

# EXECUTIVE SUMMARY

Development of an Integrated Field Test/Modeling Protocol for  
Efficient In Situ Bioremediation Design and Performance  
Uncertainty Assessment

SERDP Project ER-2311

APRIL 2019

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## 1.0 INTRODUCTION

Widespread use of chlorinated solvents, such as tetrachloroethene (PCE) and trichloroethene (TCE), in dry cleaning and degreasing operations has resulted in groundwater contamination at thousands of industrial facilities and government installations throughout the United States and abroad (ITRC, 2011; NRC, 2005). In most cases, chlorinated solvent spill sites are conceptualized as consisting of two main regions, a highly contaminated source zone that often contains free product, commonly referred to as a dense non-aqueous phase liquid (DNAPL), and a down-gradient groundwater plume that contains both dissolved- and sorbed-phase contamination (ITRC 2003). The long-term persistence of DNAPLs (as entrapped ganglia or pools) in the source zone and the high local contaminant concentrations associated with their presence also creates a strong driving force for contaminant diffusion into lower permeability layers, where dissolved and sorbed mass is subsequently sequestered. Substantial laboratory and field research has demonstrated the importance of this sequestered mass to the persistence of down gradient contaminant plumes (e.g., DiFilippo and Brusseau, 2008; NRC, 2005; Parker et al., 2008; Suchomel and Pennell, 2006) and the long term performance (mass removal or transformation rates) of most remedial technologies, in particular those that require the delivery of chemical additives or amendments (e.g., Christ et al., 2010; Kaye et al., 2008; Stroo et al., 2003).

Although substantial progress has been made in the development of both noninvasive and invasive source zone characterization technologies in the past two decades (e.g., ITRC, 2003; Kavanaugh et al., 2003; Kram et al., 2002; NRC, 2005), these technologies can typically provide quantitative information on contaminant mass distributions only in the vicinity of the sampling location, which may not be representative of the entire source zone. To address the limitations associated with sparse sampling, it is now common practice to employ statistical interpolation approaches (e.g., kriging) to estimate contaminant concentration at unsampled locations using available borehole data. However, a primary drawback to such approaches is their limitation in interpolating highly sparse and discontinuous patches of DNAPL in heterogeneous domains (e.g., Maji et al., 2006).

The challenges posed by detailed (fine-scale) delineation of source zone mass have also led to the development and application of averaged characterization metrics, such as DNAPL mass spatial moments, pool fraction, trajectory-averaged saturation statistics, and ‘source strength’, that can represent the salient features of the mass distribution (e.g., Stroo et al., 2003; ITRC, 2004; Jawitz et al., 2005; Christ et al., 2006; Saenton & Illangasekare, 2007; Chen and Jawitz, 2009). Here, the hypothesis is that such metrics can be employed in upscaled mathematical models to predict source longevity and down-gradient flux evolution under natural or remedial conditions. Comparisons to laboratory data (Fure et al., 2006; Zhang et al., 2008; Christ et al., 2010; DiFilippo & Brusseau, 2011) and field data history matching exercises (DiFilippo and Brusseau, 2008; Falta et al., 2005b) suggest that such approaches may hold promise, particularly for use in screening remedial alternatives.

Unfortunately, most laboratory treatability studies do not adequately mimic the mass transfer processes, such as rate-limited dissolution, diffusion and desorption, that control elution of sequestered mass and remedial system performance in a natural heterogeneous formation. Thus, such studies tend to overestimate potential treatment effectiveness. For example, a comparison of 138 chlorinated solvent bioremediation field and laboratory studies revealed that median

laboratory rate constants were consistently higher (up to one order-of-magnitude) than observed field rate constants (Suarez and Rifai, 1999). The assumptions underlying the selection of a down-hole treatability (DHT) methodology for this research are that: (a) even advanced assessment tools, such as molecular probes, fail to provide reaction rate information necessary to predict remediation extent in complex subsurface environments; and (b) the tool or method should provide information that is relevant at the field scale and can be readily incorporated into model(s) for simulation of remediation performance and uncertainty assessment.

The above discussion highlights the urgent need for better field treatability test methods to predict potential remedial system performance and for the development of improved, cost-effective, field characterization methods and associated modeling tools that encompass all source zone mass and facilitate the identification of the most critical source zone properties that will govern mass persistence and the performance of remedial options.

## 2.0 OBJECTIVES

The overarching goal of this research project is to develop and demonstrate a remediation design and performance assessment protocol that can efficiently assess the suitability of a remediation technology and predict remedial performance (e.g., mass removal/destruction) and the uncertainty associated with such predictions. This protocol couples careful characterization of the contaminant source with down-hole treatability testing and mathematical modeling. The research directly responds to the following specific objectives in the SERDP Statement of Need:

- 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 performance.
- Development of field measurements or methodologies that provide data to optimize treatment if current operations are not expected to meet performance objectives.
- Development of assessment procedures and methodologies that aid in the decision to discontinue operation of a technology and implement an alternative technology.

The fundamental hypothesis of this work is that it is impossible to provide reliable predictions of remedial performance, and its associated uncertainty, without consideration of the complex coupling between contaminant transformation/reaction rates, contaminant mass distribution (spatial configuration and phase partitioning), and the processes influencing the accessibility of this mass (e.g., heterogeneous flow paths, diffusion). Although the project utilizes microbial reductive dechlorination as a representative *in situ* remediation technology, the developed protocol and associated modeling tools are applicable to other remediation technologies, such as monitored natural attenuation and chemical oxidation.

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### 3.0 TECHNOLOGY DESCRIPTION

The research approach involves coupling of site characterization, remediation performance assessment (reaction rates), upscaled model development, and numerical simulations of remedial performance and uncertainty. The study focused on a representative TCE-contaminated site (Commerce Street Superfund Site, Williston, VT) to facilitate the development, refinement and testing of protocols and software tools within the context of an actual field site.

To achieve its goal, the project was structured around three phases that addressed: (i) source and plume characterization, (ii) upscaled mass transfer and transformation rates, and (iii) field-scale reactivity and predictions of remedial performance. The project work plan is illustrated in Figure E-1.

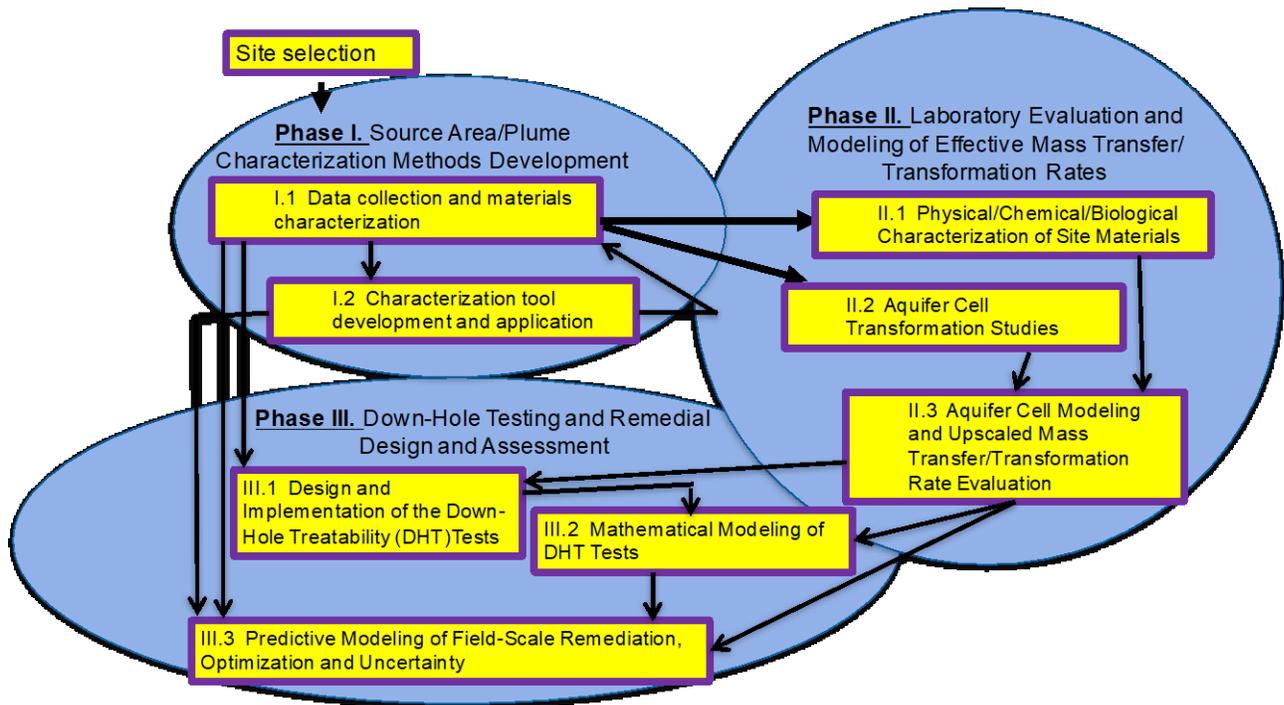


Figure E-1. Project Work Plan.

**Phase I** focused on the development and demonstration of methods/modeling tools to characterize the source zone for subsequent remedial design, implementation, and assessment. Here, the specific objective was to develop a protocol and software tools that employ measured field data to produce a representation of the subsurface source zone that captures the spatial distribution and uncertainty associated with key features (permeability, microbial activity/mass, and sequestered contamination [sorbed, immobile aqueous, and NAPL]) that control remedial performance.

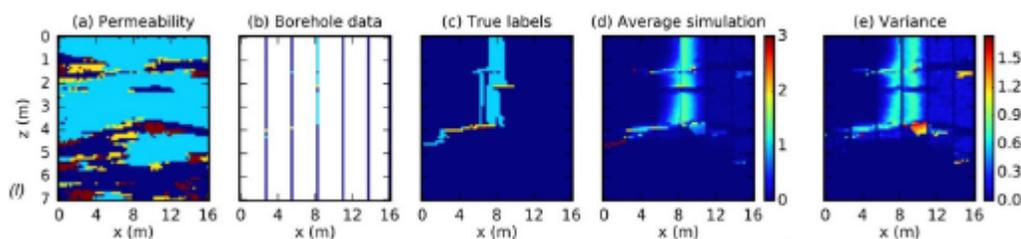
**Phase II** focused on batch and bench-scale laboratory testing, and upscaled mathematical model development to support the design and implementation of a field remediation strategy. Here, the performance of microbial reductive dechlorination was evaluated in aquifer cells that were representative of field conditions, and the resulting data were employed to develop and evaluate upscaled models to describe effective mass transfer and reaction rates.

**Phase III** focused on the estimation and application of effective rate parameters in field-scale remediation. In this phase, a downhole treatability test was conducted at the Commerce Street Superfund Site to estimate effective *in situ* transformation/reaction rates and to support the design and assessment of site remediation strategies. Here a mathematical model, refined and validated in Phase II, was employed to estimate effective field transformation rates. Estimated rates were then compared to batch- and aquifer cell-measured rates to shed light on the processes controlling remediation at the field scale. In addition, a traditional three-dimensional flow and transport simulator was adapted and employed, in conjunction with the source zone characterization and uncertainty results from Phase I, to propose an optimal sampling strategy coupling sensitivity analysis and uncertainty quantification.

## 4.0 PERFORMANCE ASSESSMENT

### 4.1 PHASE I

A novel statistical approach was developed and implemented for the reconstruction of non-aqueous phase liquid (NAPL) source zone realizations and the quantification of source zone metrics and associated uncertainty. This approach employed discriminative random field (DRF) models, originally introduced for computer vision applications, to model the spatial distributions and relationships among source zone properties (permeability, NAPL saturation and aqueous concentration distributions) consistent with commonly collected field data. Application of DRF models required a limited number of full-scale simulations to train the model parameters. Monte-Carlo sampling methods based on these trained models then provided an efficient method to generate contaminant mass realizations conditioned on measured borehole, bypassing the need to run computationally intensive, partial differential equation-based simulations of physical flow and transport. Post-processing of these realizations yielded approximations of uncertainty to inform further sampling for characterization and remediation (Phase III). The reconstructed contaminant mass realizations provided sufficient information for calculating averaged characterization metrics, such as total contaminant mass and pool fraction (PF), used to predict source zone longevity, mass recovery behavior and remedial performance. The model performance was evaluated through comparisons of these predicted source zone metrics with those obtained from the ‘true’ mass distributions generated with validated flow and transport models. These comparisons clearly demonstrated that the trained DRF model can reconstruct realistic saturation and concentration fields conditioned to borehole data for a range of NAPL spill scenarios (see example in Figure E-2). The model was also shown to significantly outperform traditional kriging approaches in reconstructing NAPL mass distributions.



**Figure E-2. Example Output of BRAINS Model for Estimation of DNAPL Saturation Distribution Profile in a Heterogeneous Formation.**

*Depicted output (d) is the average of 2000 realizations.*

#### 4.1.1 Selected Conclusions from Phase I:

- **A DRF model (BRAINS) was developed and implemented for contaminant source zone characterization and uncertainty quantification.** The DRF model is completely characterized by a small collection of parameters ( $w$  and  $v$  vectors). These parameters are determined through a ‘training’ process, employing a set of source zone spill data specific to the selected DNAPL contaminant and geologic environment. Once the DRF parameters are determined, the model can be used to generate realizations of the DNAPL saturation and aqueous phase concentration using off-the-shelf Metropolis sampling methods.

This methodology is far superior to Monte Carlo approaches, which require extensive flow and transport simulations to generate a similar set of realizations and cannot easily account for measured data.

- **Ensemble averages over realizations of the DRF model represent the expected values for concentration and saturation fields, while the variances provide a quantifiable measure of the uncertainty associated with permeability and contaminant source zone.** These uncertainty measurements were used in Phase III to identify optimal locations for further borehole sampling.
- Model performance was assessed by comparing estimated and ‘true’ metrics for contaminant mass distributions in a structured heterogeneous unconsolidated depositional aquifer environment. **The trained DRF model produced realistic saturation and concentration fields, conditioned to borehole data for a range of NAPL spill scenarios (release rates, spill ages, pool fractions). Comparison with a traditional kriging approach clearly demonstrated the superiority of BRAINS in reconstructing DNAPL saturation distributions and associated DNAPL architecture metrics.**

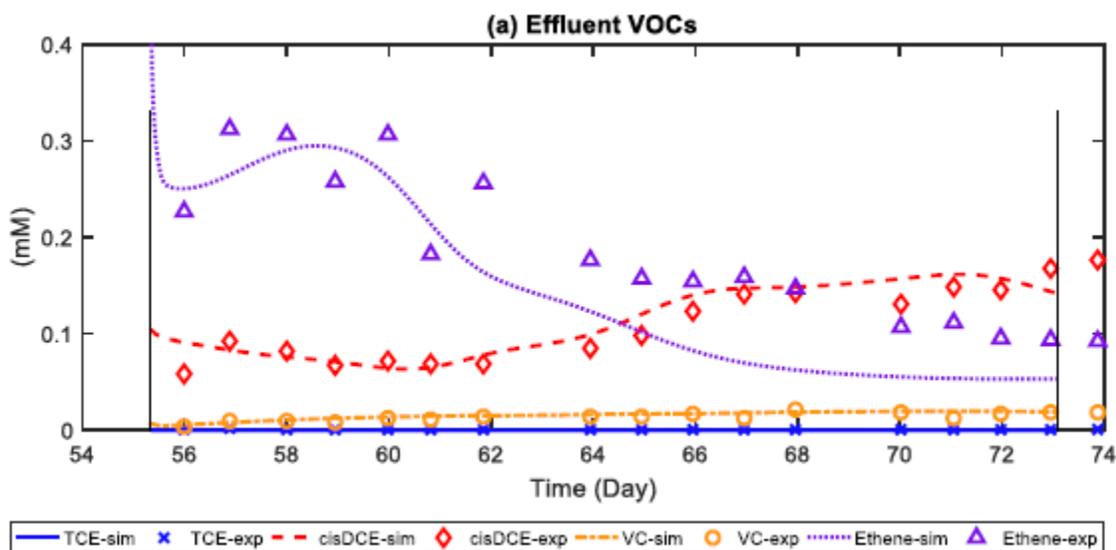
## 4.2 PHASE II

Microcosms were provided with lactate and TCE to derive dechlorination rates in a batch system and one set was amended with SiREM KB-1®. Microcosm and batch reactor experiments demonstrated the need for bioaugmentation and biostimulation at the site to transform TCE to ethene. The native microbial population was capable of transforming TCE to 1,2-Dichloroethene (*cis*-DCE) using the dissolved organic carbon in site groundwater but completed the transformation more quickly when supplied with lactate as an electron donor. The absence of continued dechlorination in most reactors indicated a low population of *Dehalococcoides* (*Dhc*) harboring the RDase genes necessary to produce vinyl chloride (VC) and ethene and a non-uniform distribution of organisms at the site. Bioaugmentation of reactors with KB-1® or Bio-Dechlor INOCULUM (BDI) was successful, facilitating the transformation of TCE to ethene in an average of 37 days. A robust numerical model incorporating adsorption of contaminants to soil and partitioning into the bottle headspace was created to simulate microbial reductive dechlorination in the batch reactors and microcosms. The numerical model and Matlab fitting routine were able to match the chlorinated ethene and ethene concentrations observed in the KB-1® bioaugmented microcosms, providing culture-specific yield coefficients and substrate utilization rates that were used in later modeling work.

Concurrently, an aquifer cell system was constructed with soil from the Commerce Street field site, loaded with TCE, and configured to mimic the field-scale downhole treatability test. The aquifer cell was provided with lactate and then bioaugmented with KB-1®. Effluent and side port measurements of volatile fatty acid concentrations, chlorinated ethene and ethene concentrations, and biomass abundance were used in conjunction with an enhanced version of the modular three-dimensional multispecies transport simulator MT3DMS to explore effective bio-reaction rates (e.g., maximum substrate utilization rates ( $\mu_{max}$ )). This enhanced version of MT3DMS is capable of simulating anaerobic reductive dechlorination of multiple contaminants in heterogeneous environments, incorporating consumption of the carbon source by a competitor culture. Microbial reductive dechlorination is modeled with a modified Monod kinetic expression that accounts for limitations due to electron donor availability and daughter product inhibition.

Model simulations employing batch-measured rates provided a good prediction of aquifer cell behavior (average relative error of 19%) only when heterogeneity was explicitly modeled and TCE and cis-DCE inhibition of VC transformation was neglected (see Figure E-3). This result was attributed to spatial variations in microbial population and substrate availability created by the presence of physical heterogeneity. Comparison of simulation results for models employing both heterogeneous and uniform domain properties, incorporating the same domain size and transformation rate parameters, revealed that ethene production was underpredicted by the uniform property model. This result contrasts with literature reports of field-scale reductions in observed effective transformation rates. Coupling of laboratory observations with modeling results suggests that transformation to ethene varied spatially within the domain, primarily associated with low permeability layers (zones with longer residence times). This variation demonstrates the influence of local heterogeneity on dechlorination prediction accuracy. To investigate the effect of the residence time on dechlorination, the flow rate was reduced by 50%, increasing the proportion of ethene in the aquifer cell (molar basis) from 26% to 54%.

Also in this project phase, upscaled modeling was undertaken to develop solutions and correlations to quantify effective mass transfer coefficients that describe back-diffusion/desorption and bioenhanced NAPL dissolution under a range of heterogeneous formation conditions.



**Figure E-3. Comparison Between Simulated and Experiment Effluent Concentrations for Chlorinated Ethenes and Ethene Components.**

*Competitive inhibition was neglected in this simulation.*

#### 4.2.1 Selected Conclusions from Phase II

- An industry-standard groundwater transport simulator, MT3DMS, was adapted to incorporate multi-order Monod kinetics coupled with a microbial growth model to account for biotransformation of multiple components by multiple microbial populations.

- **Bioenhanced desorption and back diffusion of chlorinated solvents play an important role in mass release in heterogeneous formations.** For the examined experimental conditions, the magnitude of this enhancement was observed to vary spatially and temporally (from 6-55%), with the largest enhancement measured at interfaces with fine-textured, highly sorptive media. These results demonstrate that bioenhanced desorption/back diffusion can significantly reduce plume persistence and remedial cleanup timeframes.
- **Temporal and spatial population shifts in the predominant strain of *Dhc* are observed with changes in electron acceptor abundance.** These observations demonstrate the importance of maintaining a robust dechlorinating community harboring multiple RDase genes. When the necessary genes are present, the microbial population is able to adapt to changes in electron acceptor availability associated with varying up gradient concentrations or the back diffusion of chlorinated ethenes from low permeability and highly sorptive materials.
- ***Dhc* cells are capable of penetrating low permeability porous media, including clays.**
- **Observed aquifer cell microbial transformation rates were consistent with microcosm (batch)-fitted values, when permeability variations were incorporated in the model. Thus, models must incorporate heterogeneity to make accurate predictions of dechlorination.**
- **Competitive inhibition was found to be of little significance in heterogeneous-packed formations,** attributed to microenvironments in the aquifer cell and differences in soil/water ratios between microcosm and aquifer cell experiments.
- **Accurate representation of sorption processes (extent, rate limitations, and nonlinearity) in transport models is crucial to the accurate prediction of plume longevity,** particularly for the prediction of post-DNAPL dissolution longevity; (de)sorption processes were observed to dominate the rate of mass release (back diffusion) to transmissive zones, following DNAPL dissolution.
- **An upscaled model was developed and parameterized to describe effective mass transfer (desorption) rates in three dimensional heterogeneous systems.** This Multi-Rate Mass Transfer (MRMT) model, with two constant-in-time first-order rates, was shown to successfully reproduce breakthrough curves.
- **A screening level model was developed and implemented to estimate bioenhancement of DNAPL dissolution.** Nomographs were presented to facilitate graphical estimation of bioenhancement factor expressions for zero-order, first-order, and full Monod transformation kinetics as a function of the Péclet and Damköhler Numbers.

### 4.3 PHASE III

A DHT test was conducted at the Commerce St site and test observations were used, in conjunction with the enhanced MT3DMS model, to estimate effective *in situ* biotransformation rate parameters. Simulations of the field pilot test, using aquifer cell-calibrated rate parameters that had been adjusted for temperature effects, resulted in an over-prediction of ethene production by a factor of 2. Model sensitivity analyses suggested that this discrepancy, observed between laboratory and field transformation rates despite the comparable sizes of the aquifer cell and pilot test treatment zone, was associated with unmodeled heterogeneity in flow and biomass distributions.

Similar to the behavior observed in the cell experiment, when the flow rate in the test zone was reduced by 50%, the observed proportion of ethene increased from 17% to 78% at the end of the treatment zone. These data demonstrate that controlling residence time is essential to completely detoxify TCE to ethene.

Also, in this project phase, adjoint sensitivity analysis was employed, in conjunction with a first-order second-moment (FOSM) uncertainty analysis method, to develop a systematic approach to optimize borehole sampling for prediction of down-gradient flux-averaged concentration (FAC) evolution at a contaminated site. In this approach, an initial conditioned spatial distribution of contaminant mass is first generated by averaging realizations of the DRF model developed in Phase I. The adjoint state method is then used to quantify the importance of local system properties on down-gradient FAC. The FOSM method, which uses linear approximations to directly propagate parameter and data uncertainties into system states via sensitivity matrices, is employed to estimate the uncertainty of FAC predictions. Both permeability and source zone mass compartments are treated as random variables to account for aquifer heterogeneity, flow irregularity, source zone morphology, and their interlinkages. Then in the decision process, data worth analysis is used to develop an optimal borehole sampling strategy by selecting additional measurements that yield the largest reduction in FAC uncertainty. The entire approach was implemented in the widely-used transport modeling platform MT3DMS to facilitate future adoption by practitioners and site managers. The utility of this approach was demonstrated using numerically generated, two-dimensional, heterogeneous DNAPL source zones. Results reveal that the model-guided sampling strategy recommends additional sampling locations that vary with the prediction time window; optimal borehole measurements are chosen further down-gradient for early time predictions, while up-gradient measurements have larger impact at later times. Locations with low permeability values and high DNAPL saturations are generally good potential candidates for additional measurements. Comparison of predictions associated with the optimized versus a uniform sampling approach reveals that the FOSM model yields better estimates of down-gradient flux averaged concentration, associated with a significant reduction in variance. This innovative sampling strategy, coupling sensitivity analysis and uncertainty quantification, shows promise for enhancement of our ability to guide characterization of source zones under realistic field conditions.

Finally, in this phase, project results were integrated into a source zone remediation feasibility framework to guide practitioners on the use of the developed modeling methodologies (see description in next section). This framework provides an efficient method to perform site characterization and obtain screening-level forecasts of site behavior, with and without implementation of treatment remedies. Application of the framework to a realistic synthetic field scenario in Section VII.A. of the report demonstrated its feasibility and potential benefits during conceptual site model refinement and remedial site management.

#### 4.3.1 Selected Conclusions from Phase III

- **A FOSM uncertainty analysis modeling framework was developed and implemented to estimate variance in predicted flux averaged concentration along a transect down gradient of a DNAPL source zone.** The method honors borehole observations and enables consideration of the coupling among aquifer heterogeneity, flow irregularity, and source zone mass distribution (morphology). The FOSM model was coupled with data worth assessments and implemented in the modeling framework to guide acquisition of additional site data.

- **Application of the FOSM method to numerically generated, field-scale, source zone scenarios revealed that hydraulic conductivity variations and DNAPL saturation distributions tend to dominate FAC predictions.**
- **Down Hole Test results were consistent with trends observed in the aquifer cell experiment.** Bioaugmentation with KB-1<sup>®</sup> successfully provided a large, viable *Dhc* population capable of transforming *cis*-DCE to ethene over the duration of the pilot test. Lactate pulses were rapidly fermented and provided a growth substrate to increase the *Dhc* population. Growth stalled when the residence time was insufficient to increase the degree of *cis*-DCE dechlorination. A reduction in pumping rate, increased the extent of transformation of *cis*-DCE to ethene and allowed the *Dhc* population to continue to increase in abundance.

## 5.0 IMPLEMENTATION ISSUES

This research provides site managers, regulatory officials, and the scientific community with protocols and software tools to (a) efficiently characterize site conditions, (b) obtain relevant reaction rates and develop upscaled models, and (c) predict remedial performance and associated uncertainty. The developed models and their associated implementation protocols are equally applicable to any remedial technology whose application is hindered by interphase mass transfer limitations, i.e., by heterogeneity in formation properties and contaminant mass distributions.

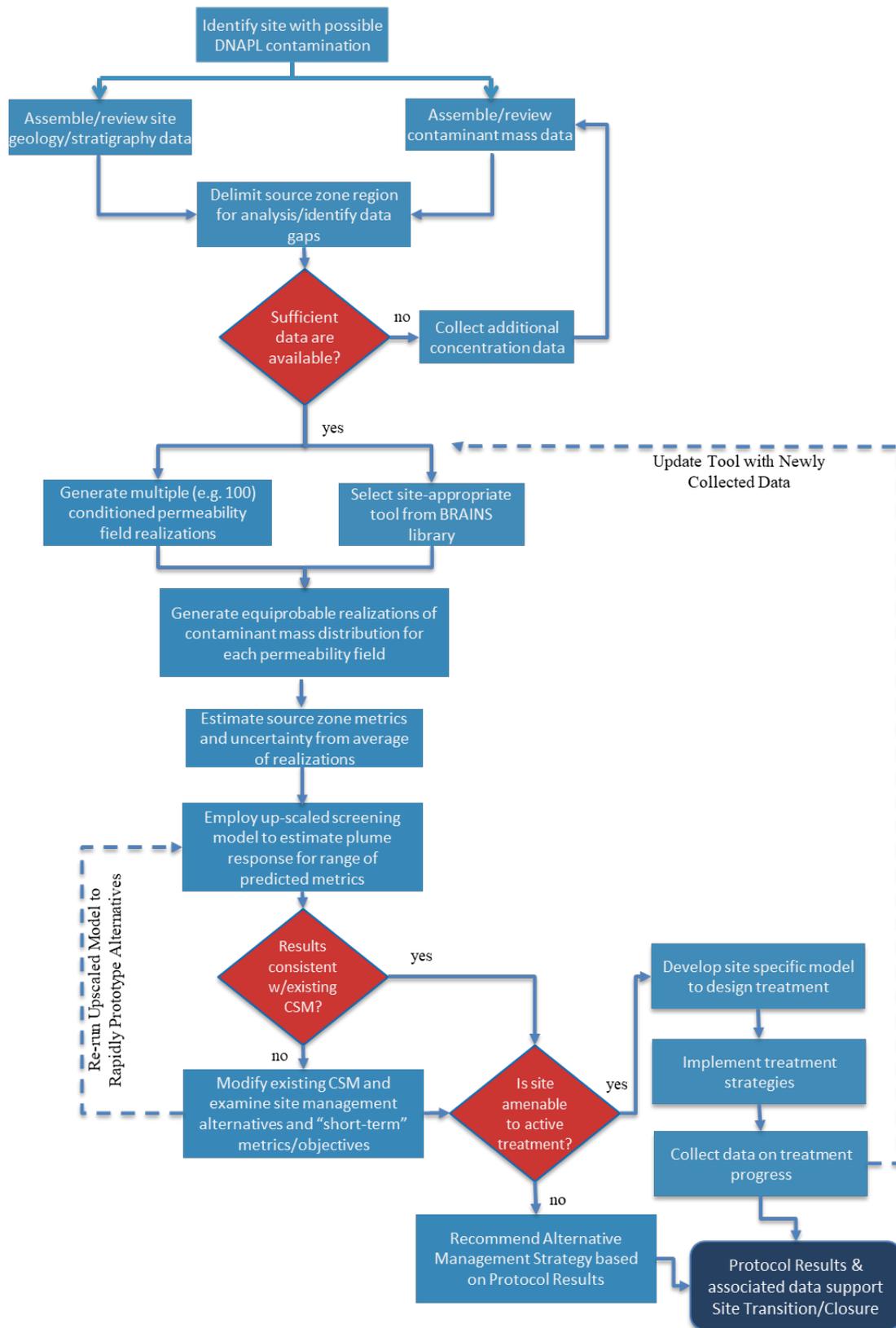
A straightforward framework (Figure E-4) was presented for implementation of the developed mathematical models for near-source site characterization and plume response prediction. This framework couples the 2D BRAINS model with an existing upscaled mass transfer model previously developed under SERDP sponsorship (Christ et al., 2010). The trained BRAINS model is used to generate a set of 2D representations of contaminant mass distributions along a plume centerline. These results enable the estimation of effective, or upscaled, parameters employed in the screening model, as well as the estimation of the uncertainty associated with screening model predictions.

Figure E-4 represents the work flow for site characterization and screening-level FAC assessment. Here, once a DNAPL source zone site has been selected, available data on the site geology/ stratigraphy are collected and matched to a representative site subsurface permeability model. The permeability models are then linked to a library of machine learning characterization tools (BRAINS library).

After a site-matched characterization tool is obtained, BRAINS is employed, along with measured borehole data to estimate source zone metrics. This procedure requires only field-measured borehole data (permeability, saturation, sorption and aqueous concentration) as inputs, as well as some formation geostatistical characteristics. The first step in applying BRAINS to a real-world problem is to generate multiple realizations of the permeability field, conditioned on borehole measurements. Once the permeability realizations have been generated, the site-appropriate trained BRAINS model is applied to each permeability field to derive a set of equiprobable realizations of contaminant mass distribution along the plume centerline. Here all realizations are conditioned available site data (saturations and aqueous and sorbed mass concentrations).

A set of source zone characterization metrics, such as DNAPL mass spatial moments and PF, can then be calculated from the averages of the source zone (saturation and concentration) realizations. This procedure provides a simple and straightforward approach to predict the estimated range of characterization metrics across all equiprobable permeability realizations. Once the ranges for source zone metrics have been estimated, the Protocol employs an upscaled screening tool, presented by Christ et al., (2010), to predict mass recovery behavior; the case study presented in Section VII.A illustrates the use of this screening tool. Screening tool output can then guide preliminary site remediation decisions and future in-source data collection.

This research focused on the development and application of the BRAINS model for one representative heterogeneous unconsolidated formation type in 2D cross section. Thus, it should be viewed as a proof of principle for the application of this modeling approach and as the first step in generating a 3D characterization tool (i.e. library of models). It is anticipated that, while the developed features and model structure are robust, the BRAINS model itself will need to be retrained for applications to different depositional environments. Future work should focus on the development of such a library of trained models and on the design and implementation of a field demonstration of the framework.



**Figure E-4. Site Remediation Feasibility Protocol Flow Diagram.**

## 6.0 REFERENCES

- Chen, X., and Jawitz, J. W. (2009). "Convergence of DNAPL Source Strength Functions with Site Age." *Environmental Science & Technology*, 43(24), 9374–9379.
- Christ, J. A., Ramsburg, A. C., Pennell, K. D., and Abriola, L. M. (2006). "Estimating mass discharge from dense nonaqueous phase liquid source zones using upscaled mass transfer coefficients: An evaluation using multiphase numerical simulations." *Water Resources Research*, 42(11).
- Christ, J. A., Ramsburg, A. C., Pennell, K. D., and Abriola, L. M. (2010). "Predicting DNAPL mass discharge from pool-dominated source zones." *Journal of contaminant hydrology*, 114(1–4), 18–34.
- DiFilippo, E. L., and Brusseau, M. L. (2008). "Relationship between mass-flux reduction and source-zone mass removal: Analysis of field data." *Journal of Contaminant Hydrology*, 98(1–2), 22–35.
- DiFilippo, E. L., and Brusseau, M. L. (2011). "Assessment of a simple function to evaluate the relationship between mass flux reduction and mass removal for organic-liquid contaminated source zones." *Journal of Contaminant Hydrology*, 123(3–4), 104–113.
- Falta, R. W., Rao, P. S., and Basu, N. (2005). "Assessing the impacts of partial mass depletion in DNAPL source zones: I. Analytical modeling of source strength functions and plume response." *Journal of Contaminant Hydrology*, 78(4), 259–280.
- Fure, A. D., Jawitz, J. W., and Annable, M. D. (2006). "DNAPL source depletion: Linking architecture and flux response." *Journal of Contaminant Hydrology*, 85(3), 118–140.
- ITRC. (2003). "Technology Overview: An Introduction to Characterizing Sites Contaminated with DNAPLS." The Interstate Technology & Regulatory Council, Washington, DC.
- ITRC. (2004). "Strategies for Monitoring the Performance of DNAPL Source Zone Remedies." The Interstate Technology & Regulatory Council, Washington, DC.
- ITRC. (2011). "Integrated DNAPL Site Strategy." The Interstate Technology & Regulatory Council, Washington, DC.
- Jawitz, J. W., Fure, A. D., Demmy, G. G., Berglund, S., and Rao, P. S. C. (2005). "Groundwater contaminant flux reduction resulting from nonaqueous phase liquid mass reduction." *Water Resources Research*, 41(10).
- Kavanaugh, M. C., Suresh, P., and Rao, C. (2003). *THE DNAPL REMEDIATION CHALLENGE: IS THERE A CASE FOR SOURCE DEPLETION?* U.S. ENVIRONMENTAL PROTECTION AGENCY, Office of Research & Development, WASHINGTON, DC.

- Kaye, A. J., Cho, J., Basu, N. B., Chen, X., Annable, M. D., and Jawitz, J. W. (2008). "Laboratory investigation of flux reduction from dense non-aqueous phase liquid (DNAPL) partial source zone remediation by enhanced dissolution." *Journal of Contaminant Hydrology*, 102(1–2), 17–28.
- Kram, M. L., Keller, A. A., Rossabi, J., and Everett, L. G. (2002). "DNAPL Characterization Methods and Approaches, Part 2: Cost Comparisons." *Groundwater Monitoring & Remediation*, 22(1), 46–61.
- Maji, R., Sudicky, E. A., Panday, S., and Teutsch, G. (2006). "Transition Probability/Markov Chain Analyses of DNAPL Source Zones and Plumes." *Ground Water*, 44(6 Understanding), 853–863.
- NRC. (2005). *Contaminants in the Subsurface: Source Zone Assessment and Remediation*. The National Academies Press, Washington, DC.
- Parker, B. L., Chapman, S. W., and Guilbeault, M. A. (2008). "Plume persistence caused by back diffusion from thin clay layers in a sand aquifer following TCE source-zone hydraulic isolation." *Journal of Contaminant Hydrology, Partial Source Zone Removal*, 102(1), 86–104.
- Saenton, S., and Illangasekare, T. H. (2007). "Upscaling of mass transfer rate coefficient for the numerical simulation of dense nonaqueous phase liquid dissolution in heterogeneous aquifers." *Water Resources Research*, 43(2).
- Stroo, H. F., Unger, M., Ward, C. H., Kavanaugh, M. C., Vogel, C., Leeson, A., Marqusee, J., and Smith, B. P. (2003). "Remediating chlorinated solvent source zones." *Environmental Science & Technology*, 37(11), 224A-230A.
- Suarez, M. P., and Rifai, H. S. (1999). "Biodegradation Rates for Fuel Hydrocarbons and Chlorinated Solvents in Groundwater." *Bioremediation Journal*, 3(4), 337–362.
- Suchomel, E. J., and Pennell, K. D. (2006). "Reductions in Contaminant Mass Discharge Following Partial Mass Removal from DNAPL Source Zones." *Environmental Science & Technology*, American Chemical Society, 40(19), 6110–6116.
- Zhang, C., Werth, C. J., and Webb, A. G. (2008). "Investigation of surfactant-enhanced mass removal and flux reduction in 3D correlated permeability fields using magnetic resonance imaging." *Journal of Contaminant Hydrology*, 100(3–4), 116–126.