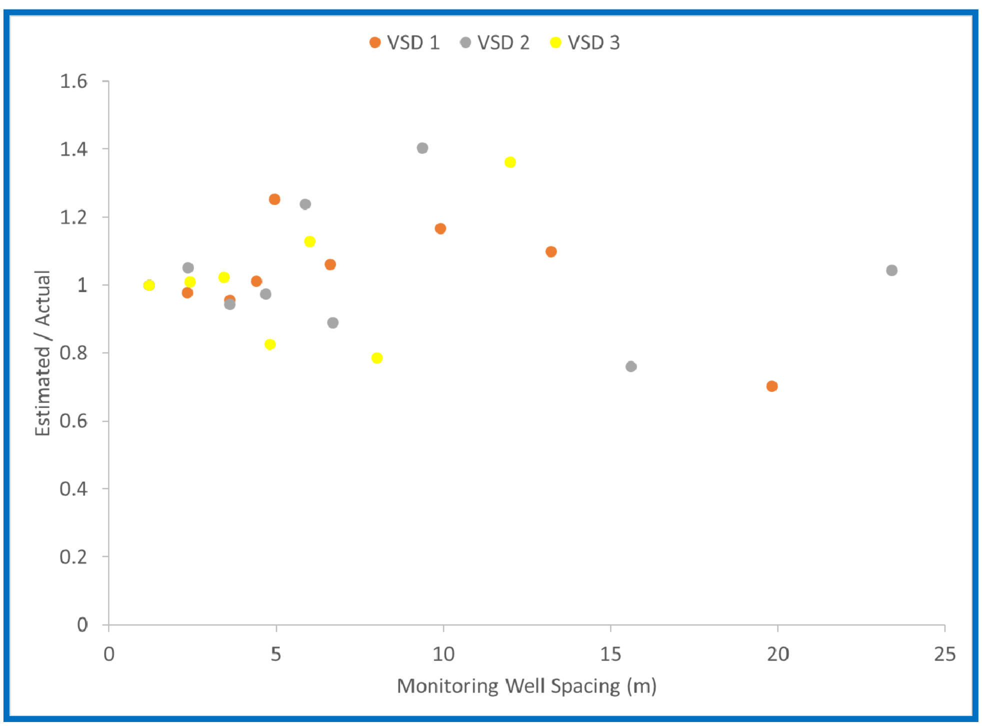

Figure 1: Uncertainty estimates (using the PFM approach) in source zone discharge derived from the DIVER project

Appendix B

Background Information on DNAPL3D-RX Model (ESTCP ER-0424)

DNAPL3D-RX Model Equations

Multiphase Flow Equations (Kueper and Frind, 1991; Gerhard and Kueper, 2003; Grant and Gerhard, 2007):

$$\frac{\partial}{\partial x_i}\left[\frac{k_{ij} k_{rw}}{\mu_w}\left(\frac{\partial P_w}{\partial x_j} + \rho_w g \frac{\partial y}{\partial x_j}\right)\right] + \rho_w (\alpha + \theta\beta) \frac{\partial P_w}{\partial t} = 0$$

$$\frac{\partial}{\partial x_i}\left[\frac{k_{ij} k_{rnw}}{\mu_{nw}}\left(\frac{\partial (P_w + P_c)}{\partial x_j} + \rho_{nw} g \frac{\partial y}{\partial x_j}\right)\right] + (1 - S_w)(\alpha) \frac{\partial P_w}{\partial t} + \theta \frac{\partial S_w}{\partial t} = -J_{nw}$$

$i, j = x, y, z$

where P is pressure {M[1]L[-1]T[-2]}, P_c is capillary pressure {M[1]L[-1]T[-2]}, k_{ij} is the intrinsic permeability tensor {L[2]}, k_r is the relative permeability {-}, μ is dynamic viscosity {M[1]L[-1]T[-1]}, ρ is fluid density {M[1]L[-3]}, θ is porosity {-}, S is phase saturation {-}, g is gravitational acceleration {L[1]T[-2]}, α is porous medium compressibility {M[-1]L[1]T[2]}, β is wetting phase compressibility {M[-1]L[1]T[2]}, t is time {T[1]}, J is the solute mass flux from the immiscible liquid phase to the aqueous phase {M[1]L[-3]T[-1]}. *x,y,z* represent spatial coordinates {L[1]} where x represents the longitudinal direction, z represents the lateral direction and y represents the vertical direction. Subscripts w and nw represent both wetting and non-wetting phases, respectively.

Solute Transport Equations (Clement, 1997; Clement et al., 1998):

$$\frac{\partial (\theta C^n_m)}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D^n_{ij} \frac{\partial C^n_m}{\partial x_j}\right) - \frac{\partial}{\partial x_i}\left(\theta v_i C^n_m\right) + q_s C^n_s + \sum \mathbb{R}_m + J$$

$$\frac{\partial (\theta C^n_{im})}{\partial t} = \sum \mathbb{R}_{im}$$

$i, j = x, y, z$

where D_{ij} is the hydrodynamic dispersion tensor {L[2]T[-1]}, v_i is the average linear groundwater velocity {L[1]T[-1]} obtained from the multiphase flow model component, q_s is the source/sink term represented as a volumetric flux {T[-1]}, $\mathbb{R}$ is the rate of all reactions {M[1]L[-3]T[-1]}, t is time {T[1]}. Superscript n represents species number, and subscripts m and im represent mobile and immobile species, respectively. *x,y,z* represent spatial coordinates {L[1]} where x represents the longitudinal direction, z represents the lateral direction and y represents the vertical direction.

Reaction Equations (Pre-Remedy VSDs):

The following equations outline the first-order biotic decay equations used during the simulation of the pre-remedy VSD domains:

$$\frac{\partial\partial[TTCCTT]}{\partial\partial\partial\partial} = \frac{-kk_{TTTTTT}}{RR_{TTTTTT}}[TTCCTT]$$

$$\frac{\partial\partial[ccDDCCTT]}{\partial\partial\partial\partial}^{TT} = \frac{kk_{TTTT}}{RR_{ccccTTTT}}[TTCCTT]$$

where k_{TCE} is the first-order biotic decay coefficient{T^{-1}}, R_{TCE} is the retardation factor for trichloroethene, R_{cDCE} is the retardation factor for cis-dichloroethene, t is time {T^{1}}. Square brackets represent molar concentrations (mol L^{-3}).

Reaction Equations (EISB Remedy VSDs):

The following equations outline the Monod kinetic and reaction rate expressions utilized for the simulation of the DM teams' VSD EISB remedy designs. The sequential reductive dechlorination of trichloroethene (TCE) → cis-dichloroethene (cDCE) → vinyl chloride (VC) → ethene (ETH) is represented using dual-Monod kinetics, dependent on both chlorinated ethene and electron donor (assumed to be only hydrogen (H_2) in this case) concentrations. The model tracks the growth/decay of three bacterial species: lactate fermenters (FERM), dechlorinators (DECH) and methanogens (METH). Square brackets represent molar concentrations (mol L^{-3}) and biomass concentrations (X_n) were calculated in units of milligrams cells per litre.

<u>Monod Kinetic Equations:</u>

$$\Re_{FFTTFFFF} = qq_{FFTTFFFF} XX_{FFTTFFFF} \left\{\frac{[LLLLCCTTLLTTTT]}{KK_{LLLLTTTTLLTTTT} + [LLLLCCTTLLTTTT]}\right\} e^{-\left\{\frac{[HH_2]}{HH_2^{ssssssssss}}\right\}} ff(XX_{nn})$$

$$\Re_{FFTTTTHH} = qq_{FFTTTTHH}\frac{XX_{FFTTTTHH}}{II_{FFTTTTHH}}\left\{\frac{[HH_2] - HH^*_{FFTTTTHH}}{KK_{FFTTTTHH} + [HH_2] - HH^*_{FFTTTTHH}}\right\} ff(XX_{nn})$$

$$\Re_{TTTTTT} = qq_{TTTTTT} XX_{ccTTTTHH}\left\{\frac{[TTCCTT]}{KK_{TTTTTT}II_{TTTTTT} + [TTCCTT]}\right\}\left\{\frac{[HH_2] - HH^*_{ccTTTTHH}}{KK_{HH_2} + [HH_2] - HH^*_{ccTTTTHH}}\right\} ff(XX_{nn})$$

$$\Re_{ccccTTTT} = qq_{ccccTTTT} XX_{ccTTTTHH}\left\{\frac{[ccDDCCTT]}{KK_{ccccTTTT}II_{ccccTTTT} + [ccDDCCTT]}\right\}\left\{\frac{[HH_2] - HH^*_{ccTTTTHH}}{KK_{HH_2} + [HH_2] - HH^*_{ccTTTTHH}}\right\} ff(XX_{nn})$$

$$\Re_{VVTT} = qq_{VVTT} XX_{ccTTTTHH}\left\{\frac{[VVCC]}{KK_{VVTT}II_{VVTT} + [VVCC]}\right\}\left\{\frac{[HH_2] - HH^*_{ccTTTTHH}}{KK_{HH_2} + [HH_2] - HH^*_{ccTTTTHH}}\right\} ff(XX_{nn})$$

Additional Notes/Discussion:

1) The fermentation reaction equation contains an additional exponential term related to the inhibition of fermentation due to H_2 concentrations. H_2^{scale} is representative of the inhibitory aqueous electron donor concentration for substrate fermentation. Similar methodology was used by Kouznetsova et al. (2010) where this parameter was calibrated to microcosm experiments involving a linoleic acid substrate.

   The H_2^{scale} parameter for this work was estimated following the study by Fennell (1998). Fennell (1998) evaluated different organic substrates (ethanol, lactic acid, butyric acid and propionic acid) to assess H_2 electron donor production. Kouznetsova et al. (2010) briefly discussed that both linoleic acid and propionate required very low H_2 partial pressures for fermentation to occur. Fennell (1998) observed the following peak H_2 partial pressures which were dependent on the ratio of electron donor to PCE contaminant:

   a. At a 1:1 and 2:1 ratio, propionic acid produced a peak H_2 level of approximately $10^{-5.1}$ atm.
   b. At a 1:1 ratio, lactic acid produced a peak H_2 level of 10^{-4} atm. At a 2:1 ratio, lactic acid produced a peak H_2 level of approximately 10^{-3} atm.

   Similar to Kouznetsova et al. (2010), the exponential term in this fermentation reaction equation represents a simplification (the reader is referred to this paper for a more in-depth explanation). Based on the greater substrate concentrations utilized during the DIVER test simulations, the 10^{-3} atm peak H_2 level for lactate fermentation was selected for this work. This value was not based on calibration to laboratory experiments but represents a threshold limit where the electron donor production rate declines exponentially based on the H_2 concentrations already present. The 10^{-3} atm H_2 partial pressure was converted to an approximate molar concentration of 0.8 mM (8×10^{-7} M) using a Henry's Constant (at 25°C) of 1282.05 L●atm/mol.

2) $f(X_n)$ terms were added to each biological reaction equation based on the methodology presented in Malaguerra et al. (2011). Malaguerra et al. (2011) introduced the following equation in the biological kinetics for non-dechlorinating bacteria:

$$f(X_n) = \frac{X_n^{max} - X_n}{X_n^{max}}$$

   where: X_n is the current biomass concentration of biological species "*n*", X_n^{max} is a calibrated model biomass parameter based on biological species "*n*".

   In this work the biomass function was applied to all species. This term represents a simplification as it is utilized to maintain biomass cellular concentrations at realistic levels. X_n^{max} was a calibrated parameter determined by Malaguerra et al. (2011). For the DIVER remedy simulations, X_n^{max} was based on the biomass concentration that resulted in producing a *Dehalococcoides* gene copies count of 1×10^{11} gene copies/L. The upper limit of the bacterial mass range presented by Malaguerra et al. (2011) of 1172×10^{-15} g biomass/cell was used to back-calculate an appropriate X_n^{max} for this project. This conversion factor used differs from the actual determined value of 4.2 x 10^{-15} g cells/copy for *Dehalococcoides* from Duhamel et al. (2004). However, since the dechlorinator population used in this project is more representative of a dechlorinating biomass consortium, a higher conversion factor was more suitable as it allowed for a greater limit on the maximum biomass concentration (X_n^{max}).

Inhibition Coefficients:

$$II_{FFTTTTHH} = 1 + \frac{[TTCCTT]}{KK_{ii}^{TTTTTT}}$$

$$II_{TTTTTT} = 1 + \frac{[ccDDCCTT]}{KK_{ii}^{ccccTTTT}} + \frac{[VVCC]}{KK_{ii}^{VVTT}}$$

$$II_{ccccTTTT} = 1 + \frac{[VVCC]}{KK_{ii}^{VVTT}} + \frac{[TTCCTT]}{KK_{ii}^{TTTTTT}}$$

$$II_{VVTT} = 1 + \frac{[ccDDCCTT]}{KK_{ii}^{ccccTTTT}} + \frac{[TTCCTT]}{KK_{ii}^{TTTTTT}}$$

Reaction/Degradation Rates:

$$\frac{\partial\partial[TTCCTT]}{\partial\partial\partial\partial} = -\frac{\Re_{TTTTTT}}{RR_{TTTTTT}}$$

$$\frac{\partial\partial[ccDDCCTT]}{\partial\partial\partial\partial} = \frac{(\Re_{TTTTTT} - \Re_{ccccTTTT})}{RR_{ccccTTTT}}$$

$$\frac{\partial\partial[VVCC]}{\partial\partial\partial\partial} = \frac{(\Re_{ccccTTTT} - \Re_{VVTT})}{RR_{VVTT}} - \frac{\lambda\lambda_{VVTT}[VVCC]}{RR_{VVTT}}$$

$$\frac{\partial\partial[TTTTHH]}{\partial\partial\partial\partial} = \frac{\Re_{VVTT} - kk_{TTTTHH}[TTTTHH]}{RR_{TTTTHH}}$$

$$\frac{\partial\partial[CCCC-]}{\partial\partial\partial\partial} = \Re_{TTTTTT} + \Re_{ccccTTTT} + \Re_{VVTT}$$

$$\frac{\partial\partial[LLLLCCTTLLTTTT]}{\partial\partial\partial\partial} = -\Re_{FFTTFFFF}$$

$$\frac{\partial\partial[MMTTTTHH]}{\partial\partial\partial\partial} = \Re_{FFTTTTHH}$$

$$\frac{\partial\partial[HH_2]}{\partial\partial\partial\partial} = FF_{FFTTFFFF}\,\Re_{FFTTFFFF} - (FF_{TTTTTT}\,\Re_{TTTTTT} + FF_{ccccTTTT}\,\Re_{ccccTTTT} + FF_{VVTT}\,\Re_{VVTT} + FF_{FFTTTTHH}\,\Re_{FFTTTTHH})$$

$$\frac{\partial\partial XX_{FFTTFFFF}}{\partial\partial\partial\partial} = YY_{FFTTFFFF}\,\Re_{FFTTFFFF} - \lambda\lambda_{XX_{FFFFFFFF}}\,XX_{FFTTFFFF}$$

$$\frac{\partial\partial XX_{ccTTTTHH}}{\partial\partial\partial\partial} = (YY_{TTTTTT}\,\Re_{TTTTTT} + YY_{ccccTTTT}\,\Re_{ccccTTTT} + YY_{VVTT}\,\Re_{VVTT}) - \lambda\lambda_{XX_{ddssssh}}\,XX_{ccTTTTHH}$$

$$\frac{\partial\partial XX_{FFTTTTHH}}{\partial\partial\partial\partial} = YY_{FFTTTTHH}\,\Re_{FFTTTTHH} - \lambda\lambda_{XX_{FFFFMMMM}}\,XX_{FFTTTTHH}$$

Nomenclature:

FF_{cc} – stoichiometric production or use coefficient of H_2 (mol H_2 mol c^{-1})
HH_{nn}^* – H_2 threshold to reflect H_2 utilization efficiency for microbial species *n* (M^1 L^{-3})
II_{cc} – inhibition coefficient due to species *c* (dimensionless)
$K_{ii}K^{cc}$ – inhibition constant due to chemical species *c* (M^1 L^{-3})
KK_{cc} – half-saturation constant (M^1 L^{-3})
qq_{nn} – maximum utilization rate of microbial species *n* for chemical species *c* (mol *c* M_{bio}^{-1} T^{-1})
RR_{cc} – retardation coefficient for chemical species *c* (dimensionless)
XX_{nn} – biomass concentration of microbial species *n* (M^1 L^{-3})
YY_{nn} – yield coefficient of microbial species *n* per chemical species *c* (M_{bio}^1 mol c^{-1})
$\lambda\lambda_{XX_{nn}}$ – decay coefficient for microbial species *n* (T^{-1})
$\Re_{ii}$ – molar rate of biological degradation due to microbial process *i* (mol L^{-3} T^{-1})
kk_{TTTTHH} – first-order degradation rate of ethene (T^{-1}); based on model testing, this parameter corresponded to half-life of 1 day.

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Appendix C

Phase 1 ESA Reports

PHASE I ENVIRONMENTAL SITE ASSESSMENT

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Project Number TR0489

May 2017

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1. INTRODUCTION

Geosyntec Consultants (Geosyntec) was retained to perform a Phase I Environmental Site Assessment ("Phase I ESA") at a former auto parts manufacturing facility owned by CM AutoParts, Incorporated. The facility is located at 123 Smith Street, Springfield, North Dakota (referred to herein as the "Site").

1.1 Purpose

This Phase I ESA was conducted in general accordance with the scope and limitations of the guidance contained within the ASTM International Standard Practice for Environmental Site Assessments: Phase I Environmental Site Assessment Process (hereafter, ASTM E1527-13). Any exceptions or deviations to the guidance contained in ASTM E1527-13 are described in Section 7. The Phase I ESA was conducted to identify, to the extent feasible, "Recognized Environmental Conditions[1]" (RECs) at the Site, as the "REC" term is defined by ASTM E1527-13. This REC definition eliminates from consideration a number of conditions that could fall under the general definition of "environmental" issues and focuses the Phase I ESA on known or potential releases of hazardous substances.

1.2 Scope of Services

The Phase I ESA scope of work included: (i) reviewing pertinent information/documents provided by CM AutoParts; (ii) reviewing environmental databases for the Subject Property and surrounding properties pursuant to ASTM E1527-13; (iii) reviewing historical land usage via historical aerial photographs, fire insurance rate maps, city directories, and United States Geological Survey (USGS) topographic maps, as available; (iv) a visual reconnaissance of the major interior and exterior features of the Site; and (v) reviewing Site operations and existing permits and plans provided by the Site owner or representative, and evaluating compliance with applicable state and federal environmental programs. The Site visit was conducted in November 2016.

1.3 Significant Assumptions

No significant assumptions were made while conducting this Phase I ESA.

1.4 Limitations and Exceptions

This Phase I ESA report contains a description and history of the Site, an environmental database review, a summary of visual observations made during the reconnaissance of the Site, and a

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[1] As defined by ASTM E1527-13, a Recognized Environmental Condition is: "the presence or likely presence of any hazardous substances or petroleum products in, on, or at a property: (1) due to any release to the environment; (2) under conditions indicative of a release to the environment; or (3) under conditions that pose a material threat of a future release to the environment. *De minimis* conditions are not Recognized Environmental Conditions."

description of information obtained during interviews of persons knowledgeable with the Site. The findings and conclusions presented in this Phase I ESA report are the result of professional interpretation of the information collected at the time of this study. The Phase I ESA report does not necessarily include an exhaustive search of all available records, nor does it include detailed assessment of all Phase I ESA findings.

1.5 Special Terms and Conditions

No special terms or conditions were taken into account as part of this project.

1.6 User Reliance

This Phase I ESA report has been prepared solely for the client. No third party shall have the right to rely on opinions rendered in connection with the services described.

2. SITE DESCRIPTION

This section describes the key characteristics of the Site. These descriptions were derived from information gathered during the reconnaissance unless referenced otherwise. The Site is owned by CM AutoParts Ltd. Mr. Chris Muffler, Owner and Plant Manager, was interviewed during the Site visit, and provided some of the pertinent information referenced in this section.

2.1 Site Location and General Characteristics

The Site is located at 123 Smith Street, Springfield, North Dakota. The City of Springfield is located in the southwestern portion of the State of North Dakota. Based on information from the Springfield County Assessor's website, the Site occupies one parcel with identification number 0010-20-3-894-02 and occupies approximately 37 acres.

Land use surrounding the Site is agricultural as shown on **Figure 1**. The Site is bordered by Smith Street on the West and South Sides. There are no residential properties bordering the Site.

2.2 Site Use

The Site operated as a manufacturer of automobile parts from 1964 to 2006. During its operation, the Site contained one building, approximately 275,000 square feet under roof, situated in the northern portion of the property. Primary operations at the Site included: i) Manufacture of brake pads and shoes (1964-1980); ii) Assembly of brake calipers (1980-2006) ; iii) bulk storage of various production chemical products; iv) finished product warehousing; and v) shipping and receiving. The manufacturing plant was shut down and demolished in 2006 and no activities have been conducted on Site since that time.

Exterior bulk chemical storage areas were located south of the warehouse area of the plant. The southern portions of the Site are primarily grassy open land. A truck parking area was located to the east of the Plant and a large asphalt-paved area was located to the southeast of the building (**Figure 2**).

2.3 Description of Structures, Roads, Other Improvements

This section contains a description of the structures, roads and improvements observed by Geosyntec during the Site visit in 2016. The approximate construction dates were provided by Mr. Chris Muffler of CM AutoParts during the on-site interview. According to Mr. Muffler, CM AutoParts developed the Site on former agricultural land and began with the construction of the Plant Building in approximately 1963-1964. The Site entrance is on the Southeast portion of the Site, The eastern portion of the Site is a large paved area that was formerly for truck parking.

Storm water runoff from Site generally drains to the southeast along the paved area at the eastern side of the Site, or infiltrates or runs overland to the southeast in the grassy area south of the plant.

The Site is connected to the municipal water supply. Based on the database search, interviews, and the Site reconnaissance, there are four monitoring wells currently at the Site (locations shown in Figure 2).

The Site is connected to the municipal sanitary sewer system. Both sanitary wastewater and pre-treated industrial wastewater are discharged to the municipal sanitary sewer system. Based on the interviews and the Site reconnaissance, there are no current or historic sumps or drains at the Site that currently discharge wastewater from the building.

Solid Waste, hazardous waste, universal waste, and used oil were accumulated on Site. These wastes were disposed of by North Dakota Environmental of Springfield North Dakota.

2.4 Physical Setting

The Site is located in the Ordus Plains of the Upper Lowlands. The Ordus Plains are comprised of the Tertiary sediments of the Buffalo Springfield formation and are underlain by limestone of the Copperhead Road unit. The area is characterized by rolling plains. The Site is located approximately 8 miles north of the Dakota River, which is the major drainage basin in Springfield County.

Based on Site well logs, overburden at the site consists of layered silty sands and confining clays. The approximate depths of the various layers are as follows:

- Clay layer at surface that is approximately 7 ft thick;
- Fine sand aquifer from approximately 7 to 30 ft bgs;
- Clay from approximately 30 to 50 ft bgs;
- Silty sand aquifer from approximately 50 to 80 ft bgs; and
- Clay to the bottom of borings at 90 ft bgs.

The ground surface elevation at the Site is relatively flat at an elevation of approximately 110 feet above mean sea level (ft amsl). The ground surface topography in the Site vicinity slopes gently downward to the south and east. Ground surface elevation across the Site is shown in **Figure 3**. Based on the ground surface topography and the Site location relative to the Dakota River, the anticipated groundwater flow direction in the silt and sand aquifers is southerly towards the river.

3. USER-PROVIDED INFORMATION

This section describes the information provided to Geosyntec by the User of this Phase I ESA, who is considering the acquisition of the Site.

3.1 Title Records

A chain of title search was not included in the scope of services for this project.

3.2 Environmental Liens or Activity and Use Limitations

A search for environmental liens or activity and land use limitations (AULs) associated with the Site was conducted. No environmental liens or AULs were found.

3.3 Specialized Knowledge

Mr. Chris Muffler accompanied Geosyntec on the Site reconnaissance and interview, and supplied Geosyntec with specialized knowledge regarding the history of CM AutoParts, and general operations of the plant to the best of his knowledge.

3.4 Owner, Property Manager, and Occupant Information

The Subject Property is owned and operated by CM AutoParts.

3.5 Reason for Performing This Phase I ESA

Geosyntec understands the performance of a Phase I ESA for the Site was requested to assist in identifying potential environmental liabilities associated with the Site prior to potential acquisition of CM AutoParts.

4. RECORDS REVIEW

The records review consisted of: i) reviewing applicable federal, state, and local environmental databases; ii) reviewing readily available and identified historical aerial photographs, topographic maps, fire insurance maps and city directories; iii) reviewing readily available previous site investigation reports; and iv) reviewing potential for soil vapor impacts.

4.1 Environmental Database Search

4.1.1 Database Search Approach

Geosyntec reviewed applicable and reasonably ascertainable federal, state, and local environmental databases as part of this Phase I ESA. The environmental database search was performed to ascertain whether the Site or the surrounding properties were suspected of having environmental conditions that could have impacted the structures, soil, groundwater, or surface water at the Site.

4.1.2 Database Search Results

The significant findings of the database search as related to the Site are described below.

The Site was identified by address as 123 Smith Street, Springfield, and by name as CM AutoParts. The Site was identified in the following databases.

- Resource Conservation and Recovery Act (RCRA) environmental databases:

  CM AutoParts was identified from 1990 to 2006 as a Small Quantity Generator of wastes including: wastewater treatment sludges from chromium (D007), lead (D008), and trichloroethylene (D040).

- North Dakota Tier 2 database:

  CM AutoParts is listed in the North Dakota Tier 2 database, indicating the storage or manufacture of hazardous chemicals.

4.2 Historical Records Review

Available historical records were reviewed. No fire insurance maps or property tax maps were found for the Subject Property.

Historical aerial photographs and topographic maps for the Site area are not available. **Figure 1** shows a recent aerial photograph of the Site.

4.3 Previous Environmental Investigations

A limited Site investigation was undertaken at the request of the Owner to evaluate the condition of the Site prior to listing the property for sale. The following activities were conducted as part of this investigation:

- Installation of 4 shallow and 4 deep groundwater wells;
- Soil sampling in November 2016;
- Groundwater sampling in November 2016; and
- Groundwater levels were measured in November 2016

No report was prepared as a result of this investigation, but the data were provided and are available in Appendix A of this report. This includes soil concentration data from samples collected during well installation (Table A.1), fraction of organic carbon (foc) data from soil samples (Table A.2), groundwater elevations in November 2016 (Table A.3), and groundwater concentrations from samples collected in November 2016 (Table A.4). Concentrations were below detection limits at 3 of 4 boring locations, but trichloroethene (TCE) and cis-dichloroethene (DCE) were detected in soil at BH-4S and BH-4D and in groundwater at MW-4S and MW-4D.

5. SITE RECONNAISSANCE

5.1 Methodology and Limiting Conditions

A reconnaissance of the Site was conducted by qualified personnel with Geosyntec in November 2016.

As part of the reconnaissance, Geosyntec attempted to look for evidence of used, stored, or discarded hazardous substances, areas of disturbed or discolored soil, suspect equipment and/or building materials that may contain hazardous substances, areas of distressed vegetation, wastewater discharge areas, storage tanks/septic systems, waste management/disposal areas, lagoons, pits, sumps, surface water management areas, and stained surfaces. As the Site is demolished, much of the information was obtained through an interview with Mr. Muffler. Adjoining properties were peripherally observed from the perimeters of the Site and from public rights-of-way.

The significant findings from the reconnaissance of the Site are described below.

Manufacturing/Assembly

- The majority of the former building was used for manufacturing and assembly of auto parts. Mr Muffler noted that prior to demolition there was dark staining on the floor in the degreasing area of the plant. This Area is noted on Figure 2 as "Former Degreasing Area"

Liquid Chemical Storage Areas

- A chemical storage area room was located in the south central portion of the plant. This room had doors that were accessible both from inside and outside the plant. During the interview, Mr. Muffler noted that chemicals were stored in totes, glass, and stainless steel containers. He believed the chemical storage areas to be in good condition prior to demolition. The former chemical storage area is indicated on Figure 2.

Product Staging, Shipping, and Receiving Warehouse Areas

- Product staging, shipping, and receiving warehouse areas and the shipping and receiving dock were located in the north-east portion of the building. Mr. Muffler believed these areas were in good condition prior to building demolition.

Former Burial Ground

- A former drum burial ground is located south of the building as shown in Figure 2. Mr. Muffler indicated during interviews that this area was used to bury empty drums in the 1960s and early 1970s.

6. INTERVIEWS

During the Site reconnaissance in November 2016, Geosyntec conducted an interview with Mr. Chris Muffler of CM AutoParts. Mr. Muffler was knowledgeable about the history and operations of CM AutoParts and was forthcoming with information when asked. Pertinent information provided by Mr. Muffler is presented throughout this Phase I report.

7. EVALUATION

As required by ASTM E1527-13, this section presents the Geosyntec-identified known or suspect recognized environmental conditions (RECs), controlled recognized environmental conditions (CRECs), historical recognized environmental conditions (HRECs), and / or *de minimis* conditions at the Subject Property.

A CREC is a recognized environmental condition resulting from a past release of hazardous substances or petroleum products that has been addressed to the satisfaction of the applicable regulatory authority with certain restrictions or controls.

An HREC is a recognized environmental condition resulting from a past release of hazardous substances or petroleum products that has occurred in connection with the property and has been addressed to the satisfaction of the applicable regulatory authority, without subjecting the property to any restrictions or controls.

de minimis conditions generally do not present a threat to human health or the environment and generally would not be the subject of an enforcement action if brought to the attention of appropriate governmental agencies.

7.1 Findings

The following findings (locations shown in Figure 2) were identified as having the potential to be known RECs, CRECS, HRECs, and/or *de minimis* conditions at the Site are listed below (these are not in any particular order of importance):

FINDING A: A former degreasing area used by CM AutoParts was located in the eastern side of the former plant. Mr. Muffler recalled observing staining on the floor in this area prior to demolition.

FINDING B: A former drum burial area south of the former plant. The number and condition of drums is unknown.

FINDING C: Chlorinated solvents in soil and groundwater were detected during the November 2016 sampling events. TCE and cDCE were detected in the groundwater at monitoring wells MW-4S and MW-4D. MW-4S had TCE and cDCE concentrations of 117 and 105 milligrams per litre (mg/L), respectively, which exceeded the USEPA MCLs of 0.005 and

0.07 mg/L. MW-4D had TCE and cDCE concentrations of 99 and 97 mg/L, similarly exceeding the USEPA MCLs.

7.2 Opinions

This section includes the environmental professional's opinion(s) of on Site conditions identified in the findings section. Frequently, items initially suspected to be a recognized environmental condition are subsequently found, upon further evaluation, not to be considered a recognized environmental condition. The opinion includes the rationale for concluding that a condition is, or is not currently a recognized environmental condition.

Based on the information obtained during this investigation, Geosyntec has identified the following findings as known RECs or CRECs, based on the ASTM E1527-13 definition of a REC and CREC.

FINDING A: Former Degreasing Area is a REC, because staining was noted during the interview, however no records of decommissioning, clean-up, material disposal, or confirmation wipe sampling in this area were made available, creating a data gap.

FINDING B: Drum Burial Area is a REC because condition of the drums could not be observed during the Site visit. Potential cracking or corrosion could have led to a release to underlying soil and groundwater.

FINDING C: Chlorinated solvents in groundwater exceeding an USEPA MCL is a REC.

7.3 Data Gaps

In accordance with ASTM E1527-13, this section documents data gaps in the information obtained and reviewed as part of this Phase I ESA and discusses the associated significance. A data gap is defined as being "a lack of or inability to obtain information required by this practice [ASTM E1527-13] despite good faith efforts by the environmental professional to gather such information". The following data gaps were identified:

- **Former Degreasing Area:** data gaps exist because it was noted that dark staining was present on the floor prior to demolition and it is unknown if there were cracks or sumps in the floor that might have resulted in a release to the environment.

- **Drum Burial Area:** data gaps exist because the drums are buried and their condition could not be observed during the Site Visit. Additionally, the quantity and contents of the drums are unknown.

7.4 Conclusions

Geosyntec performed a Phase I ESA in conformance with the scope and limitations of ASTM Practice E1527-13 of the chemical manufacturing plant operated by CM AutoParts. Any exceptions to, or deviations from, this practice are described in Section 7.5 of this report. This assessment has revealed evidence of the following RECs at the Site:

FINDING A: Former Degreasing Area

FINDING B: Former Drum Burial Area

FINDING C: Chlorinated Solvents in Soil and Groundwater

7.5 Deviations

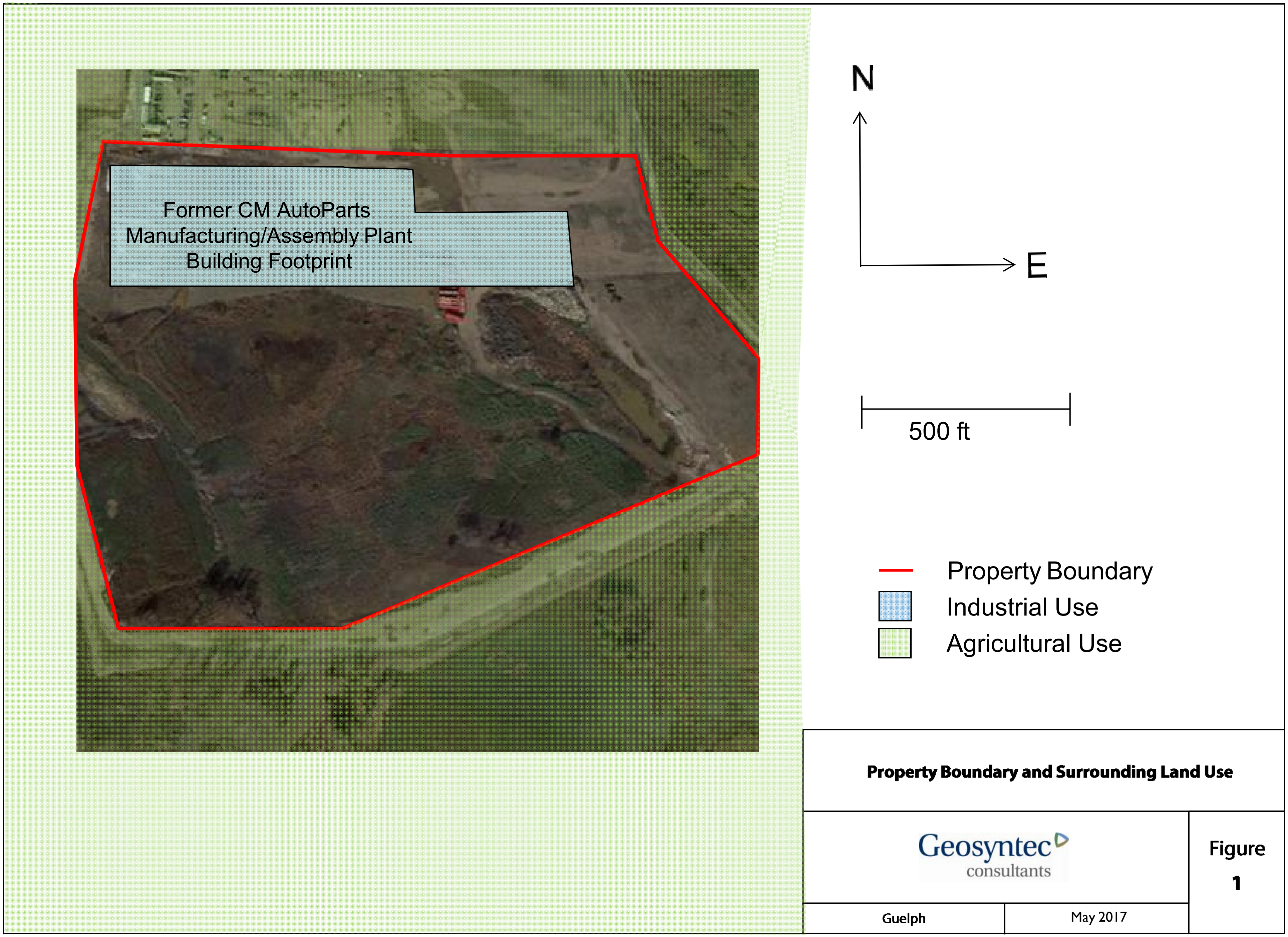
There were no exceptions or deviations from the ASTM E1527-13 standard of practice in the performance of this Phase I ESA.

7.6 Statement of Environmental Professionals

"We have the specific qualifications based on education, training, and experience to assess a property of the nature, history, and setting of the Subject Property. We have developed and performed all appropriate inquiries in conformance with the standards and practices set forth in 40 CFR Part 312."

Geosyntec consultants

FIGURES



Property Boundary and Surrounding Land Use

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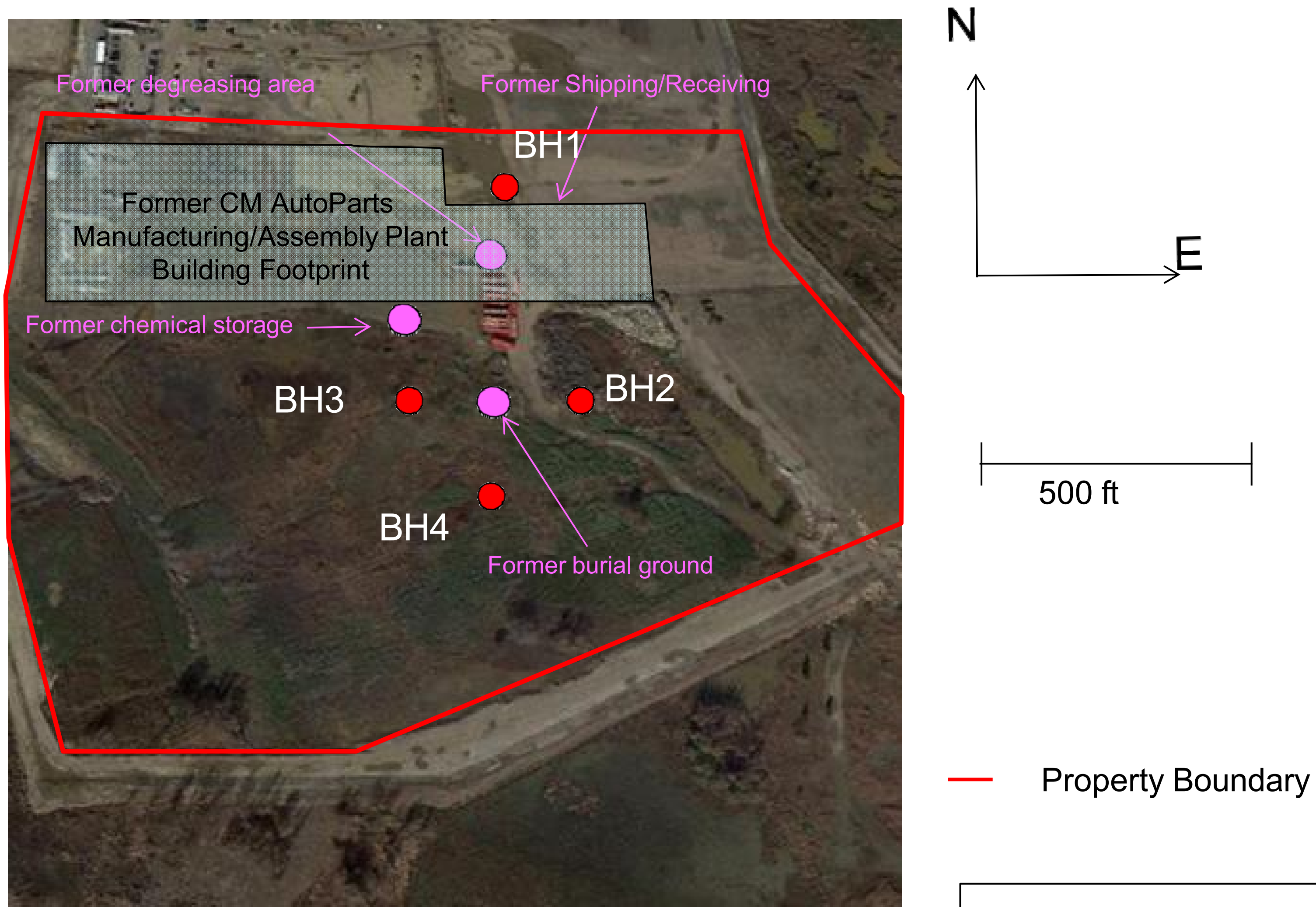
Guelph

May 2017

Figure 1

internal info: path, date revised, author



Areas of Interest and Boring Locations

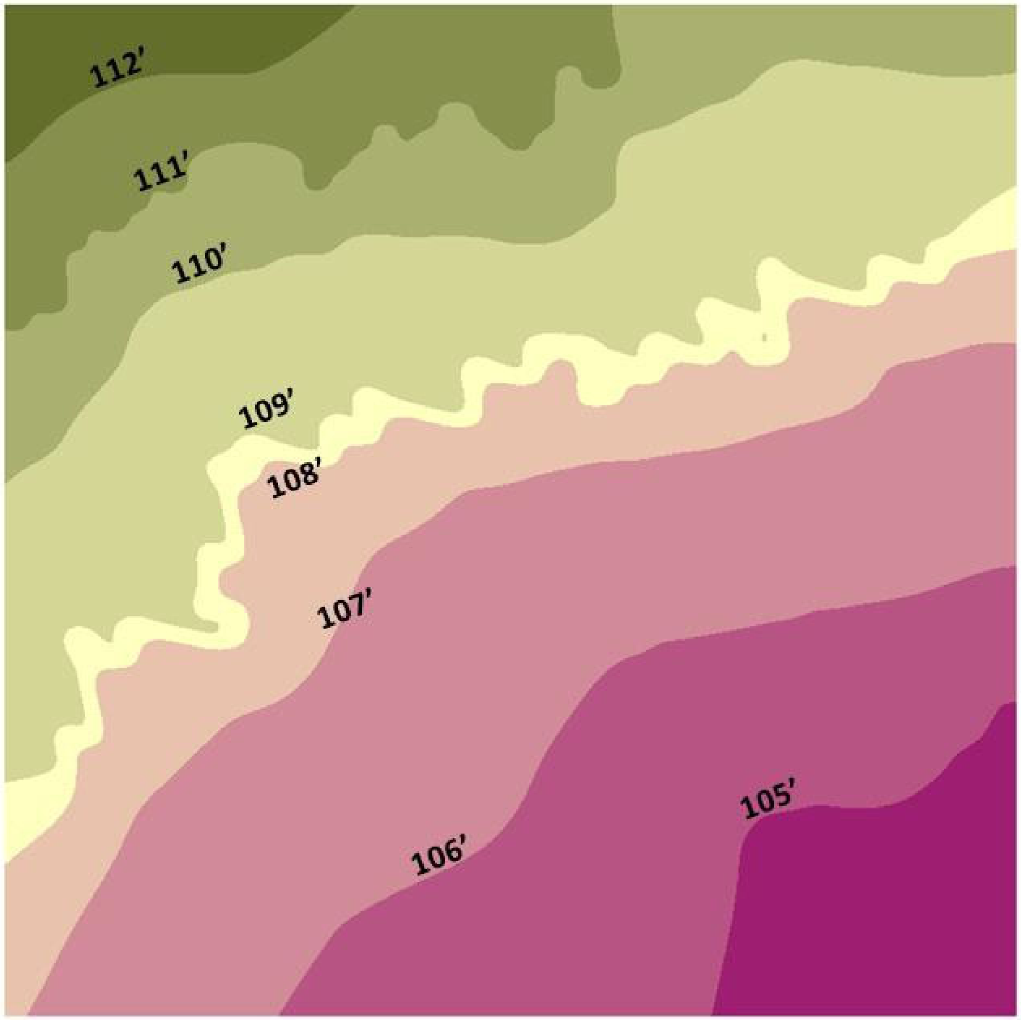
Geosyntec consultants

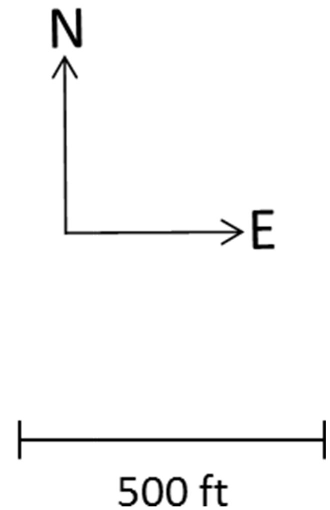
Figure 2

Guelph	May 2017

internal info: path, date revised, author

Northeast Corner:
NAD83 Easting = 101,640 ft
NAD83 Northing = 101,640 ft





Property Boundary

Southwest Corner:
NAD83 Easting = 100,000 ft
NAD83 Northing = 100,000 ft

Ground Surface Elevation	
Geosyntec consultants	Figure **3**
Guelph	May 2017

Geosyntec consultants

APPENDIX A

Site Investigation Data

Table A.1
Trichloroethene and cis-Dichloroethene Concentrations in Soil
November 2016
Former CM AutoParts Facility, Springfield

Boring Location	Sample Depth (ft bgs)	TCE (mg/kg)	cDCE (mg/kg)
BH-1S	22.85	< 0.001	< 0.001
BH-1D	35.9	< 0.001	< 0.001
BH-1D	68.75	< 0.001	< 0.001
BH-2S	19.95	< 0.001	< 0.001
BH-2D	33	< 0.001	< 0.001
BH-2D	65.9	< 0.001	< 0.001
BH-3S	20.05	< 0.001	< 0.001
BH-3D	33.1	< 0.001	< 0.001
BH-3D	66	< 0.001	< 0.001
BH-4S	19.48	35.28	25.83
BH-4D	20	29.17	21.40
BH-4D	65.45	21.62	15.71

Notes
ft bgs - feet below ground surface
mg/kg - milligrams per kilogram
< concentration below detection limit

Table A.2
Fraction of Organic Carbon in Soil
November 2016
Former CM AutoParts Facility, Springfield

Boring Location	Sample Depth (ft bgs)	f_{oc} (-)
BH-1S	22.85	3.29×10^{-3}
BH-1D	35.9	3.37×10^{-3}
BH-1D	68.75	3.16×10^{-3}
BH-2S	19.95	2.88×10^{-3}
BH-2D	33	3.17×10^{-3}
BH-2D	65.9	3.01×10^{-3}
BH-3S	20.05	3.50×10^{-3}
BH-3D	33.1	3.24×10^{-3}
BH-3D	66	2.93×10^{-3}
BH-4S	19.48	2.88×10^{-3}
BH-4D	20	3.12×10^{-3}
BH-4D	65.45	3.16×10^{-3}

Notes
ft bgs - feet below ground surface
foc - fraction of organic carbon

Table A.3
Groundwater Elevations
November 2016
Former CM AutoParts Facility, Springfield

Location	Depth to Water (ft bgs)	Water Elevation (ft amsl)
BH-1S	6.11	104.09
BH-1D	6.15	104.05
BH-2S	5.08	102.22
BH-2D	6.95	100.35
BH-3S	5.18	102.12
BH-3D	6.95	100.35
BH-4S	5.51	101.29
BH-4D	6.46	100.34

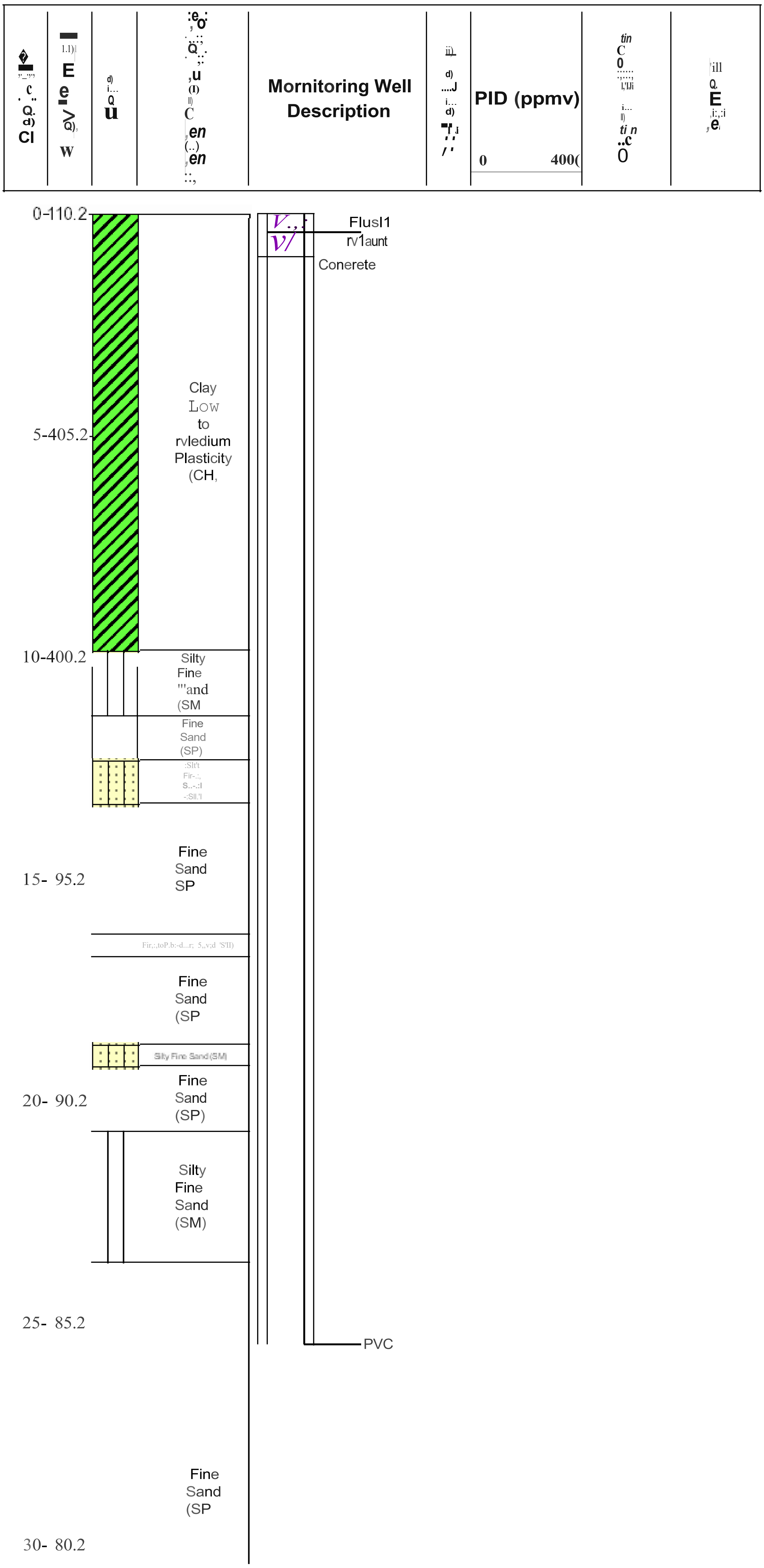
Notes
ft amsl - feet above mean sea level
ft bgs - feet below ground surface

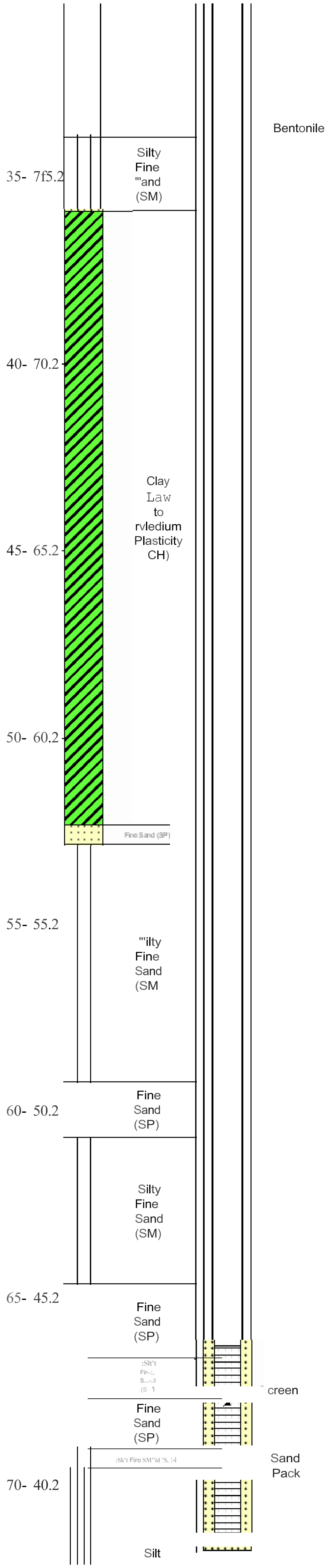
Table A.4
Trichloroethene and cis-Dichloroethene Concentrations in Groundwater
November 2016
Former CM AutoParts Facility, Springfield

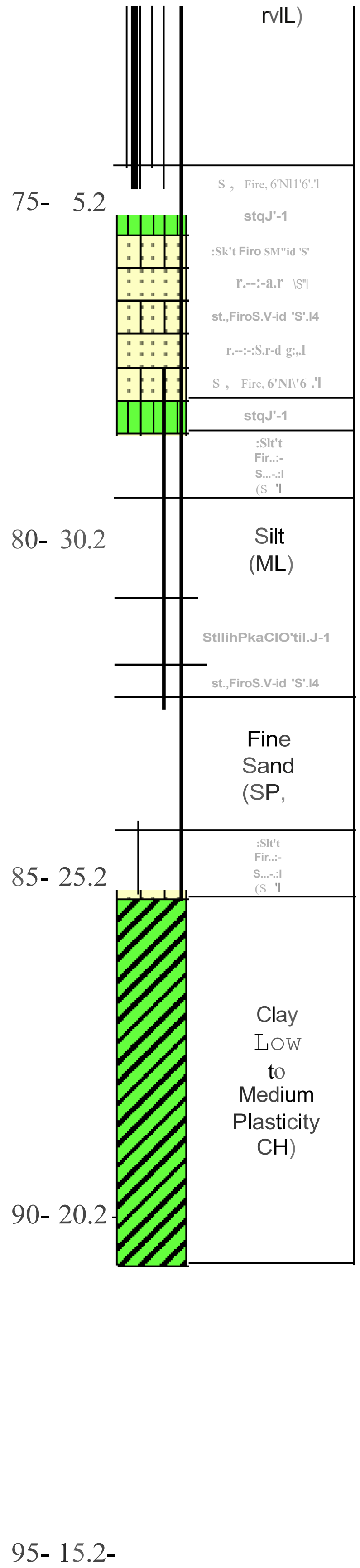
Sampling Location	Depth (ft bgs)	TCE (mg/L)	cDCE (mg/L)
MW-1S	22.85	< 0.001	< 0.001
MW-1D	68.75	< 0.001	< 0.001
MW-2S	19.95	< 0.001	< 0.001
MW-2D	65.9	< 0.001	< 0.001
MW-3S	20.05	< 0.001	< 0.001
MW-3D	66	< 0.001	< 0.001
MW-4S	19.48	116.79	105.01
MW-4D	65.45	98.66	97.11

Notes
ft bgs - feet below ground surface
mg/L - milligrams per litre
< concentration below detection limit

Projects No: GEOSYNTEC = VSD1
Borehole/Monitoring Well No: BH-1D/MW-1D
HorizontalNertical Datum: Model Domain
Northing (ft): 101313.0 **Easting (ft):** 100860.2
Drilling Equipment: SONIC DRILLING
Elevation of Ground Surface (ft): 110.22
Sampling Method: N/A
Date Started: 11/02/2016
Hammer Weight: N/A
Date Finished: 11/02/2016
Drop: N/A
Total Depth (ft):90.25
Logged by: AL **Supervising P.Eng:** HG
Measuring Point: Ground Surface
Diameter: 6"
Depth to Water in MW (ft): 6.15

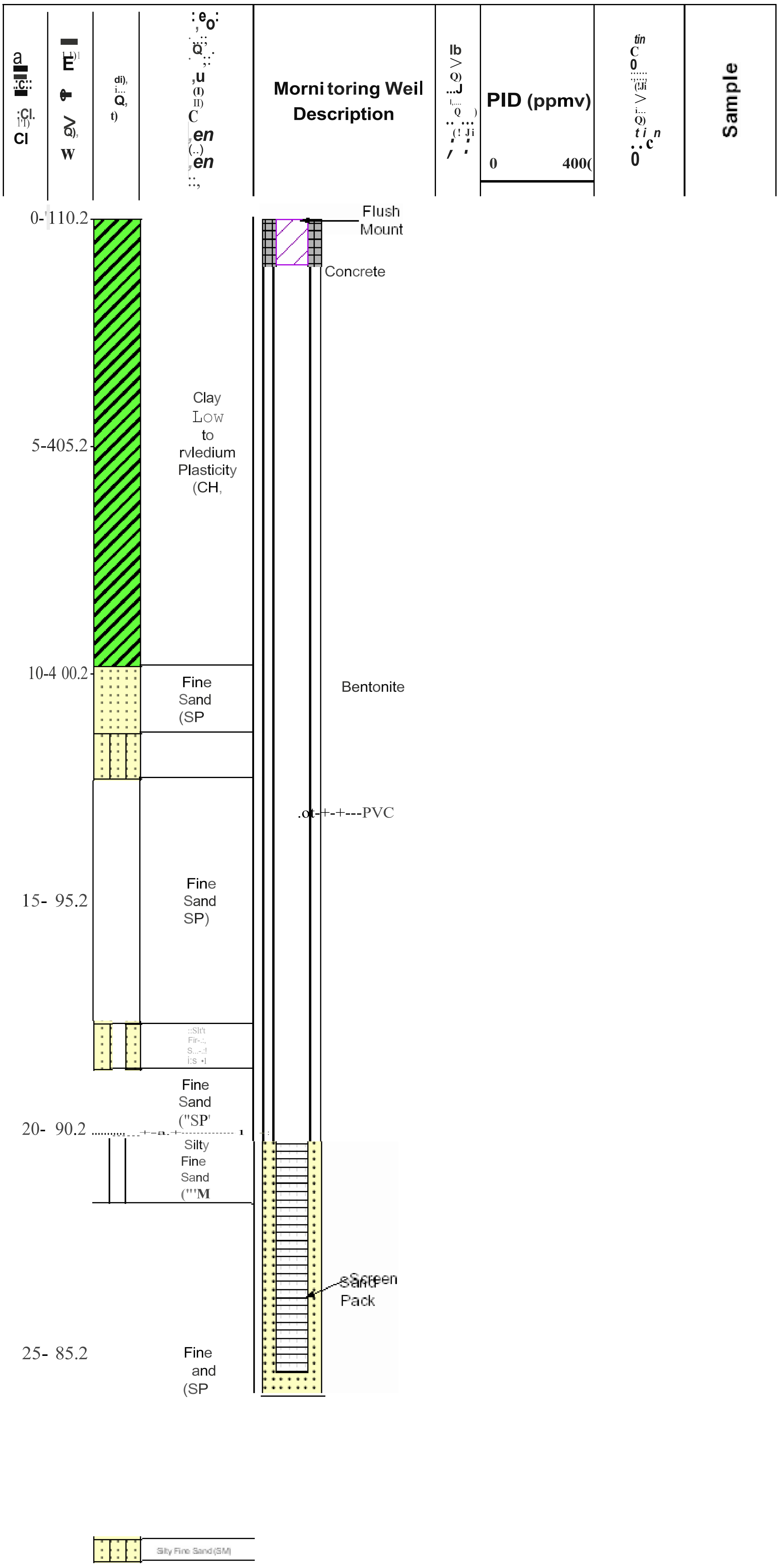


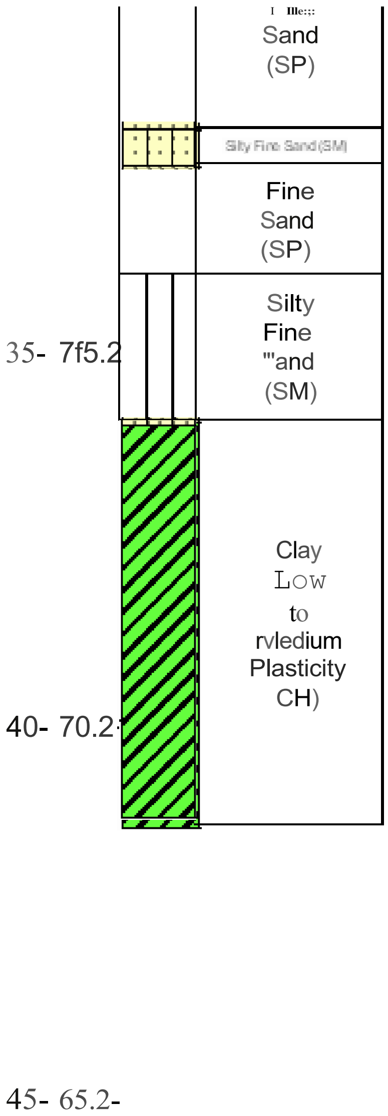

Bentonile
Silty Fine "'and (SM)
35- 7f5.2
40- 70.2
Clay Law to rvledium Plasticity CH)
45- 65.2
50- 60.2
Fine Sand (SP)
55- 55.2
"'ilty Fine Sand (SM
Fine Sand (SP)
60- 50.2
Silty Fine Sand (SM)
65- 45.2
Fine Sand (SP)
creen
Fine Sand (SP)
Sand Pack
70- 40.2
Silt



75- 5.2
80- 30.2
Silt
(ML)
Fine
Sand
(SP,
85- 25.2
Clay
Low
to
Medium
Plasticity
CH)
90- 20.2
95- 15.2-

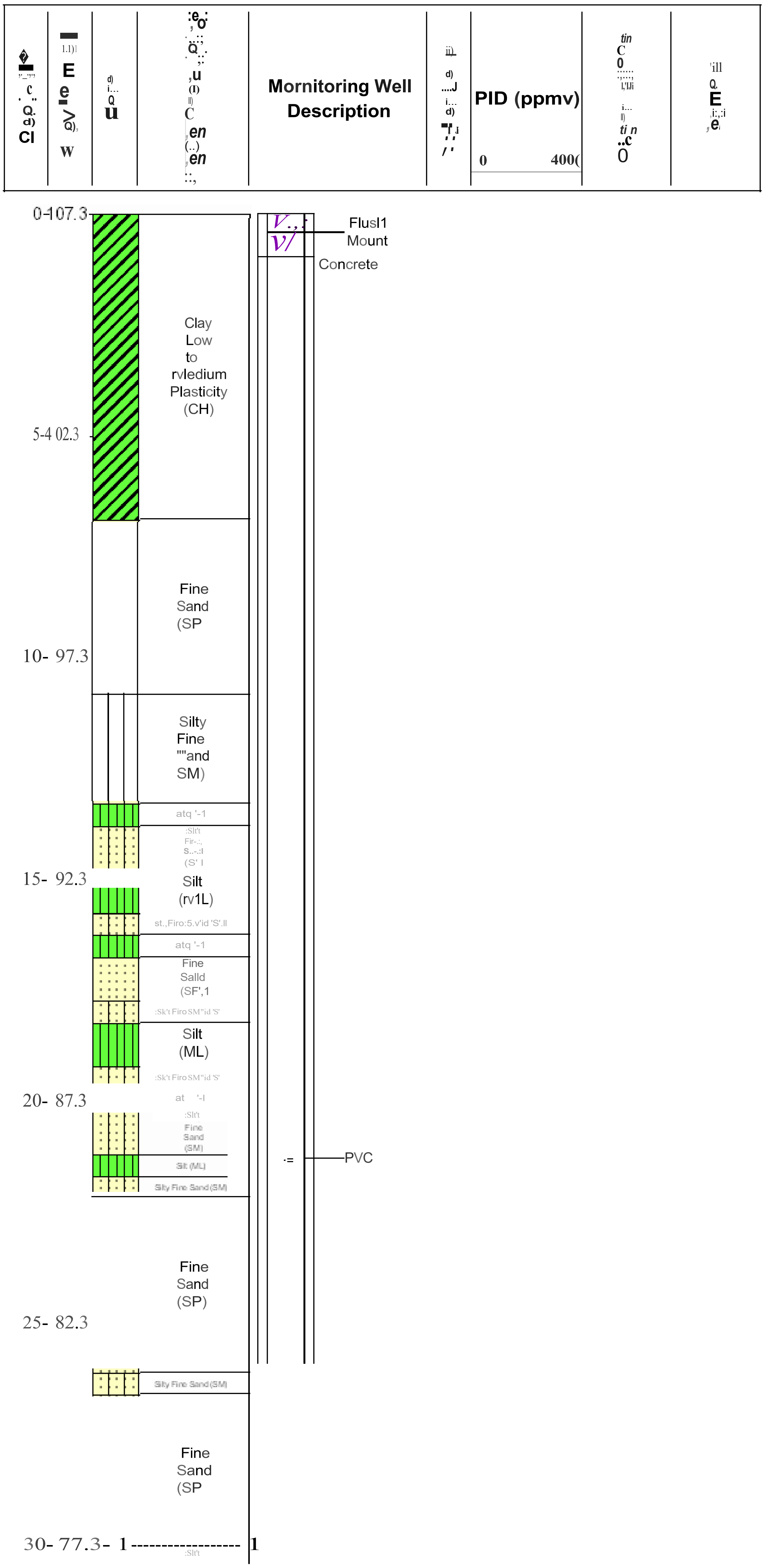
Projects No: GEOSYNTEC = VSD1
Borehole/Monitoring Well No: BH-1S/MW-1S
HorizontalNertical Datum: Model Domain
Northing (ft): 101313.0 **Easting (ft):** 100852.4
Drilling Equipment: SONIC DRILLING
Elevation of Ground Surface (ft): 110.22
Sampling Method: N/A
Date Started: 11/02/2016
Hammer Weight: N/A
Date Finished: 11/02/2016
Drop: N/A
Total Depth (ft):41.05
Logged by: AL **Supervising P.Eng:** HG
Measuring Point: Ground Surface
Diameter: 6"
Depth to Water in MW (ft): 6.11

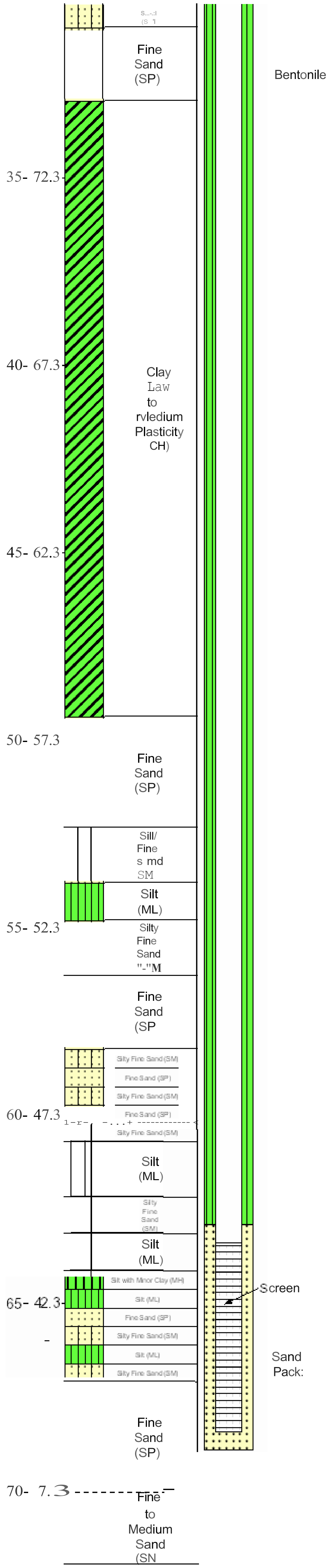




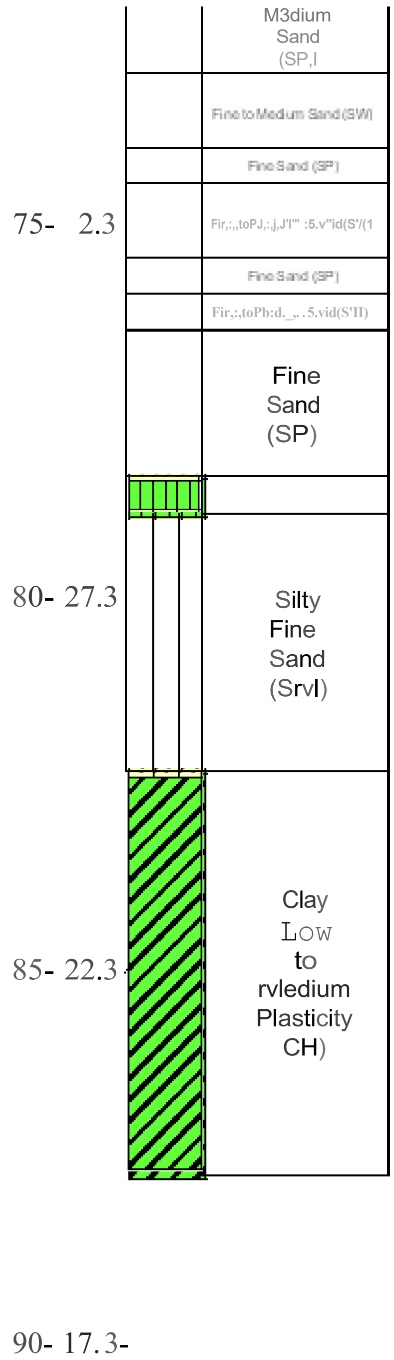
Sand
(SP)
Silty Fine Sand (SM)
Fine
Sand
(SP)
Silty
Fine
'''and
(SM)
35- 7f5.2
Clay
Low
to
rvledium
Plasticity
CH)
40- 70.2
45- 65.2-

Projects No: GEOSYNTEC = VSD1
Borehole/Monitoring Well No: BH-2D/MW-2D
HorizontalNertical Datum: Model Domain
Northing (ft): 100927.2 **Easting (ft):** 100954.7
Drilling Equipment: SONIC DRILLING
Elevation of Ground Surface (ft): 107.27
Sampling Method: N/A
Date Started: 11/02/2016
Hammer Weight: N/A
Date Finished: 11/02/2016
Drop: N/A
Total Depth (ft):87.35
Logged by: AL **Supervising P.Eng:** HG
Measuring Point: Ground Surface
Diameter: 6"
Depth to Water in MW (ft): 6.95

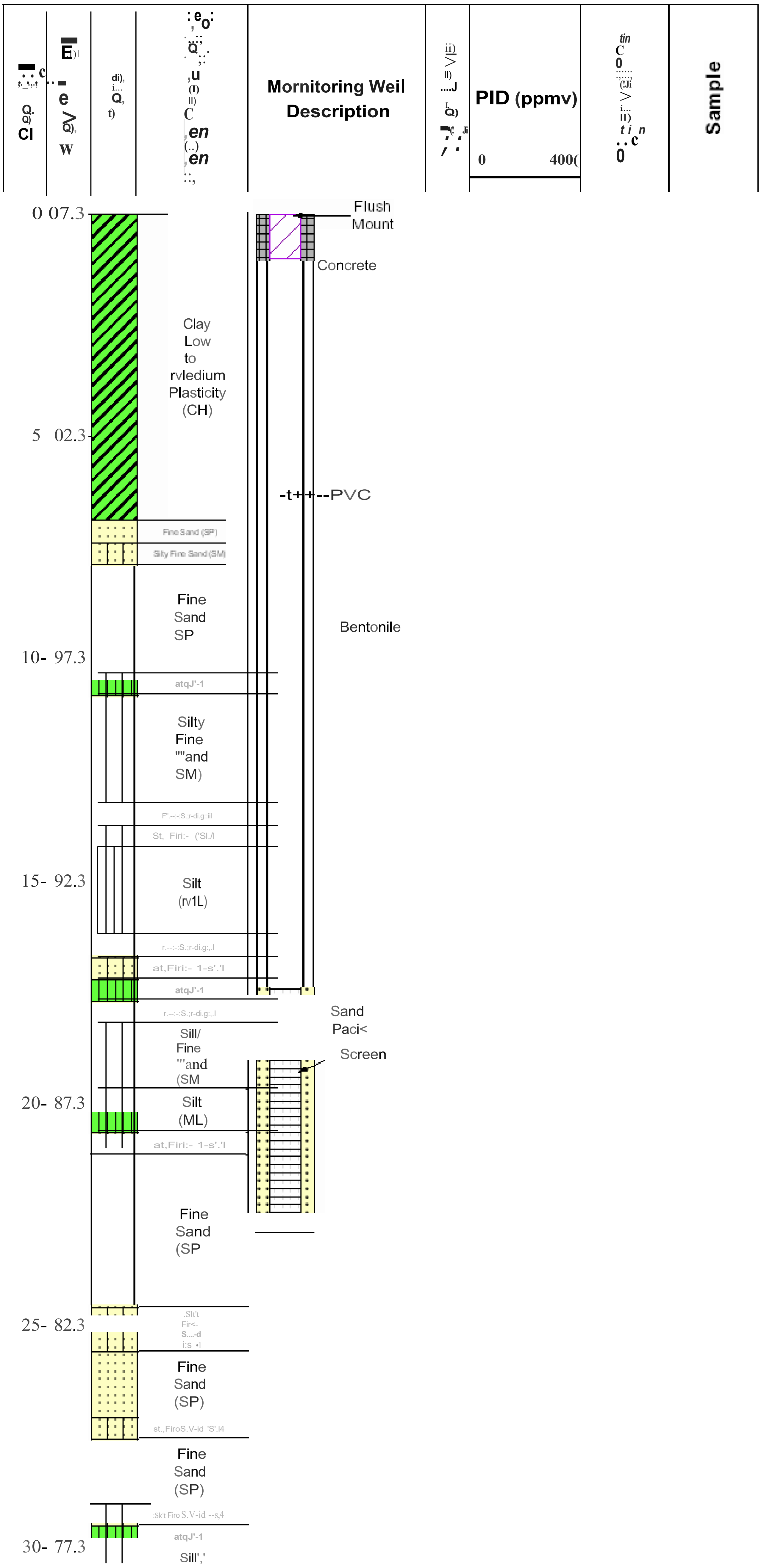


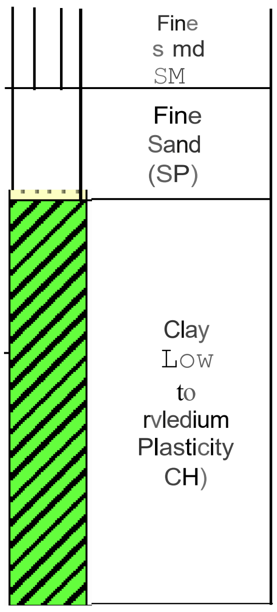


Fine
Sand
(SP)
Bentonile
35- 72.3
40- 67.3
Clay
Law
to
rvledium
Plasticity
CH)
45- 62.3
50- 57.3
Fine
Sand
(SP)
Sill/
Fine
s md
SM
Silt
(ML)
55- 52.3
Silty
Fine
Sand
"-"M
Fine
Sand
(SP
Silty Fine Sand (SM)
Fine Sand (SP)
Silty Fine Sand (SM)
60- 47.3
Fine Sand (SP)
Silty Fine Sand (SM)
Silt
(ML)
Silty
Fine
Sand
(SM)
Silt
(ML)
Silt with Minor Clay (MH)
Screen
65- 42.3
Silt (ML)
Fine Sand (SP)
Silty Fine Sand (SM)
Silt (ML)
Silty Fine Sand (SM)
Sand
Pack:
Fine
Sand
(SP)
70- 7.3
Fine
to
Medium
Sand
(SN


M3dium
Sand
(SP,I
Fine to Medium Sand (SW)
Fine Sand (SP)
75- 2.3
Fine Sand (SP)
Fine
Sand
(SP)
80- 27.3
Silty
Fine
Sand
(Srvl)
Clay
Low
to
rvledium
Plasticity
CH)
85- 22.3
90- 17.3-

Projects No: GEOSYNTEC = VSD1
Borehole/Monitoring Well No: BH-2S/MW-2S
HorizontalNertical Datum: Model Domain **Northing (ft):** 100927.2 **Easting (ft):** 100946.9
Drilling Equipment: SONIC DRILLING
Elevation of Ground Surface (ft): 107.27
Sampling Method: N/A
Date Started: 11/02/2016
Hammer Weight: N/A
Date Finished: 11/02/2016
Drop: N/A
Total Depth (ft):38.15
Logged by: AL **Supervising P.Eng:** HG
Measuring Point: Ground Surface
Diameter: 6"
Depth to Water in MW (ft): 5.08





35- 72.3-

40- 67.3-

Projects No: GEOSYNTEC = VSD1

HorizontalNertical Datum: Model Domain

Drilling Equipment: SONIC DRILLING

Sampling Method: N/A

Hammer Weight: N/A

Drop: N/A

Logged by: AL **Supervising P.Eng:** HG

Diameter: 6"

Borehole/Monitoring Well No: BH-3D/MW-3D

Northing (ft): 100927.2 **Easting (ft):** 100687.0

Elevation of Ground Surface (ft): 107.27

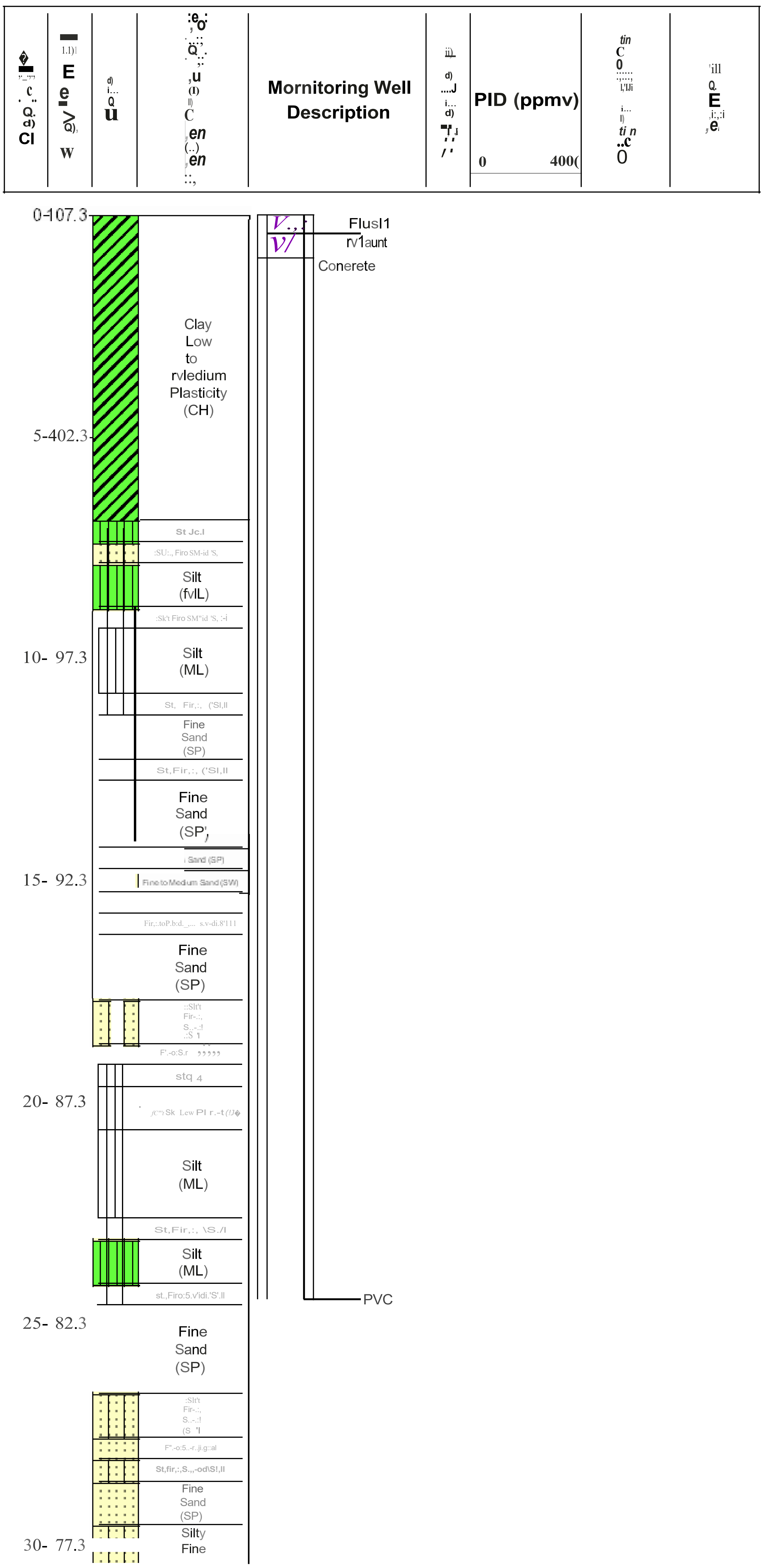
Date Started: 11/02/2016

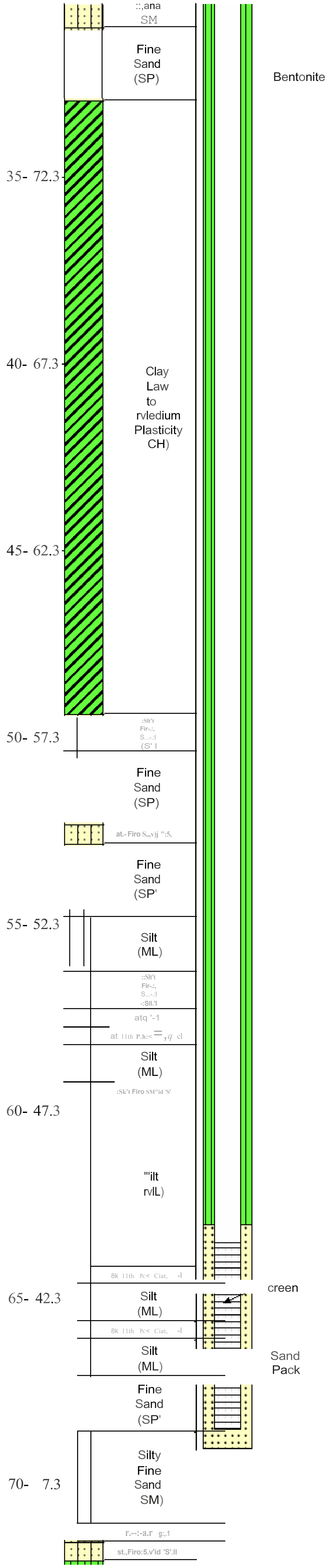
Date Finished: 11/02/2016

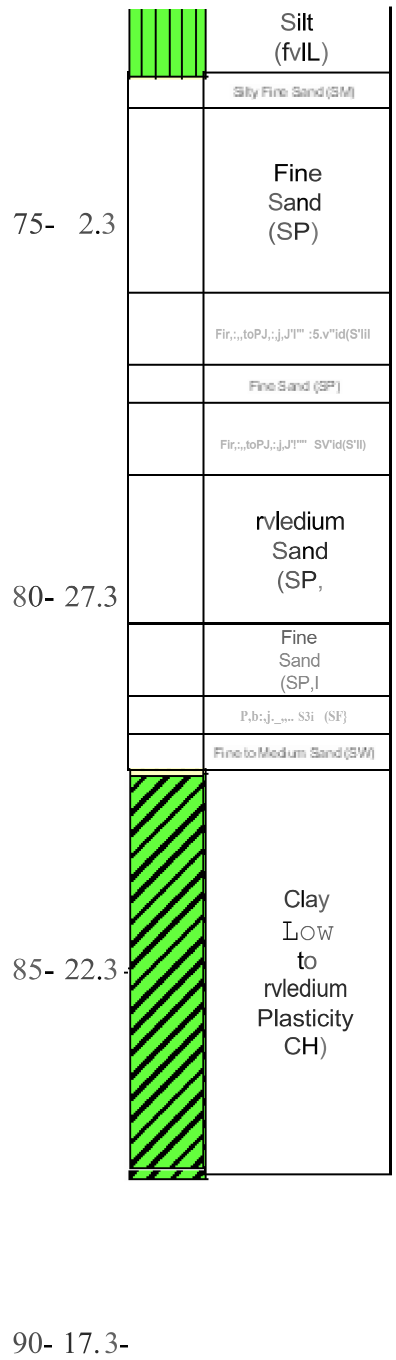
Total Depth (ft):87.46

Measuring Point: Ground Surface

Depth to Water in MW (ft): 6.95




SM
Fine Sand (SP)
Bentonite
35- 72.3
40- 67.3
Clay Law to rvledium Plasticity CH)
45- 62.3
50- 57.3
Fine Sand (SP)
Fine Sand (SP'
55- 52.3
Silt (ML)
Silt (ML)
60- 47.3
rvlL)
creen
65- 42.3
Silt (ML)
Silt (ML)
Sand Pack
Fine Sand (SP'
Silty Fine Sand SM)
70- 7.3



Silt (fvIL)
Silty Fine Sand (SM)
75- 2.3
Fine Sand (SP)
Fine Sand (SP)
80- 27.3
rvledium Sand (SP,
Fine Sand (SP,l
Fine to Medium Sand (SW)
85- 22.3
Clay Low to rvledium Plasticity CH)
90- 17.3-

Projects No: GEOSYNTEC = VSD1 **Borehole/Monitoring Well No:** BH-3S/MW-3S

HorizontalNertical Datum: Model Domain **Northing (ft):** 100927.2 **Easting (ft):** 100694.9

Drilling Equipment: SONIC DRILLING **Elevation of Ground Surface (ft):** 107.27

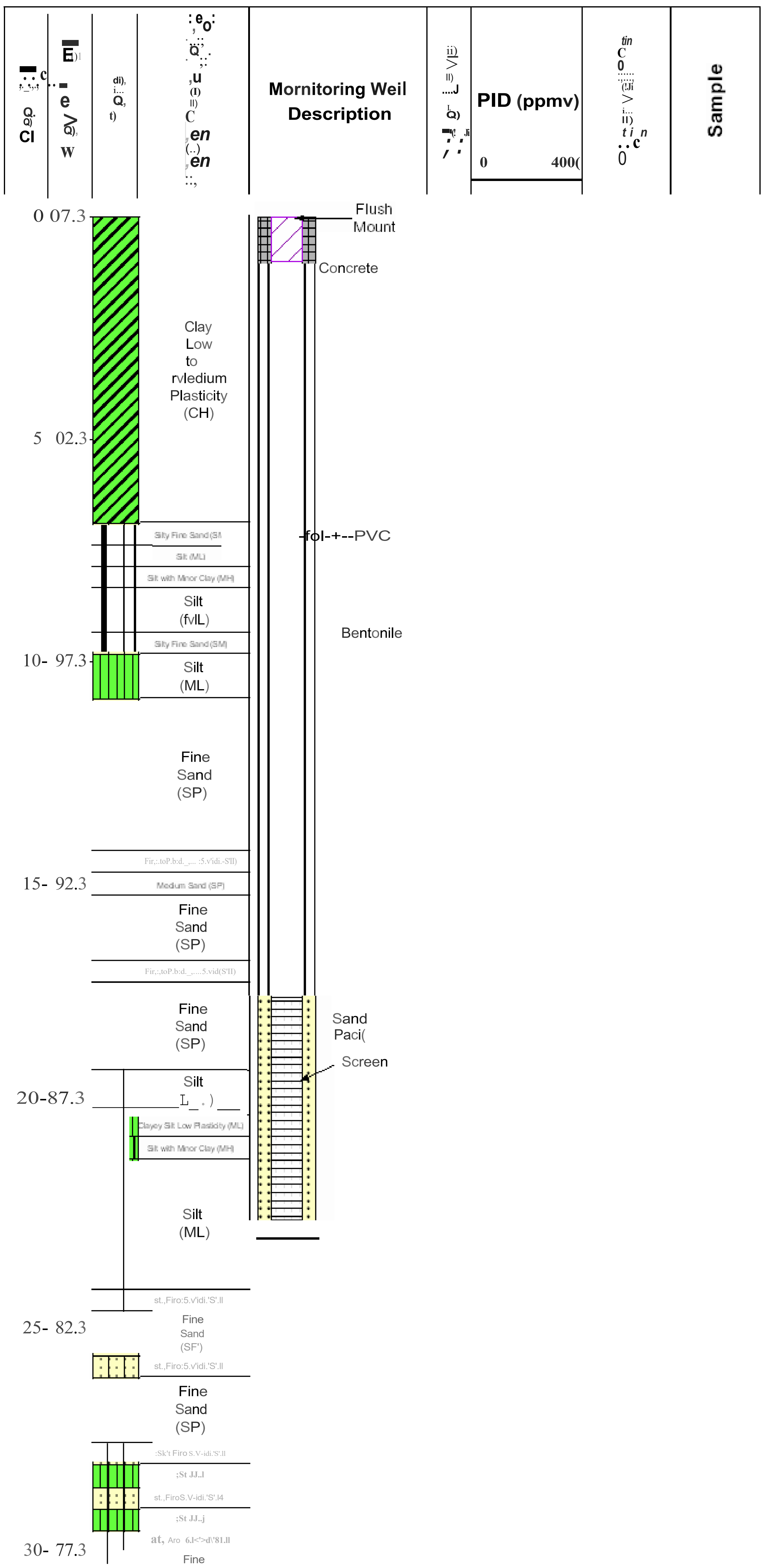
Sampling Method: N/A **Date Started:** 11/02/2016

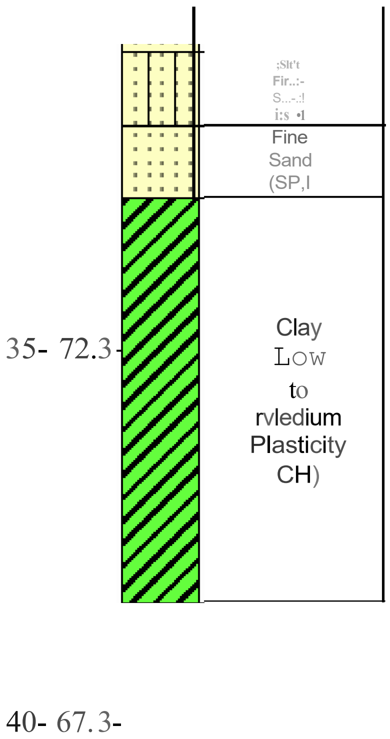
Hammer Weight: N/A **Date Finished:** 11/02/2016

Drop: N/A **Total Depth (ft):38.24**

Logged by: AL **Supervising P.Eng:** HG **Measuring Point:** Ground Surface

Diameter: 6" **Depth to Water in MW (ft):** 5.18




Fine
Sand
(SP,I
35- 72.3-
Clay
Low
to
rvledium
Plasticity
CH)
40- 67.3-

Projects No: GEOSYNTEC = VSD1

HorizontalNertical Datum: Model Domain

Drilling Equipment: SONIC DRILLING

Sampling Method: N/A

Hammer Weight: N/A

Drop: N/A

Logged by: AL **Supervising P.Eng:** HG

Diameter: 6"

Borehole/Monitoring Well No: BH-4D/MW-4D

Northing (ft): 100769.7 **Easting (ft):** 100816.9

Elevation of Ground Surface (ft): 106.78

Date Started: 11/02/2016

Date Finished: 11/02/2016

Total Depth (ft):86.93

Measuring Point: Ground Surface

Depth to Water in MW (ft): 6.46

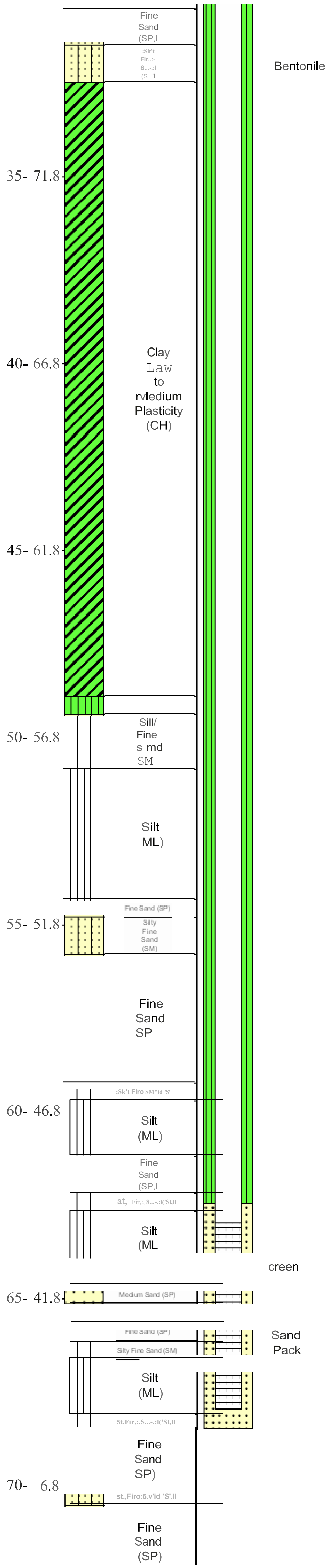
				Morni toring Well Description		PID (ppmv) 0 400(		

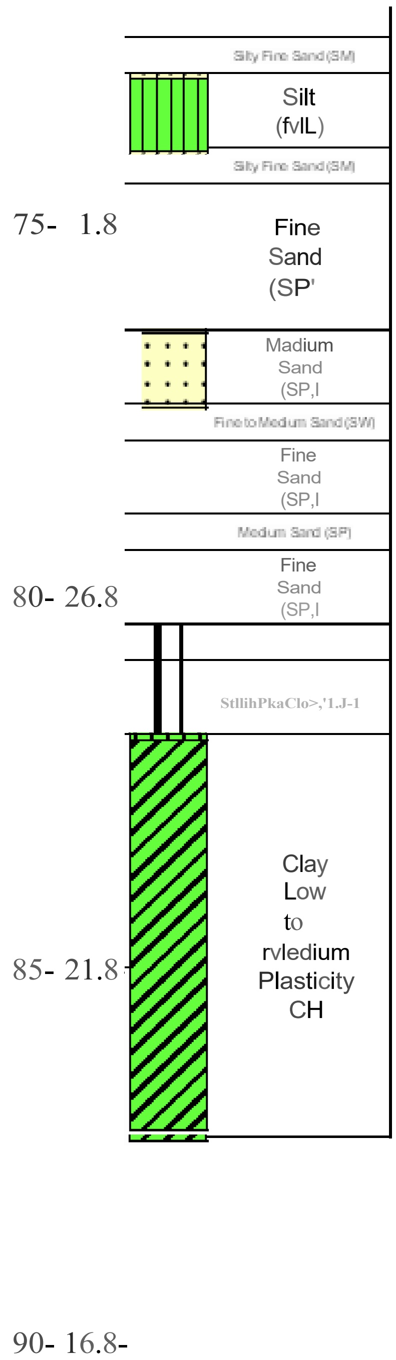
Depth - Elevation	Description
0-106.8	Clay Law to rvledium Plasticity (CH
5-4 01.8	Silty Fine Sand (SM)
	Silt (rvlL)
	Silty Fine Sand SM
10- 96.8	Silt (ML)
	Silty Fine Sand (SM)
	Silt (ML)
	Silty Fine Sand (SM)
	Silt (ML)
	Silty Fine Sand (SM)
	Fine Sand (SP)
15- 91.8	Silty Fine Sand (SM)
	Fine Salld (SF',1
	Fir.otoP 'sdtr 5.lro (.S'm
20- 86.8	Fine Sand (SP
	Silty Fine Sand (SM)
	Fine Salld (SF',1
25- 81.8	Fine Sand SP
	Silty Fine Sand (SM)
	Silt (ML)
30- 76.8	Silty Fine Sand (SM)

Flusl1 rvl aunt

Conerete

PVC


Fine
Sand
(SP,I
Bentonile
35- 71.8
Clay
Law
to
rvledium
Plasticity
(CH)
40- 66.8
45- 61.8
50- 56.8
Sill/
Fine
s md
SM
Silt
ML)
55- 51.8
Fine Sand (SP)
Silty
Fine
Sand
(SM)
Fine
Sand
SP
60- 46.8
Silt
(ML)
Fine
Sand
(SP,I
Silt
(ML
creen
65- 41.8
Medium Sand (SP)
Silty Fine Sand (SM)
Sand
Pack
Silt
(ML)
Fine
Sand
SP)
70- 6.8
Fine
Sand
(SP)


Silty Fine Sand (SM)
Silt (fvlL)
Silty Fine Sand (SM)
75- 1.8
Fine Sand (SP'
Madium Sand (SP,I
Fine to Medium Sand (SW)
Fine Sand (SP,I
Medium Sand (SP)
Fine Sand (SP,I
80- 26.8
Clay Low to rvledium Plasticity CH
85- 21.8
90- 16.8

Projects No: GEOSYNTEC = VSD1 **Borehole/Monitoring Well No:** BH-4S/MW-4S

HorizontalNertical Datum: Model Domain **Northing (ft):** 100769.7 **Easting (ft):** 100824.8

Drilling Equipment: SONIC DRILLING **Elevation of Ground Surface (ft):** 106.78

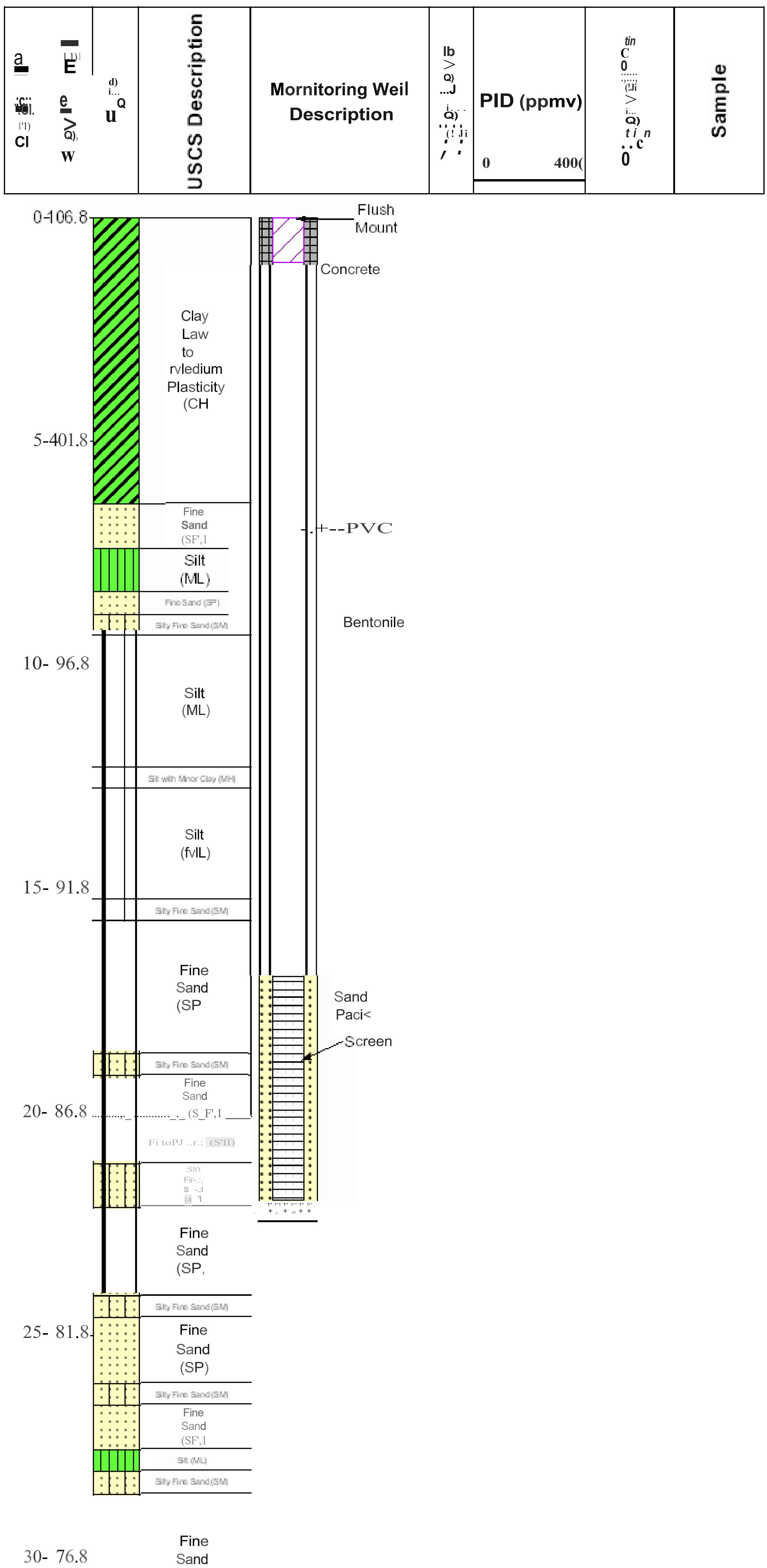
Sampling Method: N/A **Date Started:** 11/02/2016

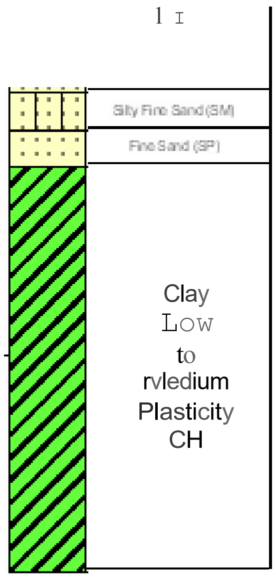
Hammer Weight: N/ A **Date Finished:** 11/02/2016

Drop: N/A **Total Depth** (ft):37.71

Logged by: AL **Supervising P.Eng:** HG **Measuring Point:** Ground Surface

Diameter: 6" **Depth to Water in MW (ft):** 5.51




Silty Fine Sand (SM)
Fine Sand (SP)
Clay
Low
to
rvledium
Plasticity
CH

35- 71.8-

40- 66.8-

PHASE I ENVIRONMENTAL SITE ASSESSMENT

MAC Storage Inc.
233 Maple Road
Jackson, Kansas 45974

Prepared by

Geosyntec consultants

130 Research Lane, Suite 2
Guelph, ON N1G 5G3

Project Number TR0637

March 2017

Geosyntec consultants

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF APPENDICES

1. INTRODUCTION

Geosyntec Consultants (Geosyntec) was retained to perform a Phase I Environmental Site Assessment ("Phase I ESA") at a former solvent storage and transfer facility owned by MAC Storage, Incorporated. The facility is located at 233 Maple Road, Jackson, Kansas (referred to herein as the "Site").

1.1 Purpose

This Phase I ESA was conducted in general accordance with the scope and limitations of the guidance contained within the ASTM International Standard Practice for Environmental Site Assessments: Phase I Environmental Site Assessment Process (hereafter, ASTM E1527-13). Any exceptions or deviations to the guidance contained in ASTM E1527-13 are described in Section 7. The Phase I ESA was conducted to identify, to the extent feasible, "Recognized Environmental Conditions[1]" (RECs) at the Site, as the "REC" term is defined by ASTM E1527-13. This REC definition eliminates from consideration a number of conditions that could fall under the general definition of "environmental" issues and focuses the Phase I ESA on known or potential releases of hazardous substances.

1.2 Scope of Services

The Phase I ESA scope of work included: (i) reviewing pertinent information/documents provided by MAC Storage; (ii) reviewing environmental databases for the Subject Property and surrounding properties pursuant to ASTM E1527-13; (iii) reviewing historical land usage via historical aerial photographs, fire insurance rate maps, city directories, and United States Geological Survey (USGS) topographic maps, as available; (iv) a visual reconnaissance of the major features of the Site; and (v) reviewing Site operations and existing permits and plans provided by the Site owner or representative, and evaluating compliance with applicable state and federal environmental programs. The Site visit was conducted in November 20146

1.3 Significant Assumptions

No significant assumptions were made while conducting this Phase I ESA.

1.4 Limitations and Exceptions

This Phase I ESA report contains a description and history of the Site, an environmental database review, a summary of visual observations made during the reconnaissance of the Site, and a description of information obtained during interviews of persons knowledgeable with the Site.

---

[1] As defined by ASTM E1527-13, a Recognized Environmental Condition is: "the presence or likely presence of any hazardous substances or petroleum products in, on, or at a property: (1) due to any release to the environment; (2) under conditions indicative of a release to the environment; or (3) under conditions that pose a material threat of a future release to the environment. *De minimis* conditions are not Recognized Environmental Conditions."

The findings and conclusions presented in this Phase I ESA report are the result of professional interpretation of the information collected at the time of this study. The Phase I ESA report does not necessarily include an exhaustive search of all available records, nor does it include detailed assessment of all Phase I ESA findings.

1.5 Special Terms and Conditions

No special terms or conditions were taken into account as part of this project.

1.6 User Reliance

This Phase I ESA report has been prepared solely for the client. No third party shall have the right to rely on opinions rendered in connection with the services described.

2. SITE DESCRIPTION

This section describes the key characteristics of the Site. These descriptions were derived from information gathered during the reconnaissance unless referenced otherwise. The Site is owned by MAC Storage Inc. Mr. John Rivers, the former Site Manager, was interviewed during the Site visit, and provided some of the pertinent information referenced in this section.

2.1 Site Location and General Characteristics

The Site is located at 233 Maple Road, Jackson, Kansas. The City of Jackson is located in the south-central portion of the State of Kansas. Based on information from the Jackson County Assessor's website, the Site occupies one parcel with identification number 0061-15-1-918-02 and occupies approximately 17 acres.

Land use adjacent to the Site is agricultural to the north, south and west, and industrial to the east, as shown on **Figure 1**. The Site is bordered by Maple Road on the East and South Sides. There are no residential properties bordering the Site.

2.2 Site Use

The Site operated as a solvent storage and transfer facility from 1990 to 2010. During its operation, the Site contained one office building, a covered transfer station situated in the eastern portion of the property attached to the office building, and a storage facility consisting of five 10,000 gallon above ground storage tanks at the southern side of the Site. An underground line connected the storage facility to the transfer station. Primary operations at the Site included the storage of trichloroethene (TCE) and transfer of TCE to small volume totes and containers for sale to local facilities. A parking lot was located west of the transfer station, and the remainder of the Site consisted of open land with grass cover (Figure 2). The facility halted operations in February 2008. In 2010, the ASTs and underground line were removed, the building was demolished and the ground surface graded flat. No commercial activities have been conducted on Site since that time.

2.3 Description of Structures, Roads, Other Improvements

This section contains a description of the structures, roads and improvements observed by Geosyntec during the Site visit in 2016. The construction dates were noted in documents provided by Mr. John Rivers of MAC Storage during the on-site interview. These documents indicate that MAC Storage was developed on former agricultural land. Construction of the facility was completed in 1989 and operations commenced in 1990. The Site entrance is on the eastern portion of the Site off Maple Road.

Storm water runoff from Site generally drains from paved areas of the Site towards storm sewers located on Maple Road, or infiltrates into ground at unpaved areas of the Site (due to the flat topography of the Site, there is little overland flow).

The Site was connected to the municipal water supply. Four monitoring wells are currently located on Site (locations shown in Figure 2).

The Site was connected to the municipal sanitary sewer system. Both sanitary wastewater and pre-treated industrial wastewater were discharged to the municipal sanitary sewer system.

2.4 Physical Setting

The area is characterized by flat lands. The lithology in the region consists of interbedded sands and clays underlain by sandstone bedrock. Based on Site well logs, overburden at the site consists of layered sands and fine sands and confining clays. The approximate depths of the various layers are as follows:

- Clay layer at surface that is approximately 3 ft thick;
- Fine to medium sand aquifer from approximately 3 to 28 ft bgs;
- Clay from approximately 28 to 52 ft bgs;
- Silt and fine sand aquifer from approximately 52 to 85 ft bgs; and
- Clay to the bottom of borings at 90 ft bgs.

The ground surface elevation at the Site is flat at an elevation of approximately 222 feet above mean sea level (ft amsl). There is no sloping of the ground surface topography in the Site. Ground surface elevation across the Site is shown in **Figure 3**.

3. USER-PROVIDED INFORMATION

This section describes the information provided to Geosyntec by the User of this Phase I ESA, who is considering the acquisition of the Site.

3.1 Title Records

A chain of title search was not included in the scope of services for this project.

3.2 Environmental Liens or Activity and Use Limitations

A search for environmental liens or activity and land use limitations (AULs) associated with the Site was conducted. No environmental liens or AULs were found.

3.3 Specialized Knowledge

Mr. John Rivers accompanied Geosyntec on the Site reconnaissance and interview, and supplied Geosyntec with specialized knowledge regarding the history of MAC Storage, and general operations of the facility to the best of his knowledge.

3.4 Owner, Property Manager, and Occupant Information

The Subject Property is owned and operated by MAC Storage.

3.5 Reason for Performing This Phase I ESA

Geosyntec understands the performance of a Phase I ESA for the Site was requested to assist in identifying potential environmental liabilities associated with the Site prior to sale of the land.

4. RECORDS REVIEW

The records review consisted of: i) reviewing applicable federal, state, and local environmental databases; ii) reviewing readily available and identified historical aerial photographs, topographic maps, fire insurance maps and city directories; iii) reviewing readily available previous site investigation reports; and iv) reviewing potential for soil vapor impacts.

4.1 Environmental Database Search

4.1.1 Database Search Approach

Geosyntec reviewed applicable and reasonably ascertainable federal, state, and local environmental databases as part of this Phase I ESA. The environmental database search was performed to ascertain whether the Site or the surrounding properties were suspected of having environmental conditions that could have impacted the structures, soil, groundwater, or surface water at the Site.

4.1.2 Database Search Results

The significant findings of the database search as related to the Site are described below.

The Site was identified by address as 233 Maple Road, Jackson, and by name as MAC Storage. The Site was identified in the following databases.

- Kansas Tier 2 database:

  MAC Storage is listed in the Kansas Tier 2 database, indicating the storage of hazardous chemicals under the Kansas and Federal Emergency Planning and Community Right to Know Act.

4.2 Historical Records Review

Available historical records were reviewed. No fire insurance maps or property tax maps were found for the Subject Property.

Historical aerial photographs and topographic maps for the Site area are not available. **Figure 1** shows a recent aerial photograph of the Site.

4.3 Previous Environmental Investigations

A limited Site investigation was completed at the request of the Owner to evaluate the condition of the Site prior to listing the land for sale. The following activities were conducted as part of this investigation:

- Installation of 4 shallow and 4 deep groundwater wells;
- Soil sampling in November 2016;
- Groundwater sampling in December 2016;
- Groundwater levels were measured in December 2016.

The data from this investigation are provided in Appendix A of this report. This includes soil concentration data from samples collected during well installation (Tables A.1), fraction of organic carbon (foc) data from soil samples (Table A.2), groundwater elevations in December 2016 (Table A.3), and groundwater concentrations from December 2016 (Table A.4). Concentrations were below detection limits at 3 of 4 boring locations, but trichloroethene (TCE) and cis-dichloroethene (DCE) were detected in soil at BH-1S and BH-1D and in groundwater at MW-1S.

5. SITE RECONNAISSANCE

5.1 Methodology and Limiting Conditions

A reconnaissance of the Site was conducted by qualified personnel with Geosyntec in November 2016.

As part of the reconnaissance, Geosyntec attempted to look for evidence of used, stored, or discarded hazardous substances, areas of disturbed or discolored soil, suspect equipment and/or building materials that may contain hazardous substances, areas of distressed vegetation, wastewater discharge areas, storage tanks/septic systems, waste management/disposal areas, lagoons, pits, sumps, surface water management areas, and stained surfaces. As the Site is demolished, much of the information was obtained through an interview with Mr. Rivers. Adjoining properties were peripherally observed from the perimeters of the Site and from public rights-of-way.

The significant findings from the reconnaissance of the Site are described below.

Transfer Station

- The majority of the former transfer station was used to transfer TCE from the storage facility into smaller totes and containers. These containers were temporarily stored at the transfer station until they were shipped off-Site. This Area is noted on Figure 2 as "Former Transfer Station"

Chemical Storage Areas

- The chemical storage area was an outdoor area consisting of five 10,000 gallon ASTs. TCE was the only chemical that is known to have been stored at this facility. Mr. Rivers noted that the tanks were refilled on a bi-weekly to monthly basis. The former chemical storage area is indicated on Figure 2.

6. INTERVIEWS

During the Site reconnaissance in November 2016, Geosyntec conducted an interview with Mr. Rivers of MAC Storage. Mr. Rivers was knowledgeable about the history and operations of MAC Storage and was forthcoming with information when asked. Pertinent information provided by Mr. Rivers is presented throughout this Phase I report.

7. EVALUATION

As required by ASTM E1527-13, this section presents the Geosyntec-identified known or suspect recognized environmental conditions (RECs), controlled recognized environmental conditions (CRECs), historical recognized environmental conditions (HRECs), and / or *de minimis* conditions at the Subject Property.

A CREC is a recognized environmental condition resulting from a past release of hazardous substances or petroleum products that has been addressed to the satisfaction of the applicable regulatory authority with certain restrictions or controls.

An HREC is a recognized environmental condition resulting from a past release of hazardous substances or petroleum products that has occurred in connection with the property and has been addressed to the satisfaction of the applicable regulatory authority, without subjecting the property to any restrictions or controls.

de minimis conditions generally do not present a threat to human health or the environment and generally would not be the subject of an enforcement action if brought to the attention of appropriate governmental agencies.

7.1 Findings

The following findings (locations shown in Figure 2) were identified as having the potential to be known RECs, CRECS, HRECs, and/or *de minimis* conditions at the Site are listed below (these are not in any particular order of importance):

FINDING A: A former storage area used by MAC Storage was located at the southeastern side of the Site.

FINDING B: A former transfer facility connected to the storage facility located to the southeast. The two facilities were connected via underground piping to transfer TCE for shipping**.** Mr. Rivers recalled observing staining on the floor of the transfer facility.

FINDING C: Chlorinated solvents in soil and groundwater were detected during the 2016 sampling event. TCE and cDCE were detected in the groundwater at monitoring well MW-1S at concentrations of 151.96 and 47.48 milligrams per litre (mg/L), respectively, which exceeded the USEPA MCLs of 0.005 and 0.07 mg/L.

7.2 Opinions

This section includes the environmental professional's opinion(s) of on Site conditions identified in the findings section. Frequently, items initially suspected to be a recognized environmental condition are subsequently found, upon further evaluation, not to be considered a recognized environmental condition. The opinion includes the rationale for concluding that a condition is, or is not currently a recognized environmental condition.

Based on the information obtained during this investigation, Geosyntec has identified the following findings as known RECs or CRECs, based on the ASTM E1527-13 definition of a REC and CREC.

FINDING A: Former Storage Facility is a REC, condition of the storage tanks could not be observed during the Site visit. Potential cracking or corrosion could have led to a release to underlying soil and groundwater.

FINDING B: Former Transfer Facility is a REC, because staining was noted during the interview. No records of decommissioning, clean-up, material disposal, or confirmation wipe sampling in this area were made available, creating a data gap.

FINDING C: Chlorinated solvents in groundwater exceeding an USEPA MCL is a REC.

7.3 Data Gaps

In accordance with ASTM E1527-13, this section documents data gaps in the information obtained and reviewed as part of this Phase I ESA and discusses the associated significance. A data gap is defined as being "a lack of or inability to obtain information required by this practice [ASTM E1527-13] despite good faith efforts by the environmental professional to gather such information". The following data gaps were identified:

- **Former Storage Facility:** data gaps exist because the storage tank was removed prior to the Site Visit and their condition could not be observed. Additionally, it is unknown if there were cracks in the tanks that might have resulted in a release to the environment.

- **Former Transfer Facility:** data gaps exist because it is unknown if a release may have occurred during the transfer process, during Site operation, prior to demolition of the facility.

7.4 Conclusions

Geosyntec performed a Phase I ESA in conformance with the scope and limitations of ASTM Practice E1527-13 of the chemical storage and transfer facility operated by MAC Storage. Any exceptions to, or deviations from, this practice are described in Section 7.5 of this report. This assessment has revealed evidence of the following RECs at the Site:

FINDING A: Former Storage Facility

FINDING B: Former Transfer Facility

FINDING C: Chlorinated Solvents in Soil and Groundwater

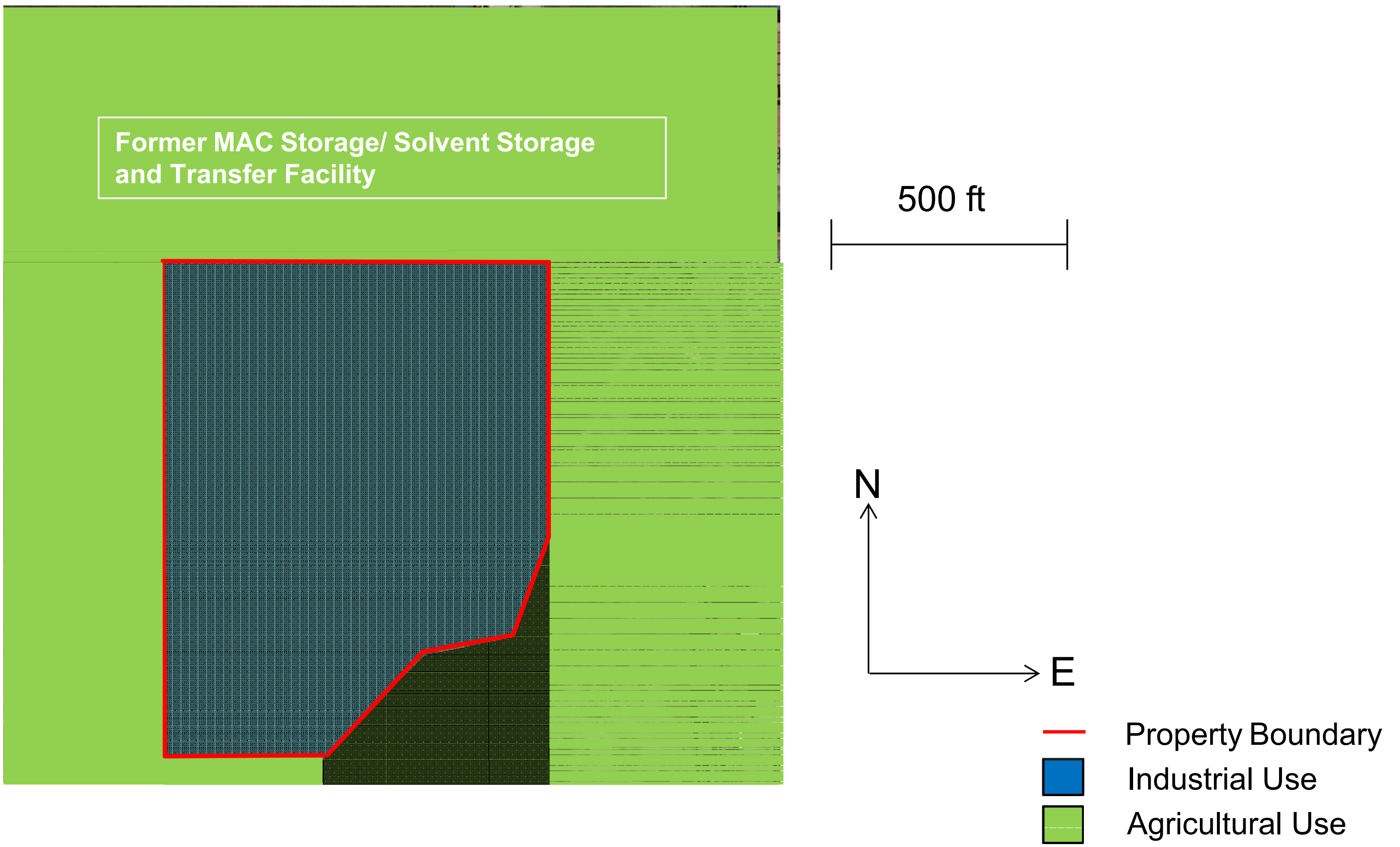
7.5 Deviations

There were no exceptions or deviations from the ASTM E1527-13 standard of practice in the performance of this Phase I ESA.

7.6 Statement of Environmental Professionals

"We have the specific qualifications based on education, training, and experience to assess a property of the nature, history, and setting of the Subject Property. We have developed and performed all appropriate inquiries in conformance with the standards and practices set forth in 40 CFR Part 312."

FIGURES



Property Boundary and Surrounding Land Use

Geosyntec consultants

Figure 1

Guelph

March 2017

internal info: path, date revised, author

Geosyntec consultants