FINAL REPORT

Decision & Management Tools for DNALP Sites: Optimization of Chlorinated Solvent Source and Plume Remediation Considering Uncertainty

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List of Acronyms

CVOC	Chlorinated Volatile Organic Chemical
DCE	cis-1,2-Dichloriethylene
DLL	Dynamic Link Library
DoD	Department of Defense
DNAPL	Dense Non Aqueous Phase Liquid
EPA	Environmental Protection Agency
GUI	Graphical User Interface
ITRC	Interstate Technology & Regulatory Council
LB	Lower Bound
LNAPL	Light Non Aqueous Phase Liquid
MCL	Maximum Contaminant Level
MNA	Monitored Natural Attenuation
NPV	Net Present Value
NRC	National Research Council
O&M	Operation and Maintenance
PAT	Pump And Treat
PCE	Tetrachloroethylene
PDF	Probability Density Function
PRB	Permeable Reactive Barrier
PREMChlor	Probabilistic Remediation Evaluation Model for Chlorinated solvents
REMChlor	Remediation Evaluation Model for Chlorinated solvents
TCE	Trichloroethylene
UB	Upper Bound
VC	Vinyl Chloride
ZVI	Zero Valent Iron

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Executive Summary

In this project, a new probabilistic remediation modeling program, Probabilistic Remediation Evaluation Model for Chlorinated solvents (PREMChlor), has been developed for simultaneously evaluating the effectiveness of source and plume remediation considering the uncertainties in all major parameters, thereby supporting the remediation selection process.

The technical foundation of PREMChlor is the EPA REMChlor (for Remediation Evaluation Model for Chlorinated solvents) model. REMChlor is a significant improvement on previous chlorinated solvent transport models, because it can simultaneously account for both source and plume remediation. REMChlor includes a source model based on a power function relationship linking the source mass to the source discharge and an analytical plume model based on one-dimensional advection, with three-dimensional dispersion. The plume model simulates natural attenuation or plume remediation temporarily and spatially for parent and daughter compounds in the first-order sequential decay chain. The plume model also calculates the cancer risks posed by carcinogenic compounds assuming that the contaminated water is used in a house for drinking, bathing, and other household uses.

PREMChlor was developed by linking the analytical model REMChlor to a Monte Carlo modeling package GoldSim via a FORTRAN Dynamic Link Library (DLL) application. In PREMChlor, all of the uncertain input parameters are treated as stochastic parameters represented by probability density functions (PDFs). The outputs from PREMChlor are also probability distributions and summary statistics of the distributions. Cost analysis of common technologies for DNAPL source removal and dissolved plume treatment are included. PREMChlor gives users a single platform where cost, source treatment, plume management, monitored natural attenuation, and risk assessment can all be evaluated together, and where uncertainty can be incorporated into the site decision making process. A license-free file containing the user-friendly graphical user interface (GUI) has been generated to make PREMChlor available for use by others.

Model demonstration examples are used to illustrate the different probabilities of meeting a remediation goal for different combinations of source and plume remediation scenarios considering uncertainties in input parameters. PREMChlor has been applied to a trichloroethene (TCE) plume in a shallow aquifer at a manufacturing plant. The calibrated model using a deterministic approach is able to closely match the pre-remediation site condition. Probabilistic simulations predict the effects of remediation and capture most uncertainties in key parameters based on estimated PDFs. The PREMChlor model has also been used to conduct sensitivity analyses by assessing the influence or relative importance of each input parameter on plume behavior, in terms of contaminant mass concentration, for three different plume types. It is found that the degree of influence of different input parameters on the contaminant mass concentration varies widely for different plume types.

1.0 INTRODUCTION

1.1 BACKGROUND

The Department of Defense (DoD) is currently responsible for cleanup of groundwater contaminated with chlorinated solvents (chlorinated volatile organic compounds, CVOCs) at thousands of sites nationwide. Much recent research has focused on technology development for both source and plume remediation (e.g. thermal methods, chemical oxidation, surfactant/cosolvent flooding, soil vapor extraction, air sparging, pump-and-treat (PAT), enhanced in-situ biodegradation) [Reddi, 1996; Brusseau et al., 1999; Wiedemeier et al. 1999; National Research Council (NRC), 2000; Kaluarachchi, 2001; US EPA, 2004b; Mayer and Hassanizadeh, 2005; Alvarez and Illman, 2006].

Process and parameter uncertainty and the expensive cost of source and plume remediation efforts have limited our ability to make effective decisions about DNAPL site remediation alternatives. For many sites, a robust, cost-effective remediation design requires some combination of source and plume remediation while considering the uncertainties that arise from hydrological and biogeochemical properties, from the site history and conditions, and from the effects of remediation.

Analytical site modeling tools have played important role in the remediation selection process. Recently, a new analytical screening level model, REMChlor has been developed [Falta et al., 2005a, b and Falta, 2008]. REMChlor is a significant improvement on existing analytical chlorinated solvent transport models such as BIOCHLOR [Aziz et al. 2000], because it can simultaneously account for both source and plume remediation.

In this project, REMChlor was used as the technical foundation to develop a quantitative decision making process that allows for quick evaluation of different combinations of source and plume remediation scenarios in the face of uncertainty.

This project was complementary to and made use of knowledge gained from other ESTCP and SERDP projects that were focusing on selecting, designing, and evaluating the performance and estimating the cost of DNAPL source remediation.

Unlike many other ESTCP projects, this project does not involve a field demonstration of a particular technology nor is it linked to any specific sites. The final products, PREMChlor software and User's Manual, and this document, therefore, are non-site-specific.

1.2 OBJECTIVE OF THE DEMONSTRATION

Having greatly expanded the functionality of REMChlor by using it in a probabilistic optimization framework, a new probabilistic remediation modeling program, PREMChlor, has been successfully developed. PREMChlor gives users a single platform where cost, source treatment, plume management, monitored natural attenuation, and risk assessment can all be evaluated together, and where uncertainty can be incorporated into the site decision making

process. A license-free file containing the user-friendly graphical user interface (GUI) has been generated to make PREMChlor available for use by others.

Included in this report also are the summary of model application to a actual field site, and the summary of the sensitivity analysis that explores the importance of key input variables on the source and plume behavior by assessing the influence or relative importance of each input parameter on the effectiveness of both source and plume remediation in terms of different plume categories.

1.3 REGULATORY DRIVERS

The Department of Defense (DoD) is currently responsible for managing thousands of chlorinated solvent sites. The CVOCs typically are believed to be carcinogens, and they have low maximum contaminant levels (MCLs) in drinking water. Much recent research has focused on technology development for both source and plume remediation, and there is ongoing debate as to the relative effectiveness of these efforts. This model will help site owners and regulators evaluate the likely performance of source and plume remediation efforts including the effects of uncertainty.

2.0 TECHNOLOGY

2.1 TECHNOLOGY DESCRIPTION

In this project, a new probabilistic remediation modeling program, PREMChlor was developed. PREMChlor takes into account the uncertainties in all major parameters and allows for quick simulations of different combinations of source and plume remediation scenarios to evaluate remediation alternatives. PREMChlor is developed by linking the analytical model REMChlor to a Monte Carlo modeling package GoldSim [http://www.goldsim.com/] via a FORTRAN Dynamic Link Library (DLL) application.

The REMChlor model is the technical foundation of the new probabilistic model. This transport model fully couples the source remediation to the plume remediation. It is not specific to any remediation technology. The contaminant source remediation is simulated as a fractional removal of source mass at a future time after the initial release; plume remediation is modeled by considering time and distance dependent decay rates of parent and daughter compounds in the first-order sequential decay chain [Falta, 2008]. The source model is based on a mass balance of the source zone where mass is removed by dissolution and advection with additional decay in the source zone [Falta, 2008]:

$$\frac{dM(t)}{dt} = -Q(t)C_s(t) - \lambda_s M(t) \tag{1}$$

where $Q(t)$ is the water flow rate through the source zone due to infiltration or groundwater flow, $C_s(t)$ is the average contaminant concentration leaving the source zone, $M(t)$ is the contaminant mass in the source zone, and λ_s is the first order decay rate in the source zone.

The source mass is linked to the source discharge through a power function relationship to reflect the site architecture [Rao et al. 2001; Rao and Jawitz, 2003; Parker and Park, 2004; Zhu and Sykes, 2004; Falta et al., 2005a；Falta, 2008, Parker and Falta, 2008]:

$$\frac{C_s(t)}{C_0} = \left(\frac{M(t)}{M_0}\right)^{\Gamma} \tag{2}$$

where C_0 is the flow-averaged source concentration corresponding to the initial source mass, M_0. The exponent, Γ, determines the shape of the source discharge response to changing source mass (Figure 1). When Γ =1, the source mass and source discharge decline exponentially with time [Newell and Adamson, 2005 and Newell et al., 2006]. When Γ >1, the source is never fully depleted, and the source discharge is always greater than zero. When Γ <1, the source is eventually depleted, and the source discharge equals zero in the end. When Γ =0.5, the source discharge declines linearly with time. When Γ=0, the source discharge remains constant until the source is completely depleted [Falta et al., 2005a; Falta, 2007 and 2008].

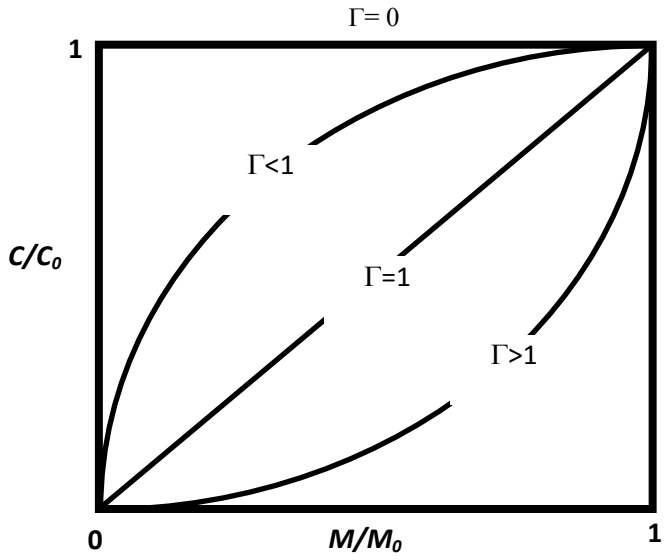


Figure 1. Power function illustration of source mass and source discharge relationship.

Field, laboratory, and theoretical evaluations of the source mass/source discharge response suggest that Γ may vary between about 0.5 and 2 at real sites [Rao and Jawitz, 2003; Falta et al., 2005a; Newell and Adamson, 2005; Fure et al., 2005; Jawitz et al., 2005; McGuire et al., 2006; Newell et al., 2006]. Simulation studies suggest that sites with DNAPL located predominantly in low permeability zones exhibit $\Gamma > 1$ and sites with DNAPL in high permeability zones exhibit $\Gamma < 1$ [Falta et al., 2005 a, b]. Park and Parker [2005] suggest Γ values greater than 1 for finger-dominated residual DNAPL and less than 1 for DNAPL pools. Essentially, Γ should be considered as an uncertain parameter, whose mean value can be roughly estimated, but whose actual value may never be precisely known at a site.

The solution of Equation 1 with the power function (Equation 2) can be used to predict the time-dependent depletion of the source zone mass by dissolution. The time-dependent mass is then used in Equation 2 to calculate the time-dependent source discharge. If Q is constant, the solutions are given by Falta et al. [2005b]:

$$M(t) = \left\{ \frac{-QC_0}{\lambda_s M_0^{\Gamma}} + \left(M_0^{1-\Gamma} + \frac{QC_0}{\lambda_s M_0^{\Gamma}} \right) e^{(\Gamma-1)\lambda_s t} \right\}^{\frac{1}{1-\Gamma}} \tag{3}$$

$$C_s(t) = \frac{C_0}{M_0^{\Gamma}} \left\{ \frac{-QC_0}{\lambda_s M_0^{\Gamma}} + \left(M_0^{1-\Gamma} + \frac{QC_0}{\lambda_s M_0^{\Gamma}} \right) e^{(\Gamma-1)\lambda_s t} \right\}^{\frac{1}{1-\Gamma}} \tag{4}$$

This source model can account for aggressive source remediation efforts (such as excavation, thermal treatment, alcohol or surfactant flooding, or chemical oxidation) that remove a certain fraction of the source mass over a short period of time [Falta et al., 2005a]. By rescaling the equations following the removal of source mass, the source mass and source discharge due to source remediation are presented by Falta et al. [2005b] as:

$$M(t) = \left\{ \frac{-QC_2}{\lambda_s M_2^{\Gamma}} + \left(M_2^{1-\Gamma} + \frac{QC_2}{\lambda_s M_2^{\Gamma}} \right) e^{(\Gamma-1)\lambda_s (t-t_2)} \right\}^{\frac{1}{1-\Gamma}} \tag{5}$$

$$C_s(t) = C_2 \left(\frac{M(t)}{M_2} \right)^{\Gamma} \tag{6}$$

$$M_2 = (1-X)M_1 \tag{7}$$

$$C_2 = C_0 \left(\frac{(1-X)M_1}{M_0} \right)^{\Gamma} \tag{8}$$

where t_2 is the time when the remediation ends; M_1 is the source mass before remediation, and M_2 is the source mass at t_2; X is the fraction of source mass removed during the remediation. This approach is not technology specific, and it allows for a realistic and mass conservative assessment of the effects of source remediation on source longevity and discharge. The source model serves also as a time-dependent mass flux boundary condition to the analytical plume model.

The plume model considers one-dimensional advection, retardation, and three-dimensional dispersion with first order decay of parent compound into daughter products. The governing equation for the dissolved concentration of each contaminant compound in the plume is as follows [Falta et al., 2005b and Falta, 2008]:

$$R\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + \alpha_x v\frac{\partial^2 C}{\partial x^2} + \alpha_y v\frac{\partial^2 C}{\partial y^2} + \alpha_z v\frac{\partial^2 C}{\partial z^2} + rxn(x,t) \tag{9}$$

where C is the dissolved concentration, and R is the retardation factor, α_x, α_y and α_z are the longitudinal, transverse, and vertical dispersivities, respectively, v is the pore velocity, and $rxn(x,t)$ is the rate of generation (+) or destruction (–) of the dissolved compound due to biological or chemical reactions that may vary temporally and spatially. The model considers a parent compound, and 3 daughter compounds that are produced by first order decay.

A streamtube approach is used to decouple the solute advection and reactions from the longitudinal dispersion. The one-dimensional advective streamtube model is characterized by a constant pore velocity and solute retardation factor. Plume reactions are included in this advective streamtube model. The entire plume is divided into different zones where the reaction rates are time and distance dependent (Figure 2). Cancer risks posed by carcinogenic compounds in the plume are calculated assuming that the contaminated water is used in a house for drinking, bathing, and other household uses [Falta, 2007].

By linking REMChlor to a probabilistic simulation package GoldSim, which uses a Monte Carlo approach to propagate the uncertainty in the input parameters of a system to the predicted results and performance, PREMChlor allows all of the uncertain input parameters are treated as stochastic parameters represented by probability density functions (PDFs). The outputs from PREMChlor are also probability distributions and summary statistics of the distributions. Cost analysis of common technologies for DNAPL source removal and dissolved plume treatment are included. PREMChlor gives users a single platform where cost, source treatment, plume management, monitored natural attenuation, and risk assessment can all be evaluated together, and where uncertainty can be incorporated into the site decision making process. A license-free file containing the user-friendly graphical user interfaces (GUI) has been generated to make PREMChlor available for use by others.

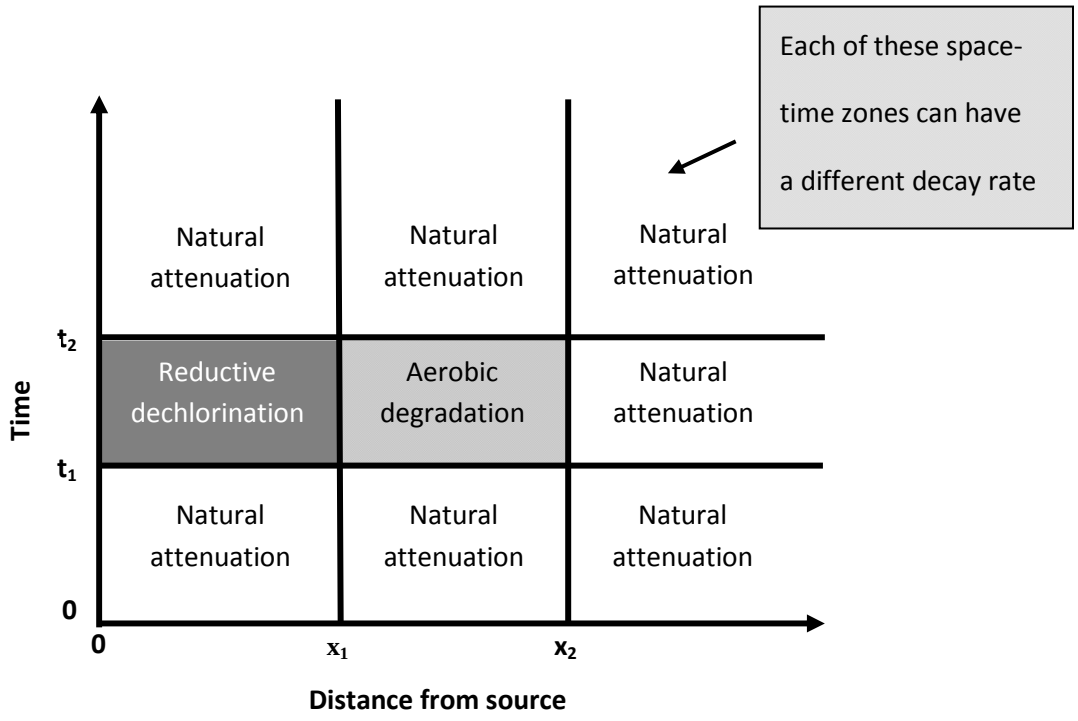


Figure 2. Illustration of plume space-time zones.

2.2 TECHNOLOGY DEVELOPMENT

Linkage between REMChlor and GoldSim

Technically, the REMChlor analytical model was compiled as FORTRAN DLL application and then linked to GoldSim. A probabilistic simulation consists of hundreds or thousands of deterministic Monte Carlo realizations. Each realization is an independent and equally likely run of the system. As illustrated in Figure 3, during the probabilistic simulation, GoldSim is used to

specify the probability distributions for all stochastic parameters and to specify the Monte Carlo parameters, such as the total simulation duration, time step, and the total realization number for the probabilistic simulation. Inside the Monte Carlo loop, for each realization, GoldSim is used to sample the value for each uncertain parameter through its PDF and specify the value to each deterministic parameter and assign the values to REMChlor. The REMChlor FORTRAN source code is called via a FORTRAN DLL application to perform the analytical calculation and calculation results are passed back to GoldSim. After all of the realizations are completed, all of the results of REMChlor calculations are stored in GoldSim and assembled into probability distributions and probability statistics.

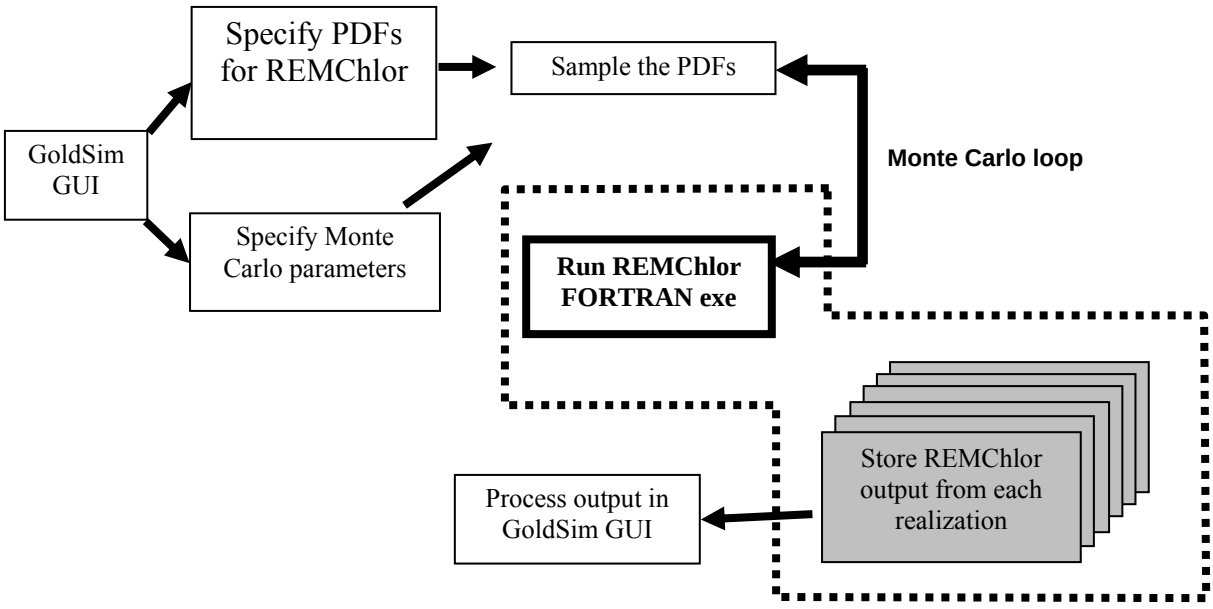


Figure 3. Flow chart of the DLL linkage during the probabilistic simulation.

PREMChlor can be run in two different modes: the probabilistic simulation mode and the deterministic simulation mode. Under the probabilistic simulation mode, model runs multiple realizations. Each realization is deterministic and uses a different probabilistic value for a stochastic parameter. Under the deterministic simulation mode, only one realization is run in which a deterministic value is used for every parameter.

PREMChlor allows two different types of input information, either deterministic or probabilistic values. Deterministic values are provided as the inputs to the model when the user knows the specific values the model requires. When the required information is uncertain, the user provides

probability distribution parameters, such as mean, standard deviation etc., as the inputs to define the distribution for a stochastic parameter.

In the PREMChlor model, a graphical user interfaces has been built to allow other users to easily enter the input values, run the model and view the results. A license-free GoldSim player file containing the graphical user interface has been generated to make the PREMChlor model available to potential users who are not familiar with details of the probabilistic model and the GoldSim simulation environment.

Unit Cost and Remediation Efficiency

PREMChlor considers common technologies for DNAPL source removal and dissolved plume treatment. Source remediation methods include thermal treatments, surfactant/cosolvent flooding, chemical oxidation/reduction, and enhanced bioremediation. The efficiency of source remediation is represented by the fraction of mass removed. In addition, efficiency of enhanced source bioremediation has another option as it can alternately be represented by the enhanced decay rate. In PREMChlor, each remediation technology corresponds to a specific unit cost (cost per volume treated) and specific remediation efficiency. These parameters are treated as uncertain variables represented by the PDFs.

The distributions and the parameters of unit costs and remediation efficiencies were derived from the literature resources. Based on the cost statistic from a comprehensive cost analysis of DNAPL source depletion technologies at 36 field sites [McDade et al.,2005], it was found that the unit cost follows a beta distribution. Based on the statistics of the concentration reduction percentages from a performance evaluation of DNAPL source remediation technologies at 59 chlorinated solvents contaminated sites [McGuire et al., 2006], it was found that the remediation efficiency follows a beta distribution. Due to lack of information, the enhanced decay rate, which is another option to represent the remediation efficiency of enhanced bioremediation, is assumed to have a triangular distribution.

The plume treatment methods mainly are enhanced biodegradation. PREMChlor can also simulate permeable reactive barriers (PRBs). Plume PRB treatment can be modeled by assigning a very high first-order degradation rate for the contaminant in a narrow reaction zone. The application of PREMChlor to a plume PRB treatment can be found in Section 4.2. Due to the lack of information, the unit cost and degradation rate for plume treatment are assumed to have triangular distributions.

Calculation of Remediation Cost

Remediation costs of source removal and plume treatment are included in the probabilistic simulation model. Remediation cost analysis is conducted outside the FORTRAN DLL link. The total remediation cost consists of the source remediation cost and the plume remediation cost. For source remediation, the probabilistic model considers a one-time capital cost, which is the product of the unit cost of the source remediation and the volume of the treated source zone. For plume remediation, cost includes a one-time capital cost and a total operation & management (O&M) cost in present net value (NPV) for a certain remediation period. The probabilistic model

allows two plume remediation zones. For each remediation zone, the one-time capital cost is the product of the unit cost of the plume remediation and the volume of the remediation zone. The calculation of the total O&M cost in NPV is based on the formula in ITRC [2006]:

$$TotalNPV = \sum_{1}^{n} \frac{AnnualCostinYeartwithInflation}{(1+InterestRate)^{t-1}} = \sum_{1}^{n} \frac{AnnualCost(1+i)^{t-1}}{(1+r)^{t-1}}$$

$$= AnnualCost \sum_{1}^{n} \frac{(1+i)^{t-1}}{(1+r)^{t-1}} = AnnualCost \frac{1-(\frac{1+i}{1+r})^{n}}{1-\frac{1+i}{1+r}} \quad (10)$$

where *AnnualCost* is the current annual cost (assumed to be constant), i is the average annual inflation rate, r is the average annual interest rate, t is the year, and n is the total period of time for plume operation and management. In Equation (10), the numerator accounts for the total O&M cost in current dollar considering inflation, and the denominator accounts for the interest rate. This formula accounts for the inflation and interest factors at the beginning of the second year.

Evaluate and Demonstrate the Model Utility

As presented in four tutorials (see the User's Manual, Appendix D), a hypothetical tetrachloroethylene (PCE) site was modeled to demonstrate the model capability. A series of simulations were conducted and simulation results show the different probabilities of meeting a remediation goal for different combinations of uncertain parameters and remediation efforts. The simulation results are summarized in Table 1.

Table 1. Summary of Model Demonstration

Simulation Scenario	Remediation Scenario	Uncertain Parameters	Probability of Meeting a Remediation Goal
Simulation 1	A very effective deterministic thermal remediation of the source that removed 97% of the source mass.	N/A	100%
Simulation 2	Identical to Simulation 1, except for adding some uncertainties to the source parameters	Initial source mass Power function exponent	>75%
Simulation 3	Identical to Simulation 2, except for making the source remediation efficiency uncertain	Initial source mass Power function exponent Source remediation efficiency	50%
Simulation 4	Identical to Simulation 3, except for adding an enhanced biodegradation of PCE and TCE in the dissolved plume	Initial source mass Power function exponent Source remediation efficiency enhanced biodegradation of PCE and TCE	95%

An example of application of PREMChlor to a real field site is given in Section 4.2 of this report.

The PREMChlor model utility has been evaluated by a test user's group consisting of experts from Noblis, the US Army Corps of Engineers, DuPont Corporation, and Camp Dresser McKee. Model feedback regarding the general usability and the utility of the model indicates that PREMChlor is functional and user friendly. Model feedback regarding the applicability of the model to the specific sites indicates that PREMChlor is believed to reasonably represent the original contaminant system and simulation results match field data.

2.3 ADVANTAGES AND LIMITATIONS OF THE TECHNOLOGY

The primary strength of PREChlor is that it allows for quick simulations of different combinations of DNAPL source and plume remediation scenarios to evaluate remediation alternatives while capturing the uncertainties in all major parameters.

PREChlor was developed from REMChlor model, it has the same limitations due to model assumptions (see REMChlor User's Manual, [Falta, 2007]). The primary limitation is that the REMChlor model assumes a simple one-dimensional flow field, and it does not consider diffusion from high velocity regions into and out of low velocity regions.

3.0 PERFORMANCE OBJECTIVES

The performance objectives for this project are listed below in Table 2.

Table 2. Performance Objectives

Performance Objective	Data Requirements	Success Criteria	Actual Performance Objective Met?
Quantitative Performance Objectives			
Develop probabilistic simulation version of the source/plume remediation model with a graphical users interface	• Source containment function • PDFs of unit costs and remediation efficiencies	• Ability to model source containment • Ability to derive the PDFs from literature resource • Ability to link REMChlor to GoldSim	Yes
Apply the model to an actual contaminant site	• Source zone parameters • Transport parameters • Remediation parameters	• Ability to simulate plume • Ability to simulate remediation effort	Yes
Qualitative Performance Objectives			
Evaluate and demonstrate and evaluate the model utility	• Feedback from usability testing group • Demonstration of model capability	• User friendly graphical interface and applicability to actual sites • Positive reviews from test users group	Yes

Developing the probabilistic simulation software involved the following tasks:

- Task 1 - Modify the current source remediation function in the REMChlor analytical model to include a source containment option.
- Task 2 - Improve the cancer risk assessment calculations in the model to include vapor transport through the vadose zone from a dissolved plume.
- Task 3 – Derive the PDFs of unit costs and remediation efficiencies for remediation technologies.
- Task 4 - Develop a probabilistic simulation version of the source/plume remediation model with a graphical users interface.
- Task 5 - Evaluate and Demonstrate the Model Utility.

The detailed discussions of the technical approach for each task are given in Section 2.2.

The ultimate goal of developing the new modeling tool was to evaluate the field remediation effort in the face of uncertainty. Application of the probabilistic model to an actual TCE site is described in Section 4.2.

Another purpose of this model is to be able to assess the sensitivity of contaminated sites to different remediation actions. Chlorinated solvents source and plume remediation are complex processes due to the many uncertain controlling variables, such as hydrogeological variables, geochemical variables and cost variables. These factors play different roles on the effectiveness

of source and plume remediation efforts. Also, the influences of parameters on the effectiveness of remediation for different types of sites are different as well. It is important to explore the influence or relative importance of input variables on the target output (e.g. contaminant mass concentration at a control plane) in terms of different plume types. The site behavior can be divided into three categories in terms of the aqueous plume behavior: a shrinking plume, a stable plume and a growing plume. For shrinking/stable plumes with the contaminant mass mostly in the source zone, the target output may be mostly sensitive to the removal efficiency of the source treatment. The growing plume is more complicated. For the scenario with the contaminant mass partly in the source zone and partly in the dissolved plume, the target output may be sensitive to the efficiency of both source removal and plume treatment. The sensitivity analysis explores the different importance of input variables to the plume behavior for different types of plumes. More detailed discussions about sensitivity analysis are presented in Section 4.3.

4.0 PERFORMANCE ASSESSMENT

The performance objectives of this demonstration included:

- Develop probabilistic simulation version of the source/plume remediation model with a graphical users interface.

- Apply the probabilistic simulation model to an actual contaminant site.

- Explore the importance of key input variables on the source and plume behavior by assessing the influence or relative importance of each input parameter on the effectiveness of both source and plume remediation in terms of different plume categories.

- Through a test user group, demonstrate that the model is useful and reasonably easy to apply.

The results from each are discussed below. Section 4.1 focuses on the model development, Section 4.2 focuses on the model application, and Section 4.3 focuses on the sensitivity analysis. The detailed comments from the test user's group are given in their entirety in Appendix B

4.1 MODEL DEVELOPEMNT

Detailed discussions about the model development are presented in the PREMChlor User's Guide (Appendix D). This section focuses on the model inputs and outputs.

Among 86 input parameters in the probabilistic model (74 are linked to the FORTRAN DLL), 18 parameters are treated as deterministic and 68 parameters are treated as stochastic. Deterministic parameters usually have less or no uncertainty and can be defined in a certain way. Stochastic parameters are normally associated with much uncertainty. In PREMChlor, four types of distributions, including the triangular distribution, normal distribution, log-normal distribution, and beta distribution, are used for stochastic parameters (Figure 4).

PREMChlor provides many intermediate and final outputs. The most useful final outputs include the concentration and mass discharge of each contaminant component as well as the total values. Contaminant concentration and mass discharge are commonly used metrics to assess the performance of the remediation. In PREMChlor, the changes of concentrations, mass discharges over time (time-histories) are calculated for any specified location (x,y,z). The final results also include the remediation costs. Each output has multiple values computed from different realizations. All these values and observations are assembled into the probability distribution and the probability statistics, including the mean, median, lower bound (LB) and upper bound (UB), and different percentiles (as shown in Figure 5). LB and UB are the lowest and highest values for an output among all of the realizations, respectively. A percentile is the value of an output below which a certain percent of observations fall. Such probability statistics are useful to evaluate the remediation alternatives.

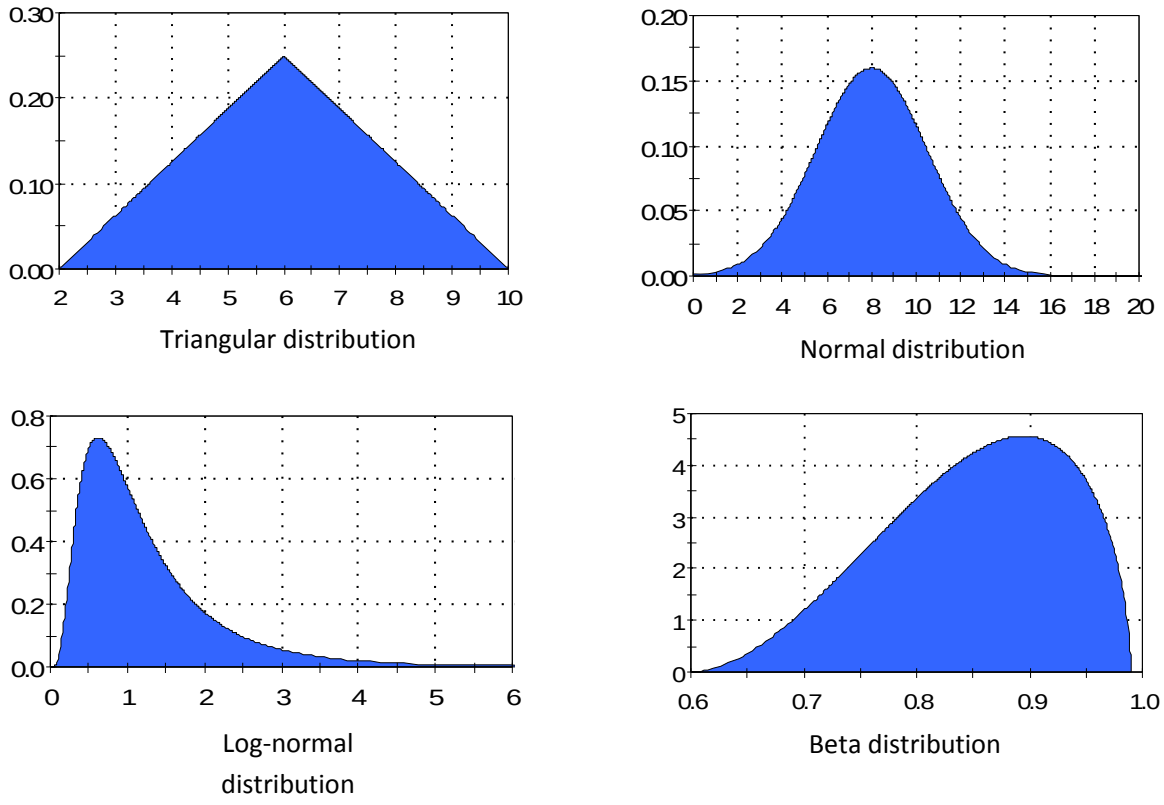


Figure 4. Probability distributions used for input parameters in PREMChlor.

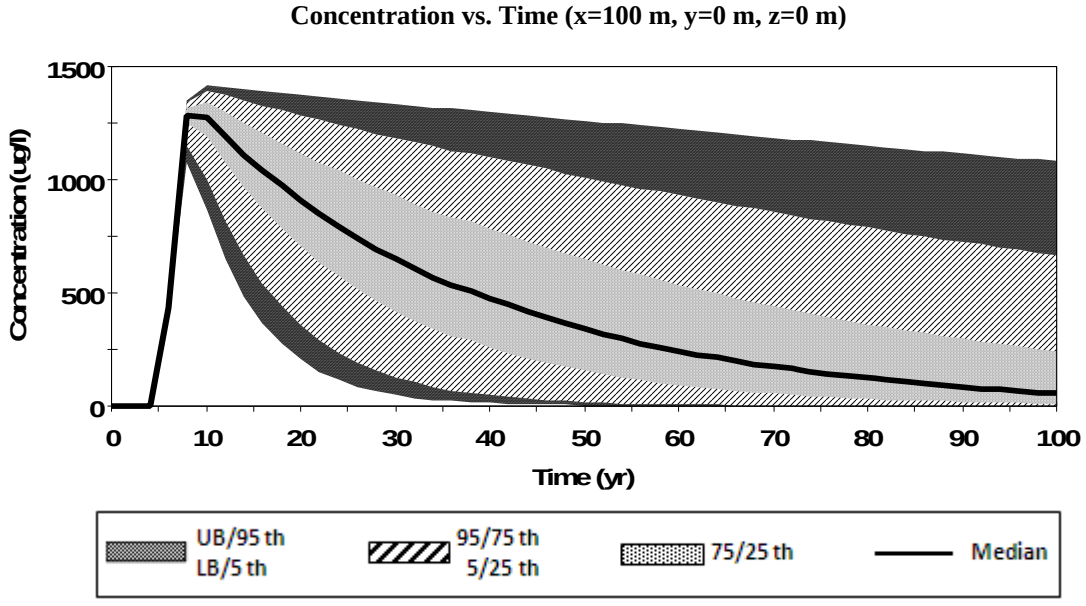


Figure 5. Probability histories of an output.

4.2 MODEL APPLICATION

In this section, the probabilistic model is applied to a shallow aquifer contaminated with TCE at a manufacturing plant in North Carolina. The simulations of field remediation were carried out in two steps. At the first step, the PREMChlor model was calibrated using a deterministic approach to represent the site condition prior to remediation activities. At the second step, the calibrated model was used to conduct the probabilistic simulation of field remediation activities considering uncertainties in seven key parameters. In this step, we pretended to not know the results of field remediation; instead we conducted probabilistic simulation to predict the performance of field remediation efforts.

Site Background and Field Remediation Activities

The site is the DuPont Kinston Plant, northeast of Kinston, Lenoir County, North Carolina. The plant began operations in 1953, and currently manufactures Dacron polyester resin and fibers. In November 1989, site investigation data indicated that the surficial aquifer beneath the manufacturing area had been impacted by a release of TCE. The impacted zone is limited to a surficial sand unit approximately 4.6 m deep overlying a thick mudstone-confining layer. An average hydraulic conductivity for the surficial aquifer is estimated to be 7.7×10^{-4} cm/sec. Groundwater Darcy velocity in the upper aquifer has been estimated to be about 1.52 to 4.57 m/yr. The regional groundwater flow direction is from southeast to northwest, with a pore velocity ranging from 5.56 to 11.13 m/yr. The water table is located at about 1.5 m below the ground surface (bgs).

TCE is the main contaminant at Kinston Site. The suspected source region was estimated to be 7.6 m in diameter and containing about 136 kg of TCE (Figure 6). The aqueous concentration of TCE in the source area showed large fluctuations over time, ranging from 0.34 mg/L to 75 mg/L. Originating from the source zone, the TCE-impacted groundwater plume extended approximately 300 m in the downgradient (northwest) direction, with a width of roughly 76 to 91 m at a downgradient distance of 89 m.

In order to clean up the site, three remediation efforts have been conducted since 1995. Initially a pump and treat (PAT) system was installed to recover and treat TCE-impacted groundwater, resulting in a TCE mass extraction of 3 lbs (1.36 kg) during a operation from 1995 to 2001, In 1999, an in-situ source area destruction pilot (a reductive dechlorination of TCE) using zero valent iron (ZVI) was conducted to destroy source zone soil contamination. In the mean time, this source ZVI treatment was implemented with a 400-foot long permeable reactive barrier (PRB) wall, which was emplaced across the groundwater plume approximately 89 m downgradient of the source area to intercept and treat contaminated groundwater (Figure 6). ZVI was injected into PRB wall to destroy contamininant.

Calibration of the Pre-Remediation Condition

The purpose of this model calibration was to use a deterministic simulation approach to match the site conditions in 1999 prior to source ZVI treatment or plume PRB wall installation. Because TCE is the major contaminant, the model calibration focused on the TCE plume. To better represent the site conditions, the monitoring well sampling data that are variable both in

space and time were used to compare with the simulation results. To be more specific, the simulated and measured time-series of TCE concentrations were compared for several monitoring wells sited in different locations in the source zone and plume (see Figure 6). During model calibration, the probabilistic model was set to use deterministic values for all parameters. Some parameters were assigned values that fall in the reported ranges from previous site investigations, some were estimated, and some were calibrated to better match the site conditions. Source, transport and natural attenuation parameters used in model calibration are shown in Table 3.

After model parameters have been estimated or calibrated, the probabilistic model was run in a deterministic way to match the site condition prior to source ZVI treatment or plume PRB wall installation. The comparison of the historical time-series of TCE concentration from 1989 to 1998 between the calibrated simulation results and the historical field sampling data for several monitoring wells are shown in Figure 7. Given the facts that 1) the compared monitoring wells are located in different locations in the source zone and plume over a large area, and 2) the compared time-series of TCE concentration covered a period of time from 1989 to 1998, the agreement of time-series of TCE concentration between modeled results and field sampling data in monitoring wells MW-29, MW-35, MW-37 and MW-36 show that with the given combination of parameters as discussed above, the calibrated model with a relatively simple flow field is able to match the pre-remediation site condition in terms of time-series of TCE concentration.

The discrepancy of the TCE concentration in the source well MW-30A is probably caused by the initial source concentration used in the model. There is large uncertainty associated with this value. The disagreement of the TCE concentration in the plume well MW-38 suggests that the initial source concentration might be too high or the TCE plume natural degradation rate might be too low. The TCE natural degradation rate used during the model calibration is an averaged estimate for the entire plume. Because the plume is heterogeneous in terms of the TCE degradation rate, this averaged estimate is also associated with some degree of uncertainty. The uncertainties in other transport parameters could also cause such concentration inconsistency for MW-38. There are likely to be other possible combinations of parameters that could match or represent available well data. To capture the uncertainties of these parameters, the probabilistic simulation of field remediation activities were conducted and are presented in the next section.

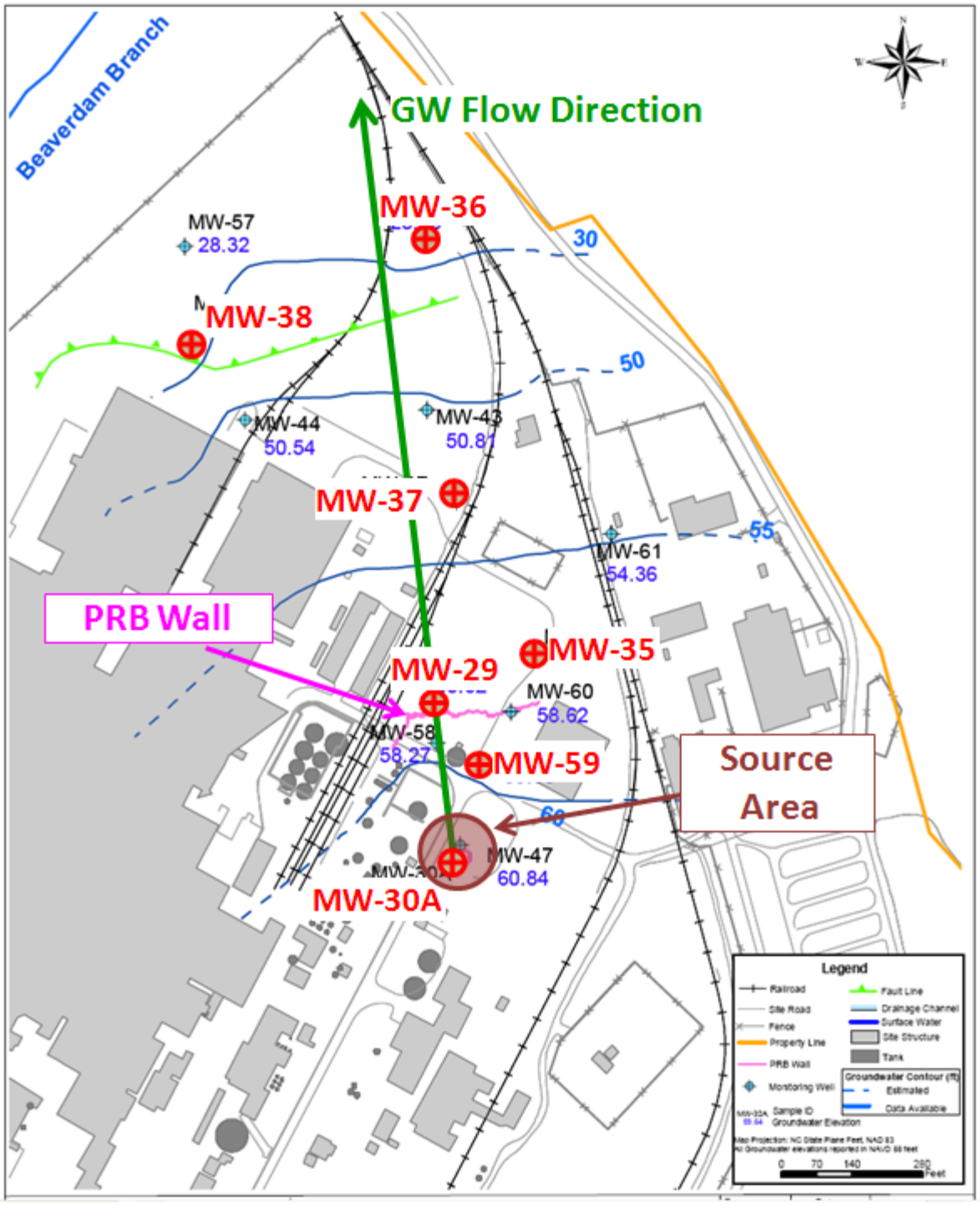


Figure 6. Site map of Kinston plant with monitoring wells.

Table 3. Source, transport and natural attenuation parameters used in model calibration.

Parameter	Value	Comment
Initial source concentration, C_0 (mg/l)	6	Estimated
Initial source mass, M_0 (kg)	136	From site reports [DERS, 1994]
Power function exponent, Γ	1	Estimated
Source width, W (m)	8	From site reports [CRG, 2002]
Source depth, D (m)	3.5	From site reports [DERS, 1994]
Source decay rate (yr^{-1})	0	Estimated
Darcy velocity, V_d (m/yr)	8	Calibrated; reports had estimated 1.5 to 4.6 m/yr [DERS, 1994]
Porosity, ϕ	0.333	Estimated from reported Darcy velocity and pore velocity [DERS, 1994 and 1998],
Retardation Coefficient, R	2	Estimated
Longitudinal dispersivity, α_x	x/20	Calibrated
Transverse dispersivity, α_y	x/50	Calibrated
Vertical dispersivity, α_z	x/1000	Estimated
TCE plume natural degradation rate, λ (yr^{-1})	0.125	Calibrated (equal to $t_{1/2}$ of 5.5 yrs)

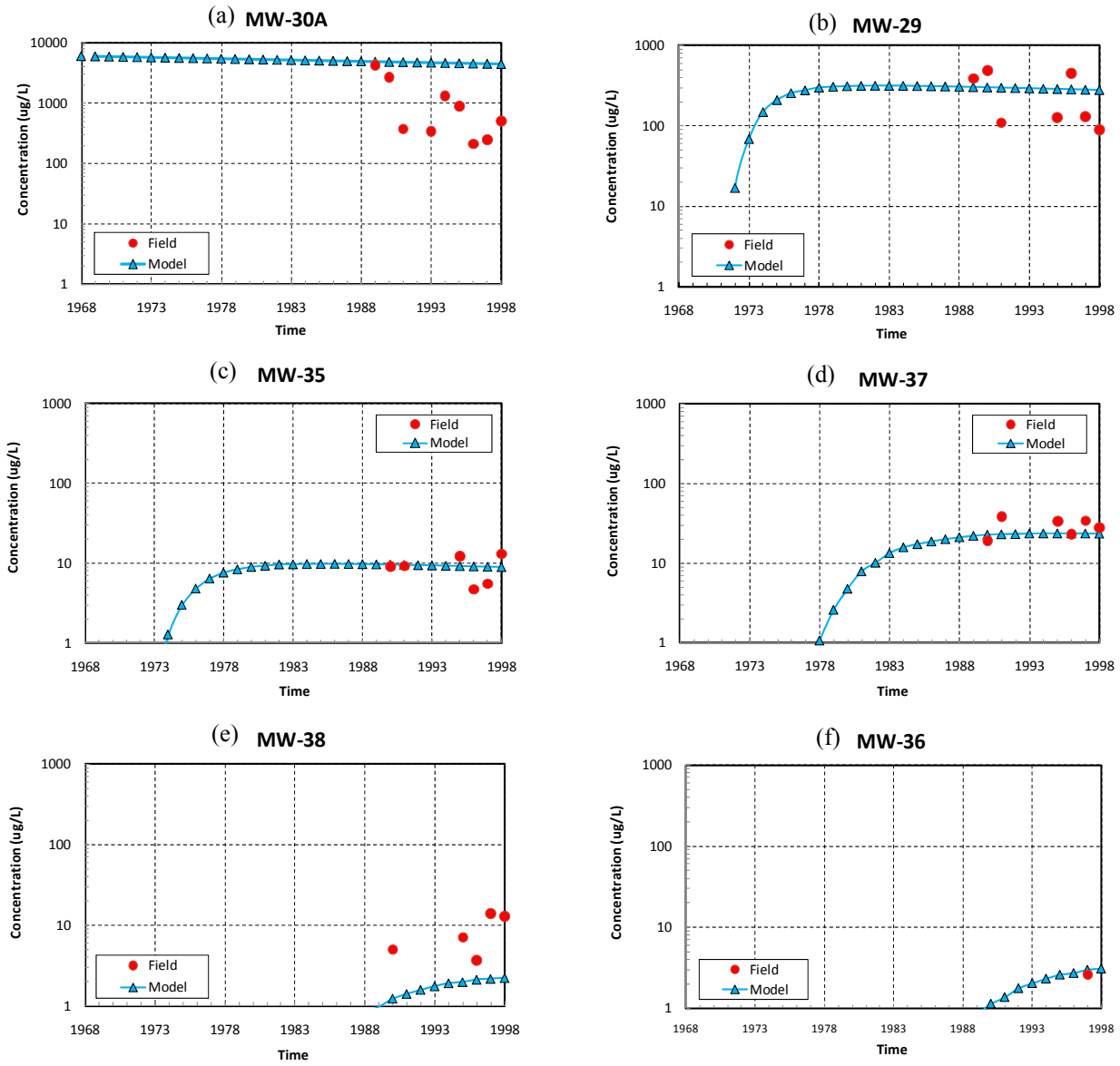


Figure 7. TCE concentrations from model calibration: a) MW-30A; b) MW-29; c) MW-35; d) MW-37; e) MW-38; f) MW-36.

Probabilistic Simulation of Field Remediation Activities

Based on the previous calibrated model, probabilistic simulations are conducted to model both the source ZVI treatment and plume PRB treatment in order to evaluate the effectiveness of field remediation efforts by considering the uncertainties in parameters. Source ZVI treatment is modeled by removing a fraction of TCE mass from the source zone in a period of 11 months starting from 1999. The Plume PRB wall is modeled by assigning a very high first-order degradation rate for TCE in a narrow reaction zone (as shown in Figure 8). The reported effective thickness of PRB wall is about 10 to 15 cm, so the PRB treatment zone starts from 89 m and ends at 89.127 m in the model.

For this site, seven key parameters, including the initial source concentration, initial source mass, power function exponent, groundwater Darcy velocity, TCE plume natural degradation rate, source mass removal percentage, and the TCE degradation rate inside the PRB wall, are associated with a high level of uncertainty, and they are treated as uncertain variables during the probabilistic simulation. All other parameters are kept as deterministic as in the model calibration. For the uncertain parameters, their mean behaviors stay consistent with the values used in model. The distributions and values of uncertain parameters are shown in Table 4 and the PDFs of distributions are shown in Figure 9. More detailed discussions about model parameters are presented in Liang [2009].

For each realization, the model simultaneously sampled different values for the seven uncertain parameters and used deterministic values for other parameters. The simulated TCE concentrations are assembled into the probabilistic statistics and are shown in Figure 10. The result of the probabilistic simulations suggest that both source ZVI injection and plume PRB wall installation have affected the TCE concentrations at the Kinston site. Simulation results of monitoring wells MW-30A and MW-59 show that TCE concentration reductions have occurred since the source ZVI injection was implemented, although the data are noisy. Simulation results of the monitoring wells MW-29, MW-35, and MW-37 show the TCE concentration reductions as a combined effect due to both source ZVI injection and plume PRB wall installation. Simulation results of the monitoring wells MW-38 and MW-36 show the remediation efforts will take effect sometime after 2011.

In summary, given a good understanding of the field hydrogeology and biogeochemistry, the calibrated model with a relative simple flow field is able to closely match the pre-remediation site condition in terms of time-series of TCE concentration for a large area of the contaminated site and a relative long period of time. Probabilistic simulations without calibration predicted the effects of remediation and captured most uncertainties in key parameters based on estimated PDFs.

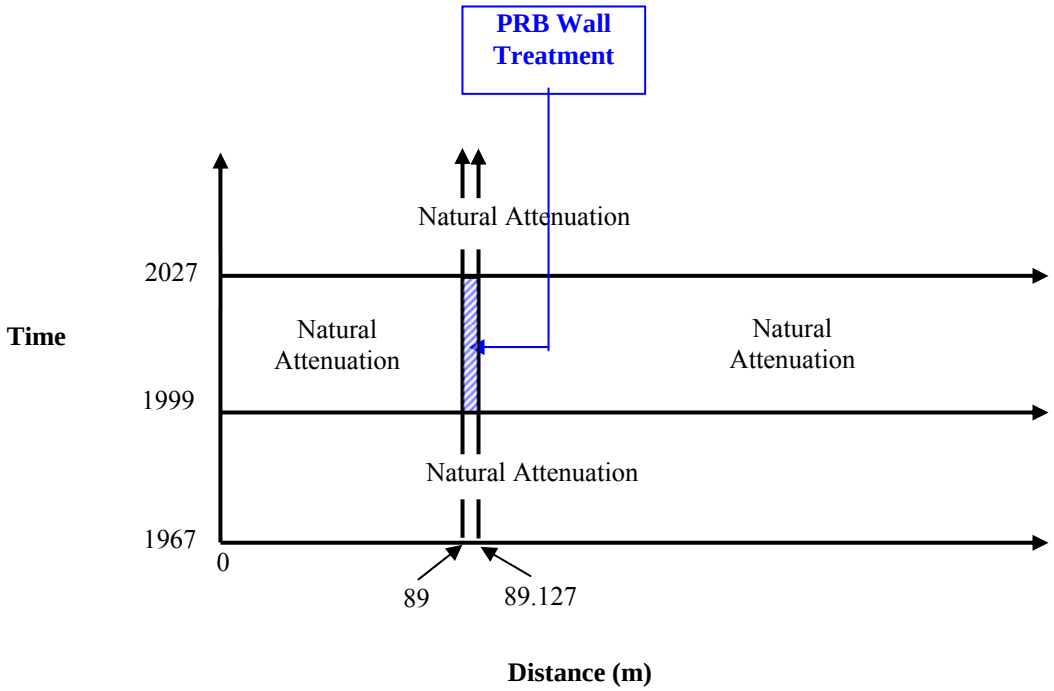


Figure 8. Plume reaction zones, including the PRB wall, modeled in probabilistic simulation.

Table 4. Uncertain parameters used in probabilistic simulation.

Parameter	Distribution	Value
Initial source concentration, C_0 (mg/l)	Triangular	min=2, most likely=6, max=10
Initial source mass, M_0 (kg)	Triangular	min=50, most likely=136, max=222
Power function exponent, Γ	Log-normal	geo mean =1, geo stdv=2
Darcy velocity, V_d (m/yr)	Normal	mean=8, stdv=2.5
TCE plume natural degradation rate, λ (yr^{-1})	Triangular	min= 0.05, most likely= 0.125, max=0.2
Fraction of source mass removal	Beta	mean=0.85, stdv = 0.08, min=0.6, max=0.99
TCE degradation rate inside PRB wall, λ_{PRB} (yr^{-1})	Triangular	min=228, most likely=436, max=644

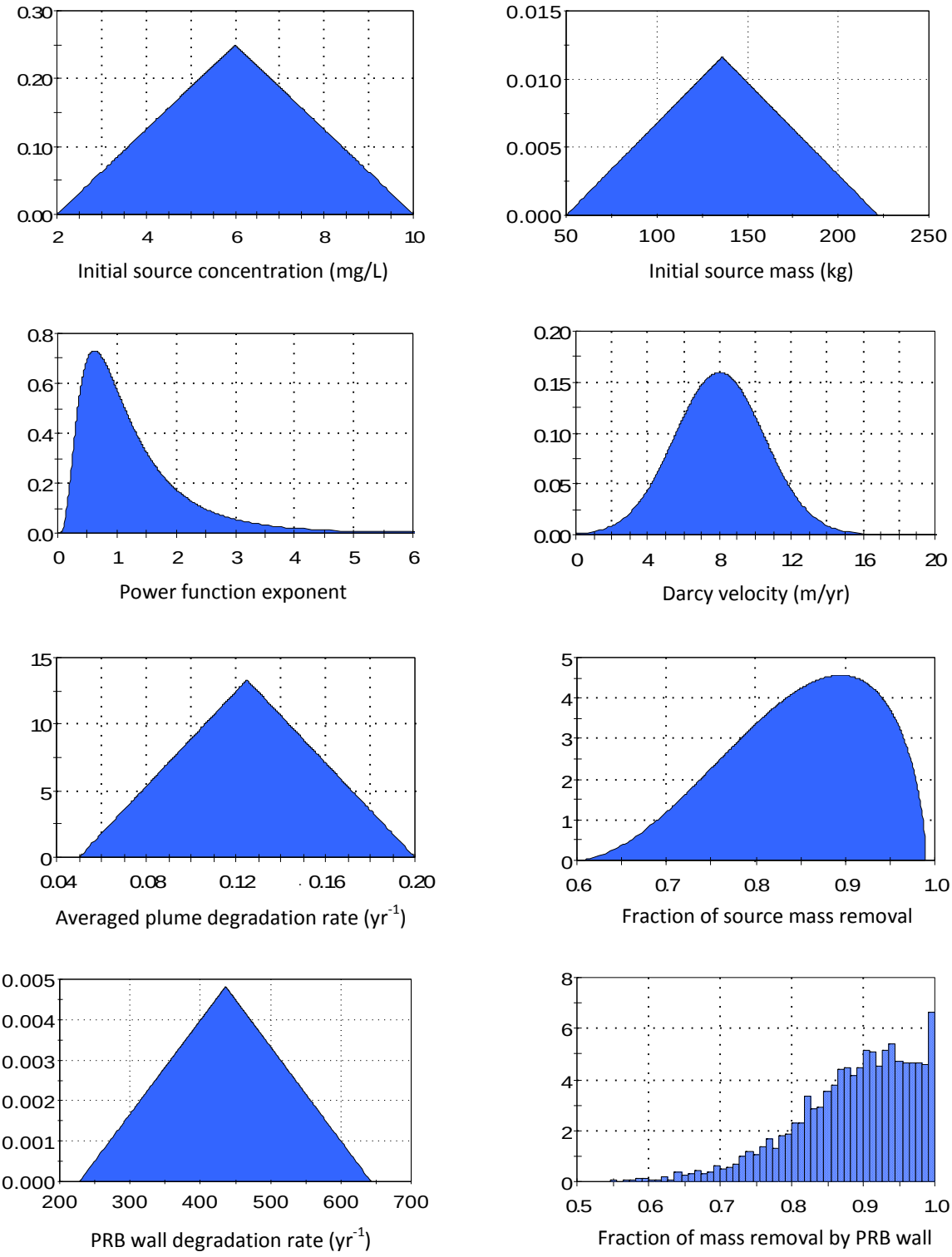


Figure 9. PDFs of uncertain parameters used in probabilistic simulation.

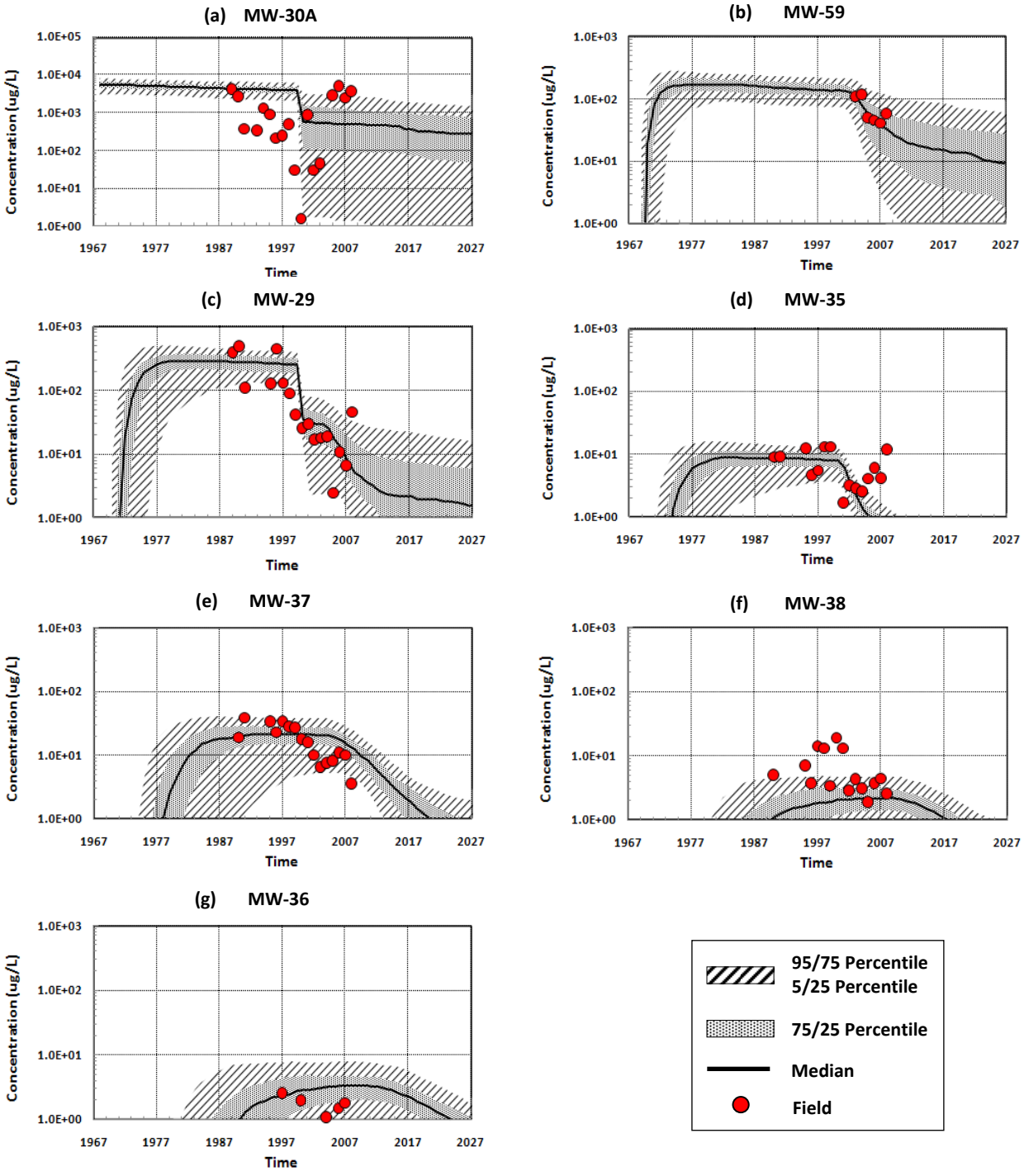


Figure 10. TCE concentrations from probabilistic simulation.

4.3 SENSITIVITY ANALYSIS FOR DIFFERENT PLUME TYPES

Different factors (hydrogeological variables, geochemical variables and cost variables) play different roles on the effectiveness of source and plume remediation efforts. In this section, the PREMChlor model is used to conduct sensitivity analyses by assessing the influence or relative importance of key input variables on the target output in terms of different plume types.

In this study, three types of plume are tested: I. A stable plume connected to the DNAPL source where the contaminant mass is partly in the source zone and partly in the plume, represented by a TCE plume; II. A growing plume that is disconnected from the source, where the most of the contaminant mass is in the plume, represented by a PCE site; and III. A growing plume that is connected to the source, where contaminant mass is partly in the source zone and partly in the plume, represented by a VC plume. For each case, a deterministic plume setting was used to represent the plume behavior as shown in Figures 11 to 13. The sensitivity analysis was then conducted based on the deterministic plume setting. During the sensitivity analysis, both source remediation and plume remediation were simulated in order to assess the influences of the input parameters on the effectiveness of the remediation efforts.

The target output specified in the sensitivity analysis is the contaminant mass concentration in the plume. Ten key input variables used to conduct the sensitivity analysis include the initial source concentration (C_0), initial source mass (M_0), power function exponent (Γ), Darcy velocity (V_d), porosity (ϕ), retardation factor (R), dispersivity parameters (longitudinal (α_x), transverse (α_y) and vertical (α_z), plume overall degradation rate without remediation (λ), source removal fraction (X_{rem}) and plume treatment rate (λ_{rem}). In PREMChlor, the longitudinal, transverse and vertical dispersivities are all scale-dependent. Each of them is equal to a different dispersivity parameter times the travel distance. The distributions and parameter values of tested input parameters are shown in Table 5 to 7.

Based on the sensitivity analysis from the three different cases, it is found that the degrees of the influence of different input parameters on the plume response are not equal. The observations for three plume types are summarized in Table 8. For a stable plume that is connected to the source and a growing plume that is disconnected from the source, the parent compound concentration or the total concentration in the downgradient plume is primarily sensitive to the initial source concentration, the power function exponent, the plume degradation rate, and the chemical travel velocity, which is determined by groundwater Darcy velocity, porosity and retardation factor. For a growing plume that is connected to the source, the concentration of a daughter compound (VC) is greatly affected by its degradation rate, the degradation rate of its direct parent (DCE) and transport parameters. The power function exponent affects the VC concentration greatly and source removal fraction plays more important role than several other parameters.

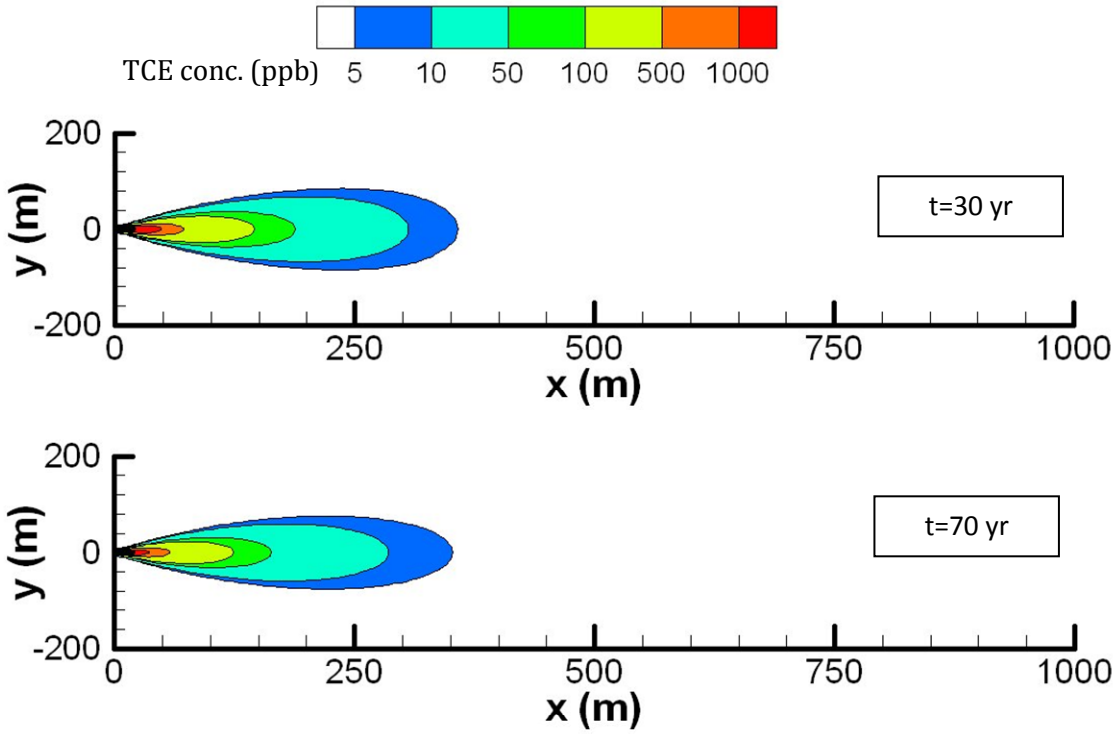


Figure 11. Plume evolution over time without remediation (Case I).

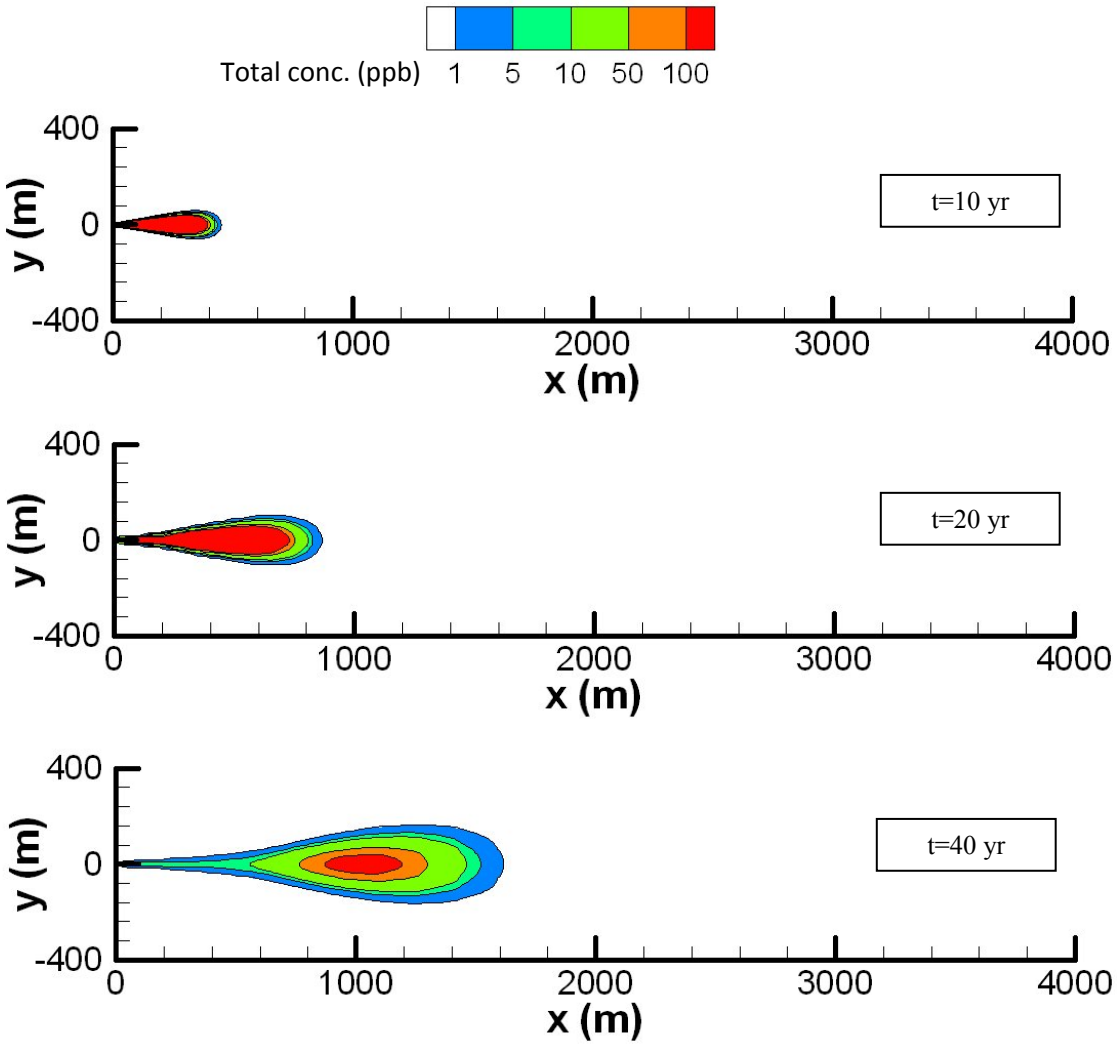


Figure 12. Plume evolution over time without remediation (Case II).

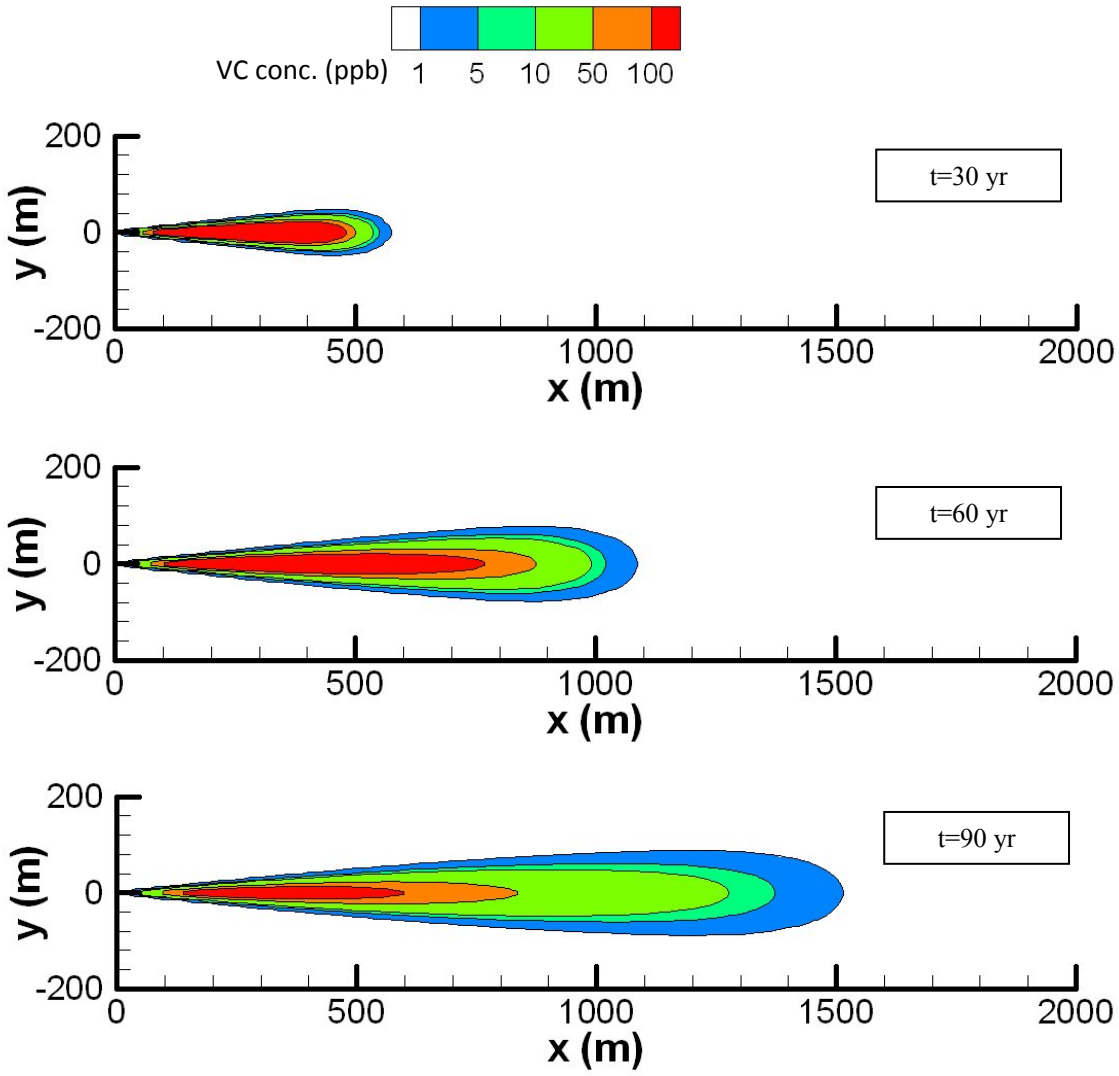


Figure 13. Plume evolution over time without remediation (Case III).

Table 5. Input parameters tested in sensitivity analysis (Case I).

Parameters	Base Case	Sensitivity Analysis	
		Distributions	Distribution Parameters
C_0 (mg/l)	6	Triangular	min=2, most likely=6, max=10
M_0 (kg)	136	Triangular	min=50, most likely=136, max=222
Γ	1	Log-normal	geo mean =1, geo stdv=2
X_{rem}	0.85	Beta	mean=0.85, stdv = 0.08, min=0.6, max=0.99
V_d (m/yr)	8	Normal	mean=8, stdv=2.5
ϕ	0.33	Triangular	min=0.28, most likely=0.33, max=0.41
R	2	Triangular	min=1.5, most likely=2, max=2.5
α_x	x/20	Triangular	min=x/100, most likely=x/20, max=x/10
λ_{TCE} (yr-1)	0.125	Triangular	min= 0.05, most likely= 0.125, max=0.2
λ_{TCE_rem} (yr-1)	436	Triangular	min=228, most likely=436, max=644

Table 6. Input parameters tested in sensitivity analysis (Case II).

Parameters	Base Case	Sensitivity Analysis	
		Distributions	Distribution Parameters
C_0 (mg/l)	100	Triangular	min=50, most likely=100, max=150
M_0 (kg)	324	Triangular	min=162, most likely=324, max=486
Γ	1	Log-normal	geo mean =1, geo stdv=1.52
X_{rem}	0.9	Beta	mean=0.9, stdv = 0.0, min=0.7, max=0.99
V_d (m/yr)	20	Normal	mean=20, stdv=3
ϕ	0.33	Triangular	min=0.28, most likely=0.33, max=0.41
R	2	Triangular	min=1.5, most likely=2, max=2.5
α_x	x/100	Triangular	min=x/200, most likely=x/100, max=x/67
λ (yr^{-1})	0.1	Triangular	min= 0.05, most likely= 0.1, max=0.15
$\lambda_{\_rem}$ (yr^{-1})	1	Triangular	min=0.5, most likely=1, max=1.5

Table 7. Input parameters tested in sensitivity analysis (Case III).

Parameters	Base Case*	Sensitivity Analysis	
		Distributions	Distribution Parameters
C_0 (mg/l)	100	Triangular	min=33, most likely=100, max=167
M_0 (kg)	1620	Triangular	min=540, most likely=1620, max=2700
Γ	1	Log-normal	geo mean =1, geo stdv=1.52
X_{rem}	0.9	Beta	mean=0.9, stdv = 0.05, min=0.7, max=0.99
V_d (m/yr)	10	Normal	mean=10, stdv=2
ϕ	0.33	Triangular	min=0.25, most likely=0.33, max=0.45
R	2	Triangular	min=1.5, most likely=2, max=2.5
α_x	x/200	Triangular	min=x/500, most likely=x/200, max=x/125
λ_{PCE} (yr^{-1})	0.4	Triangular	min= 0.13, most likely= 0.4, max=0.67
λ_{TCE} (yr^{-1})	0.15	Triangular	min= 0.05, most likely= 0.15, max=0.25
λ_{DCE} (yr^{-1})	0.1	Triangular	min= 0.03, most likely= 0.1, max=0.17
λ_{VC} (yr^{-1})	0.2	Triangular	min= 0.07, most likely= 0.2, max=0.33
λ_{PCE_rem} (yr^{-1})	1.4	Triangular	min= 0.47, most likely= 1.4, max=2.33
λ_{TCE_rem} (yr^{-1})	1.5	Triangular	min= 0.5, most likely= 1.5, max=2.5
λ_{DCE_rem} (yr^{-1})	3.5	Triangular	min= 1.17, most likely= 3.5, max=5.83
λ_{VC_rem} (yr^{-1})	3.6	Triangular	min=1.2, most likely=3.6, max=6

* base case values from Falta [2008].

Table 8. Summary of sensitivity analysis for three plume types.

Sensitivity	Case I		Case II		Case III	
	Before remediation	**After remediation**	**Before remediation**	**After remediation**	**Before remediation**	**After remediation**
Most	C_0	Γ	V_d	V_d	V_d	λ_{vc_rem}
	Γ	λ_{tce_rem}	C_0	R	C_0	λ_{dce_rem}
	λ_{tce}	X_{rem}	Γ	ϕ	λ_{dce}	V_d
	V_d	V_d	ϕ	$\lambda_{\_rem}$	ϕ	ϕ
	M_0	R	R	M_0	λ_{tce}	Γ
	α_x	C_0	M_0	Γ	λ_{vc}	λ_{pce_rem}
	ϕ	λ_{tce}	α_x	X_{rem}	λ_{pce}	λ_{tce_rem}
	R	M_0	λ	C_0	Γ	X_{rem}
	X_{rem}	ϕ	X_{rem}	α_x	M_0	R
	λ_{tce_rem}	α_x	$\lambda_{\_rem}$	λ	R	M_0
					α_x	λ_{dce}
					X_{rem}	C_0
					λ_{pce_rem}	α_x
					λ_{tce_rem}	λ_{tce}
					λ_{dce_rem}	λ_{pce}
Least					λ_{vc_rem}	λ_{vc}

4.4 SUMMARY OF PERFORMANCE ASSESSMENT

In this project, a new probabilistic remediation model, PREMChlor, has been developed. This is achieved through linking the analytical model REMChlor to a Monte Carlo modeling simulation package GoldSim via a FORTRAN Dynamic Link Library (DLL) application. PREMChlor can simultaneously evaluate the effectiveness of source and plume remediation considering uncertainties in all major parameters. In PREMChlor, all of the key input parameters, including source parameters, transport parameters and remediation parameters, are treated as uncertain parameters represented by probability density functions (PDFs). The outputs from the PREMChlor model, including contaminant mass concentration, contaminant mass discharge, cancer risk posed by a contaminant over time at a specific location and remediation costs, are also probability distributions and probability statistics. Such results are much more useful to decision-makers who utilize the simulation results. In the PREMChlor model, a graphical user interface has been built to allow other users to easily enter the input values, run the model and view the results. A license-free GoldSim player file containing the graphical user interface has been generated to make the PREMChlor model available to potential users who are not familiar with details of the probabilistic model and the GoldSim simulation environment.

This probabilistic simulation model has been applied to a TCE plume in a shallow aquifer at a manufacturing plant. Given a good understanding of the field hydrogeology and biogeochemistry, the calibrated model with a relatively simple flow field is able to closely match the pre-remediation site condition in terms of time-series of TCE concentration for a large area of the contaminated site and a relative long period of time. Probabilistic simulations predict the effects of remediation and capture most uncertainties in key parameters based on estimated PDFs.

The PREMChlor model has also been used to conduct sensitivity analyses by assessing the influence or relative importance of each input parameter on plume behavior, in terms of contaminant mass concentration, for three different plume types. It is found that the degree of influence of different input parameters on the contaminant mass concentration varies widely for different plume types. For a stable plume that is connected to the source and a growing plume that is disconnected from the source, the parent compound concentration or the total concentration in the downgradient plume is primarily sensitive to the initial source concentration, the power function exponent, the plume degradation rate, and the chemical travel velocity, which is determined by groundwater Darcy velocity, porosity and retardation factor. For a growing plume that is connected to the source, the concentration of a daughter compound (VC) is greatly affected by its degradation rate, the degradation rate of its direct parent (DCE) and transport parameters. The power function exponent affects the VC concentration greatly and source removal fraction plays more important role than several other parameters.

5.0 IMPLEMENTATION ISSUES

The PREMChlor model is freely available, and it includes a comprehensive user's guide and a Graphical User Interface. It is recommended that new users first familiarize themselves with the EPA REMChlor model before using PREMChlor. For users who are already familiar with REMChlor, it should be possible to have PREMChlor up and running in an hour or two.

6.0 COST ANALYSIS

The PREMChlor model was designed to be used without extensive training in computer modeling. The underlying deterministic model, REMChlor, was released by the EPA in late 2008. Since then, REMChlor has been downloaded nearly 2000 times, and we have been involved in 3 one or two day short courses where we teach consultants, regulators and scientists how to use the model.

It has been our experience that it takes about 8 to 16 hours of instruction and training for a groundwater or remediation professional to become proficient with the REMChlor program. This can be done through available short courses, or it may be done as a self-study, using the comprehensive REMChlor User's Guide, which contains eight tutorial examples.

Once the user is comfortable with the REMChlor program, it probably takes an additional 8 hours to become proficient with PREMChlor. Because the fundamentals of this model are the same as REMChlor, learning PREMChlor lends itself to self-study, using the PREMChlor User's Guide. This user's guide contains a complete technical description of the model, descriptions of all input variables, and four detailed tutorial examples. Our experience with the test user group (Appendix B) is consistent with our estimate of the time it takes to learn the PREMChlor program.

Because PREMChlor is analytically based, it is considerably easier and faster to use than full numerical models, particularly if those models are run in probabilistic Monte Carlo simulations. Probabilistic numerical model analyses require much more training (probably five to ten times more) before a user is competent at their use. Individual model set-up time for a probabilistic numerical model would also be much longer than for PREMChlor. However, in fairness, we should point out that PREMChlor is limited to problems involving relatively simple flow fields that do not change in time. There are sites where it would be more appropriate to apply a probabilistic approach with a full numerical model, despite the much higher costs involved.

One benefit of using PREMChlor instead of a deterministic approach is that remediation designs can be made more robust. That is, they can be designed so that they will still work even if some of the site parameters are different from initial estimates. While it is difficult to quantify the economic benefit of increased robustness, remediation efforts are expensive. Reducing the likelihood of remediation system failure should have a strong economic benefit.

PREMChlor was designed to be used to help optimize remediation designs. The basic procedure follows three steps: 1) initial deterministic model calibration to site data; 2) probabilistic simulation of several remediation alternatives (including cost functions); and 3) comparison of costs of remediation alternatives that meet the site constraints. This probabilistic cost optimization process is illustrated by a detailed example below.

6.1 COST OPTIMIZATION EXAMPLE

Introduction

A planning level assessment of remedial alternatives was performed to address chlorinated solvents found in shallow groundwater using PREMChlor. The data used for this analysis is based on the Cape Canaveral Air Station, Florida treatability study (Parsons, 1997).

Several remediation technologies were evaluated based on performance and cost:

1) Monitored natural attenuation (MNA),
2) Thermal treatment of the source area,
3) Bioremediation of the source area, and
4) Installation of a zero valent iron (ZVI) barrier wall adjacent to the river.

Area Description

Cape Canaveral Air Station is located on a barrier island on the east coast of Florida and bounded on the east by the Atlantic Ocean and on the west by the Banana River (Figure 14). The area of interest for this study is the former fire training area CCFTA-2, located approximately 336 m (1,000 ft) from the Banana River. Between about 1965 and 1985, this area was used for firefighting training (Parsons, 1997).

Groundwater sampling has indicated the presence of chlorinated hydrocarbons including trichloroethene (TCE), cis-1,2-dichloroethene (DCE) and vinyl chloride (VC). Additionally, light non-aqueous phase liquids (LNAPLS) have also been detected at the site (Parsons, 1997).

Objectives

The objective of this study was to develop a planning level evaluation of remediation alternatives for remediating chlorinated solvents at the site. The technologies evaluated were:

1) monitored natural attenuation,
2) thermal treatment of the source area,
3) bioremediation of the source area, and
4) installation of a ZVI permeable reactive barrier (PRB) wall downgradient of the plume.

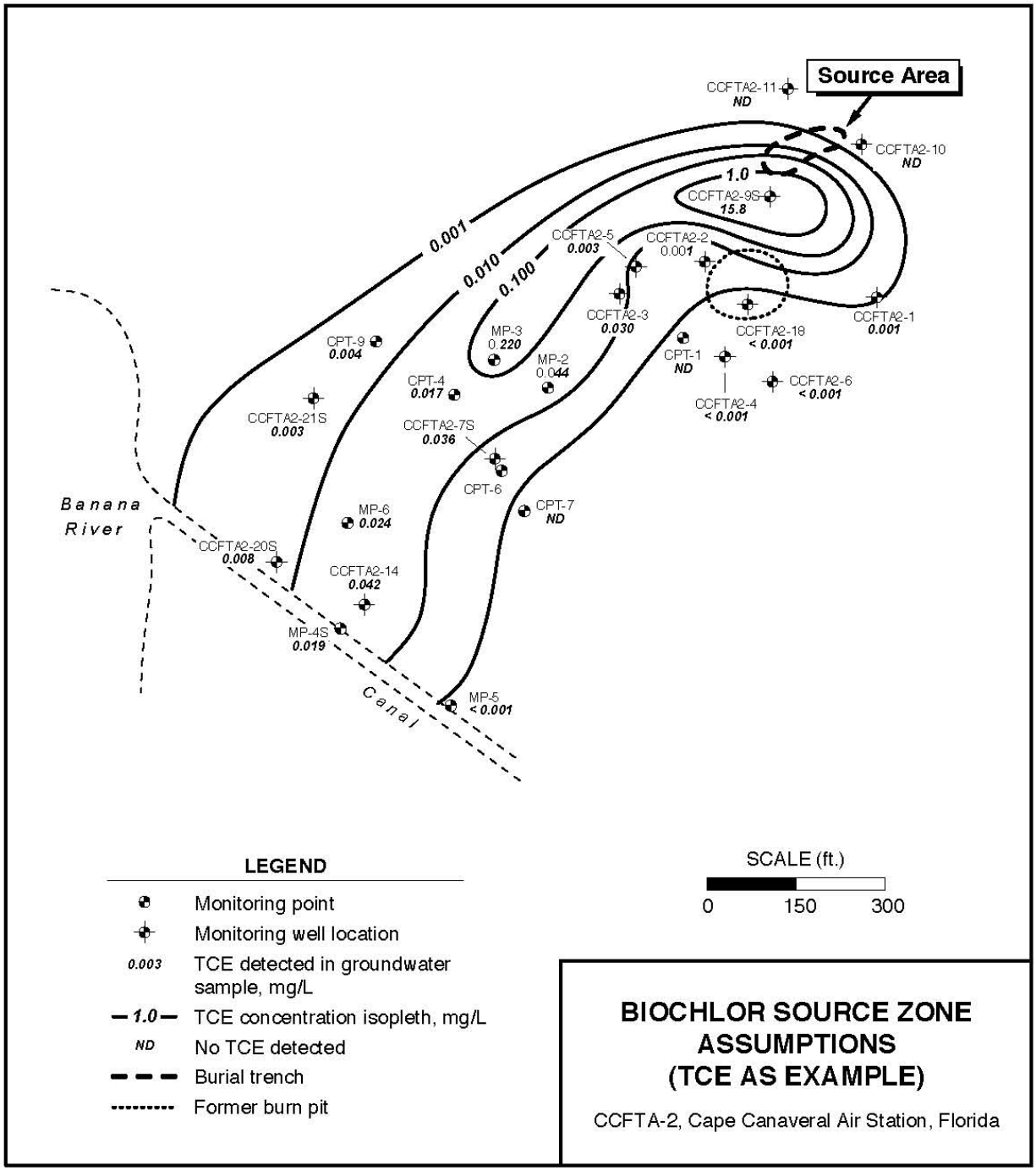


Figure 14. Model Area. Figure Adapted from the Biochlor Manual (Aziz, 2000).

Performance of the technologies was based on the metrics:

1) contaminant mass discharge into the river,
2) constituent concentration discharging into the river,
3) plume length , and
4) technology cost (including operation and management).

Model Description

PREMChlor was used to evaluate the movement of dissolved TCE, DCE, and VC migrating in the groundwater and the performance of remedial alternatives for the site.

Key model attributes, assumptions, and input data for the contaminant model are listed below. Initial data were based on the treatability study (Parsons, 1997) and the Biochlor manual (Aziz et al., 2000).

- A source depth of 17 m, and length of 79.2 m were based on figures in the treatability study. Although a source width of 32 m was used initially based on Biochlor, a final width of 17 m was used during the calibration process based on figures in the treatability study.
- Source concentration was estimated by projecting the concentration in the monitoring well CCFTA2-9S backward in time assuming a conservative first-order source decay half-life of 30 years. An initial source concentration of 32 mg/L was used. Source concentration was adjusted during model calibration.
- Initially, the monitoring well CCFTA2-9S was assuming to lie in the source zone based on Biochlor, however, during calibration, and based on the site figures, this well was assumed to be 25 m downgradient of the source area (Figure 1).
- Source mass was estimated by projecting the observed soil TCE concentrations backward in time assuming a conservative first-order source decay half-life of 30 years. Initially, a source mass of 1204 kg was used in the model. Source mass was adjusted during model calibration.
- A conservative source power function of 1.0 was used initially. The source power function was adjusted during model calibration.
- Initially, the Darcy velocity of 6.8 m/yr reported in the Biochlor manual was used in the model. Darcy velocity was adjusted during model calibration.
- An effective porosity of 0.2 was used in the model.
- Initially, the retardation factor of 2.87 reported in the Biochlor manual was used in the model. This value was adjusted during model calibration.
- The PREMChlor default values of scale-dependent longitudinal (0.01), transverse (0.001), and vertical (0.0001) dispersivities were initially used in the model. These parameters were adjusted during model calibration.
- No additional source decay was assumed in the model.
- Initially, the dissolved phase biodegradation rate of 0.18 yr^{-1} for both TCE and DCE, reported in the treatability study, and the VC degradation rate of 0.4 yr^{-1} reported in

Biochlor were used in the model. These parameters were adjusted during model calibration.

- Yields of DCE from TCE of 0.74, VC from DCE of 0.64, and ethene from VC of 0.45 were used in the model.
- Concentration observation wells, CCFTA2-9S, MP-3, CPT-4, MP-6, CCFTA2-14, and MP-4S, located in the centerline of the TCE plume were used for the calibration (Figure 1). For this purpose, the concentrations for each constituent observed in 1996 were used for comparison of simulated to measured concentrations.

Model Calibration

Calibration is the process of adjusting model parameters until the difference between modeled outputs and site-specific data are reduced to an acceptable level.

Both qualitative and quantitative comparisons were made between the model and site-specific information. Qualitative comparisons included comparison of observed centerline plume distribution to the distribution of the simulated plume. Quantitative comparisons included the comparison of simulated concentrations to measured concentrations and a comparison of the root mean square (rms) error between the two. Concentration data collected during 1996 were used for a more detailed calibration in the site area.

For calibration purposes, the model was run in deterministic mode. Over 200 deterministic simulations were run during the calibration process using various combinations of input parameters. The model was calibrated in the sequence described in the following sections.

Quantitative Calibration 1

Initially, the model was run in deterministic mode and only TCE was calibrated. For this purpose source mass, scale-dependent longitudinal and vertical dispersivities, and plume degradation rates were adjusted individually until the best possible agreement between simulated and measured concentrations was achieved.

After a trial and error process, increasing the source mass to 5,157 kg, decreasing the scale-dependent longitudinal dispersivity to 0.006 and vertical to 1×10^{-7}, and using a rate constant of 0.92 yr^{-1} throughout the dissolved plume yielded a better comparison between simulated and observed TCE concentrations (Figure 2) with an rms error of 45 ug/L. However, although a good comparison was obtained for TCE, the DCE concentration at the source well could not be reproduced (Figure 15).

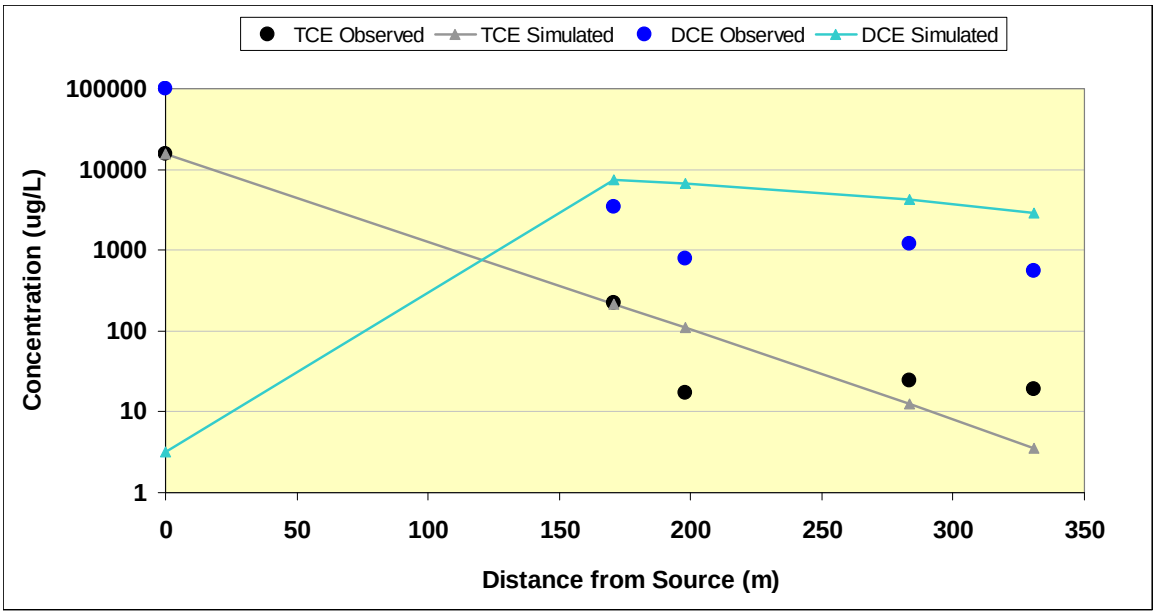


Figure 15. Comparison of Simulated and Observed TCE concentrations.

Quantitative Calibration 2

To obtain a better match for DCE and VC observed concentrations at monitoring well CCFTA2-9S, the source area was redefined based on figures in the treatability report. Next, the power function, source mass, retardation factor, and biodegradation rates were varied. Furthermore, to better match observed concentrations, the dissolved plume was divided into 3 zones and the biodegradation rate in each zone varied to obtain a better comparison with observed concentrations. After a trial and error process, a good comparison for TCE, with an rms error of 33.4 ug/L, was obtained using:

- source mass of 5,557 kg,
- source function of 0.5,
- retardation factor of 2,
- dissolved plume Zone 1 width of 25 m (distance from source edge to the first monitoring well in the plume centerline) with a biodegradation rate of 0.43 yr^{-1},
- dissolved plume Zone 2 width of 192 m (distance from CCFTA2-9S to CCFTA2-3) with a biodegradation rate of 0.95 yr^{-1}, and
- dissolved plume Zone 3 (beyond CCFTA2-3) with a biodegradation rate of 0.431 yr^{-1}

However, although a higher DCE concentration was obtained in CCFTA2-9S than Calibration 1, the simulated value was still considerably lower than the observed value: 4,367 ug/L compared to the observed value of 98,500 ug/L.

Quantitative Calibration 3: Final Calibration

Better comparison of simulated TCE, DCE, and VC concentrations to observed concentrations were obtained by:

- varying source concentration to 301 mg/L;
- using a source mass of 5,557 kg (from Calibration 2);
- using a power function of 0.5 (from Calibration 2);
- varying source width to 16 m;
- varying source length to 79.2 m;
- varying the Darcy Velocity to 2.4 m/yr (a range of 2.2 m/yr to 22.1 m/yr is reported in the treatability study (Parsons, 1997));
- using a retardation factor of 2 (from Calibration 2);
- varying the longitudinal scale-dependent horizontal dispersivity to 0.1;
- using a scale-dependent vertical dispersivity of 1 x 10^{-7} (from Calibration 1);
- dissolved plume Zone 1 length of 25 m (from Calibration 2);
- dissolved plume Zone 2 length of 215 m;
- TCE plume degradation rates of 1.14 yr^{-1}, 0.45 yr^{-1}, and 0.039 yr^{-1} for Zones 1, 2, and 3, respectively;
- DCE plume degradation rates of 0.024 yr^{-1}, 0.31 yr^{-1}, and 0 for Zones 1, 2, and 3, respectively;
- VC plume degradation rates of 0.044 yr^{-1}, 0.46 yr^{-1}, and 0 for Zones 1, 2, and 3, respectively;
- Yields of DCE from TCE of 0.74, VC from DCE of 0.64, and ethene from VC of 0.45.

A final rms error of 37 ug/L was obtained for TCE. Although much higher rms errors were obtained for DCE and VC, qualitatively, the simulated DCE concentrations are a good fit for the observed values. For VC, as can be seen in Figure 16, the observed concentrations at the downgradient wells are significantly underpredicted by the model. However, overall, the model presents a conservative estimate of actual conditions present at the site.

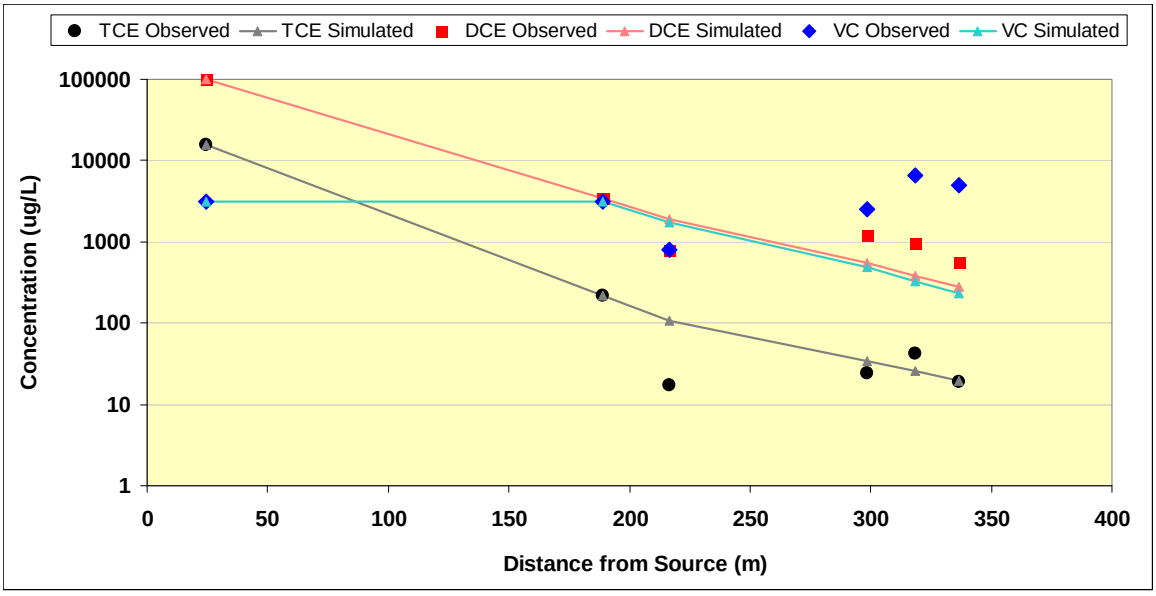


Figure 16. Final Calibration of TCE, DCE, and VC.

Probabilistic Model Development

The calibrated deterministic model was then converted to a probabilistic version based on ranges in the underlying data for each parameter (Table 9). To obtain a reasonable distribution of outputs, 1000 realizations using Latin Hypercube Sampling were run for each remedial alternative.

Remediation Alternatives

Several remedial alternatives were evaluated using the calibrated model, including:

- Monitored natural attenuation.
- Thermal treatment of the source.
- Bioremediation of the source.
- Zero valent iron PRB downgradient of source.

Key design criteria for technologies included applicability to the site and the ability to treat chlorinated ethenes. The alternatives were evaluated on the basis of Performance and Operational Cost. Performance estimates were based on:

- Contaminant mass discharge into the river.
- Concentration at the river.
- Dissolved plume length (defined as the length of the dissolved plume to the maximum contaminant level (MCL) of TCE (MCL = 5 ug/L), DCE (70 ug/L), and VC (2 ug/L)).

Performance metrics were obtained 3, 10, 30, and 60 years after the start of remediation. For purposes of this evaluation, remediation was assumed to start 32 years after the initial release of contaminants into the subsurface.

PREMChlor default source efficiencies and unit cost information were used for thermal treatment and bioremediation technologies (Table 10). For the ZVI PRB, source efficiency and unit cost information was obtained from data compiled by GSI Environmental Inc. (GSI, 2008 and 2009).

Thermal treatment was assumed to last for one year, bioremediation for two years, and the ZVI PRB for 30 years. The PRB was assumed to be 0.9 m thick, 183 m wide, and 12 m deep and installed just upgradient of the river. Over time the ZVI media loses efficiency, therefore, the total cost of implementing the ZVI PRB at the site includes the cost for maintaining the ZVI media every 10 years (GSI, 2009).

Discussion

Remedy Performance

Results of the performance metrics are presented in Table 11. PREMChlor output for TCE for each alternative, except ZVI PRB, are presented in Figure 17. The table displays the average of

the 1,000 realizations performed for each remedial option. Note that because the dissolved plume was simulated as containing three distinct zones, each with an individual biodegradation rate, and the PRB was located at the river, constituent mass discharge, plume concentration, and plume length could not be calculated for the ZVI PRB using PREMChlor.

Even though an increase in VC mass discharge to the river was observed 10 years after bioremediation, however, over time, the mass discharge decreased. Based on the modeling results, significant reductions in mass discharge to the river were observed 30 and 60 years after source remediation following thermal treatment and bioremediation for all three constituents.

- Thirty years after thermal treatment, reductions of 63%, 55%, and 46% in TCE, DCE, and VC mass discharge, respectively, were observed compared to MNA. Bioremediation resulted in 51%, 51%, and 56% reductions in TCE, DCE, and VC, respectively, compared to MNA.
- Sixty years after remediation, 97%, 94%, and 90% reductions in TCE, DCE, and VC mass discharge, respectively, were observed after thermal treatment of the source. While 95%, 90%, and 83% reductions, respectively for the three constituents, were observed after bioremediation.

Similarly, significant reductions in constituent concentrations at the river were observed 30 and 60 years after source remediation.

- Thirty years after thermal treatment, reductions of 59%, 45%, and 49% in TCE, DCE, and VC concentrations, respectively, were observed compared to MNA. Bioremediation resulted in 44%, 43%, and 41% reductions in TCE, DCE, and VC, respectively, compared to MNA.
- Sixty years after remediation, 95%, 91%, and 90% reductions in TCE, DCE, and VC mass discharge, respectively, were observed after thermal treatment of the source. While 93%, 87%, and 77% reductions, respectively for the three constituents, were observed after bioremediation.

A reduction in DCE plume length was observed 30 years after both thermal treatment and bioremediation. While a reduction in the TCE plume length was observed 60 years after both thermal treatment and bioremediation.

Remedy Cost

Total cost of each remedial alternative is presented below assuming a 30-year period.

Technology	Total Cost ($ Million)		
	25th Percentile	Median	75th Percentile
MNA	4.1	7.6	12.1
Thermal	7.0	10.7	15.1
Bioremediation	5.1	8.6	13.3
ZVI PRB	13.1	18.6	25.8

Conclusion of Cost Optimization Example

Based on planning-level cost and performance modeling, bioremediation has the best balance of performance, implementability, and cost. Key limitations of the other technologies include:

- Although MNA has a lower over cost over 30 years, there is a significant plume discharging into the river, even after 60 years.
- Thermal treatment and bioremediation indicate similar treatment results, however on average, thermal treatment will cost approximately $2 million more over 30 years.
- ZVI is prohibitively expensive.

Table 9

Parameter	Most Likely Value	Minimum Value	Maximum Value	Units	Notes
Source Zone					
Source concentration	0.30	0.15	0.62	g/L	Adjusted during calibration.
Source mass	5557.23	555.72	55572.3	kg	Adjusted during calibration.
Power function	0.5	1 (standard deviation)		-	Adjusted during calibration.
Source width	16	-	-	m	Parsons, 1997.
Source depth	17.1	8.55	34.2	m	Parsons, 1997.
Source length	79.2	-	-	m	Parsons, 1997.
Transport					
Darcy velocity	2.4	1.2 (standard deviation)		m/yr	Adjusted during calibration. Reported range: 2.2 m/yr to 22.1 m/yr (Parsons, 1997).
Porosity	0.2	0.1	0.35	-	Parsons, 1997.
Retardation factor	2	1.42	5.35	m	Adjusted during calibration. Literature range from Aziz et al., 2000.
Scale dependent longitudinal dispersivity	0.1	0.001	0.2	-	Adjusted during calibration.
Scale dependent transverse dispersivity	0.001	0.0001	0.01	-	Adjusted during calibration.
Scale dependent vertical dispersivity	1×10^{-7}	1×10^{-8}	1×10^{-6}	-	Adjusted during calibration.

Final Model Parameters

Table 9 Cont'd

Parameter	Most Likely Value	Minimum Value	Maximum Value	Units	Notes
Plume Decay Rates					
TCE: Zone 1 (0 – 25 m)	1.14	0.55	2.28	yr^{-1}	Adjusted during calibration. Literature range: 0.05 yr^{-1} to 0.9 yr^{-1} (Aziz et al., 1997).
TCE: Zone 2 (25 – 240 m)	0.45	0.23	0.91	yr^{-1}	Adjusted during calibration. Literature range: 0.05 yr^{-1} to 0.9 yr^{-1} (Aziz et al., 1997).
TCE: Zone 3 (240 m onwards)	0.039	0.02	0.079	yr^{-1}	Adjusted during calibration. Literature range: 0.05 yr^{-1} to 0.9 yr^{-1} (Aziz et al., 1997).
DCE: Zone 1 (0 – 25 m)	0.024	0.012	0.048	yr^{-1}	Adjusted during calibration. Literature range: 0.18 yr^{-1} to 3.3 yr^{-1} (Aziz et al., 1997).
DCE: Zone 2 (25 – 240 m)	0.31	0.15	0.62	yr^{-1}	Adjusted during calibration. Literature range: 0.18 yr^{-1} to 3.3 yr^{-1} (Aziz et al., 1997).
DCE: Zone 3 (240 m onwards)	0	0	3.3	yr^{-1}	Adjusted during calibration. Literature range: 0.18 yr^{-1} to 3.3 yr^{-1} (Aziz et al., 1997).
VC: Zone 1 (0 – 25 m)	0.044	0.022	0.088	yr^{-1}	Adjusted during calibration. Literature range: 0.12 yr^{-1} to 2.6 yr^{-1} (Aziz et al., 1997).
VC: Zone 2 (25 – 240 m)	0.46	0.23	0.92	yr^{-1}	Adjusted during calibration. Literature range: 0.12 yr^{-1} to 2.6 yr^{-1} (Aziz et al., 1997).
VC: Zone 3 (240 m onwards)	0	0	2.6	yr^{-1}	Adjusted during calibration. Literature range: 0.12 yr^{-1} to 2.6 yr^{-1} (Aziz et al., 1997).
Porosity	0.2	0.1	0.35		Adjusted during calibration. Reported range: 0.05 m/yr to 0.9 m/yr (Aziz et al., 1997).

Final Model Parameters

Table 10
Remedial Technology Performance and Unit Cost Parameters Using a Beta Distribution

Parameter	Performance Efficiency (Percent Removed)				Unit Cost ($/m^3)			
	Mean	Standard Deviation	Min	Max	Mean	Standard Deviation	Min	Max
MNA[1]	-	-	-	-	100,000	-	1,000	1,000,000
Thermal Treatment	97	2.5	56	100	115.1	50	41.85	392.39
Bioremediation	95	2	29	100	37.93	25	2.62	294.29
ZVI PRB[2,3]	76	29	22	99.9	2,414.07	2,255.30	145.28	8,961.25
ZVI Maintenance (Every 10 years)[2]	-	-	-	-	663.87	620.21	39.95	2,464.34

Notes:
1. Assumed annual operating and management costs.
2. GSI Environmental Inc. Oct 7, 2008 G-3243 work products. Table "Construction and O&M costs per square foot of ZVI PRB".
3. GSI Environmental Inc. Apr 7, 2009 G-3243 work product. Table "Iron wall performance data."

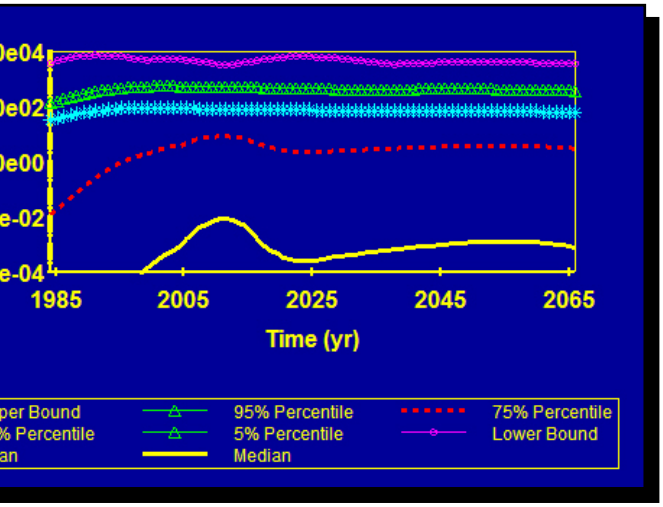
Table 11. PREMChlor Output: Performance Metrics

f r n	Mass Discharge into River (kg/yr)											
	TCE				DCE				VC			
	MNA	TT	Bio	ZVI[1]	MNA	Thermal	Bio	ZVI[1]	MNA	Thermal	Bio	ZV
	0.78	0.71	0.74	n/a	0.65	0.51	0.51	n/a	0.84	0.86	1.23	n/
	0.67	0.64	0.70	n/a	0.87	0.62	0.67	n/a	0.99	0.99	1.41	n/
	0.51	0.19	0.25	n/a	0.65	0.29	0.32	n/a	0.98	0.43	0.53	n/
	0.48	0.02	0.03	n/a	0.59	0.04	0.06	n/a	0.91	0.09	0.16	n/
f r n	Concentration at River (ug/L)											
	TCE (MCL = 5 ug/L)				DCE (MCL = 70 ug/L)				VC (MCL = 2 ug/L)			
	MNA	TT	Bio	ZVI[1]	MNA	Thermal	Bio	ZVI[1]	MNA	Thermal	Bio	ZV
	92.77	86.46	101.05	n/a	88.57	67.70	71.31	n/a	114.83	135.87	169.56	n/
	83.31	81.55	97.99	n/a	116.05	85.69	98.19	n/a	143.15	166.74	205.76	n/
	71.20	29.11	40.14	n/a	97.20	53.78	54.99	n/a	156.56	79.77	91.68	n/
	67.05	3.21	4.81	n/a	95.53	8.80	12.87	n/a	155.51	15.52	35.20	n/
f r n	Plume Length[3] (m)											
	TCE (MCL = 5 ug/L)				DCE (MCL = 70 ug/L)				VC (MCL = 2 ug/L)			
	MNA	TT	Bio	ZVI[1]	MNA	Thermal	Bio	ZVI[1]	MNA	Thermal	Bio	ZV
	>336	>336	>336	n/a	>336	331	>336	n/a	>336	>336	>336	n/
	>336	>336	>336	n/a	>336	>336	>336	n/a	>336	>336	>336	n/
	>336	>336	>336	n/a	>336	315	324	n/a	>336	>336	>336	n/
	>336	160	199	n/a	>336	196	220	n/a	>336	>336	>336	n/

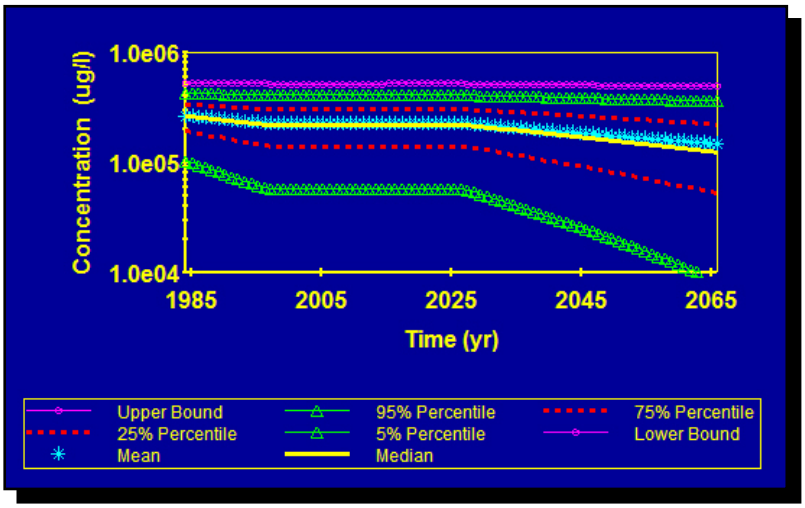
be calculated by PREMChlor because the dissolved plume was simulated as three distinct zones with individual biodegradation rates.
new ZVI PRB will be installed in 2027.
ver is approximately 336 m from the source area. Therefore, a distance of >336 assumes the plume discharges to the river.
:
remediation
ilograms per year
r

MCL = Maximum contaminant level
TT = Thermal treatment
ug/L = Micrograms per liter

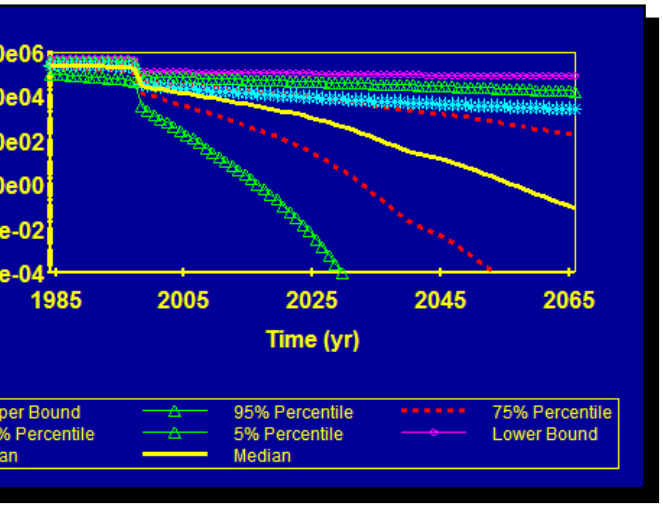
Figure 17. PREMChlor Output: TCE Concentrations



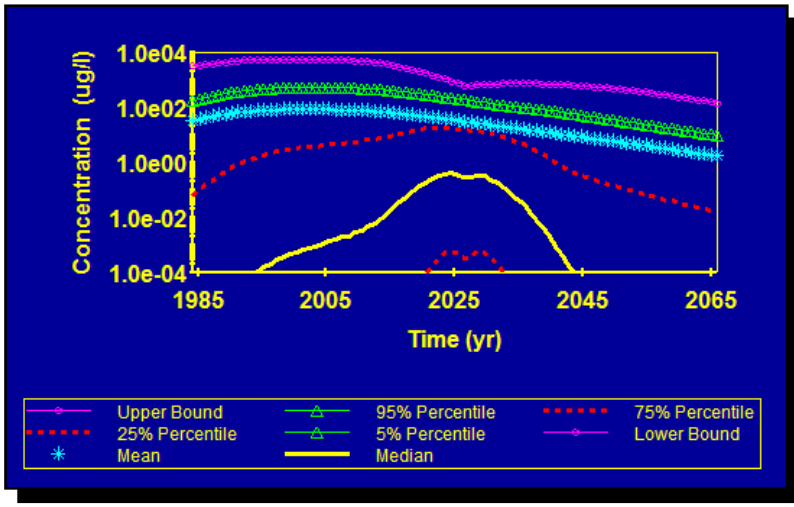
– TCE Concentrations at Source



17b. MNA – TCE Concentrations at River

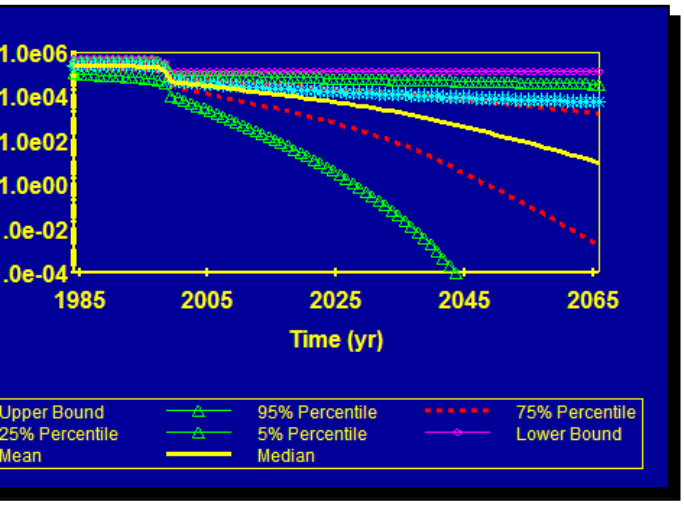


nal Treatment – TCE Concentrations at Source

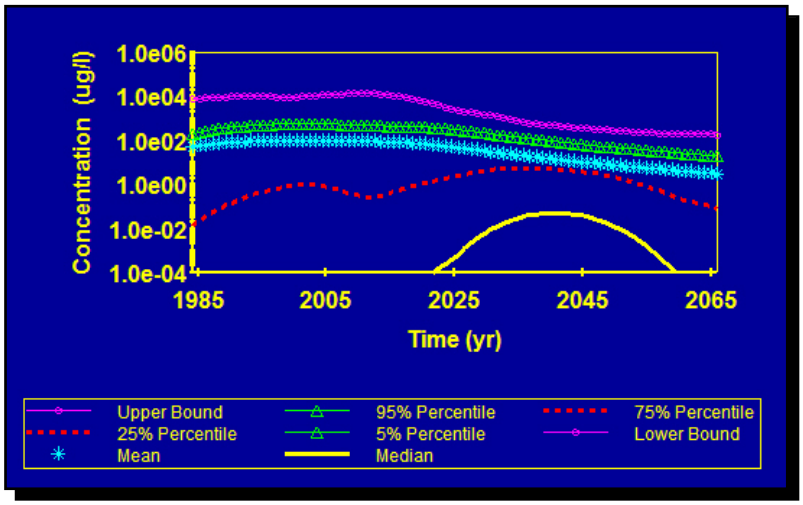


17d. Thermal Treatment – TCE Concentrations at River.

Figure 17 cont. PREMChlor Output: TCE Concentrations



oremediation – TCE Concentrations at Source



17f. Bioremediation – TCE Concentrations at River

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APPENDICES

Appendix A: Points of Contact

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Appendix B: Test User Comments on PREMChlor

MEMORANDUM FOR RECORD

SUBJECT: Evaluation of Beta Version 1.0 REMChlor/ GoldSim Player Model for Optimization of Chlorinated Solvent Source and Plume Remediation Considering Uncertainty, Using Fort Lewis East Gate Disposal Yard Site Data

PREPARED BY: Jefferey Powers, Seattle District, U.S. Army Corps of Engineers

Date: 16 October 2009

Introduction and Purpose.
The Seattle District, U.S. Army Corps of Engineers (USACE) is assisting the USACE Environmental and Munitions Center of Expertise in testing the beta version of subject modeling software developed by Dr. Ronald Falta of Clemson University. This model is a probabilistic version of the REMChlor deterministic model, also developed in part by Dr. Falta for the USEPA, which is a remediation evaluation model for chlorinated solvents that considers both source and plume treatment. Site-specific Fort Lewis East Gate Disposal Yard (EGDY) historical data was used for the evaluation. The main advantage of the REMChlor/GoldSim Player model is its ability to determine ranges of remediation efficacy dependent on uncertainty factors or parameter minimum/maximum ranges, thereby allowing the user to develop a more robust remedial strategy.

Software Tested.
GoldSim Player model beta version 1.0, utilizing GoldSim version 9.6 SP4
REMChlor version 1.0 is called and run from within the GoldSim Player model

Computer Specifications on which Software Installed.
Dell Latitude D600
Pentium processor, 1.50 GHz
1.00 GB of RAM
Microsoft Windows XP operating system

Input Parameters.
Three sub-areas of the EGDY were thermally treated in-situ by electrical resistance heating. Of the three treated sites, NAPL Area 3 data were utilized because the data set was greater and uncertainty, while still present, was thought to be better constrained than for either of the first two treatment areas, or for the three treatment areas as a whole. The EGDY was believed to be a well-characterized site, with abundant chemical and geohydrologic data to support treatment design and operation. Chemical data included pre-, during, and post-treatment contaminant histories. The principal contaminant of concern – and the principal component modeled ("Component 1") – was and continues to be TCE, a chlorinated volatile organic solvent. The thermally treated NAPL areas contained a mixture of TCE and daughter products plus petroleum hydrocarbons, although the latter occurred to a lesser extent within NAPL Area 3. The following contains model set-up and site-specific parameter values and ranges of values utilized for the probabilistic model.

Simulation Settings Interface. Under the Time tab, the time units were set to "years." The simulation duration was set to 100, with a start time (time of DNAPL source emplacement) of 1/1/1960. There were 100 time steps, each one year in duration. First a deterministic model was set up and calibrated by inputting single parameter values in the input fields and checking the box to utilize deterministic values, and checking Deterministic Simulation under the Monte Carlo tab. The final deterministic values were used as the "likely values" for the probabilistic runs. Once the model was satisfactorily calibrated using deterministic values, the boxes were unchecked and the Probabilistic Simulation was checked under the Monte Carlo tab to utilize the GoldSim Player functionality. The default settings were kept under the Monte Carlo tab. These settings were: use 100 realizations (saving all 100), use Latin Hypercube Sampling, and Repeat Sampling Sequences. Random Seed was set to one. The Globals tab was not used under the Simulation Settings Interface.

Source Zone Parameters Interface

Parameter	**Minimum Value**	**Likely Value**	**Maximum Value**
Initial Concentration (g/L)	0.1	1.1	1.3
Initial Mass (kg)	13,700	28,000	43,000
Source Width (m)	35	37	39
Source Depth (m)	8	10	12
Source Length (m)	48	50	52

Gamma: Mean of 1.9, Standard deviation of 1.41

Transport Parameters Interface

Parameter	**Minimum Value**	**Likely Value**	**Maximum Value**
Porosity	0.2	0.3	0.38
Retardation Factor	0.01	2	10
Scale-Dependent Dispersivity, Longitudinal	0.001	0.2	1
Scale-Dependent Dispersivity, Transverse	0.0001	0.02	0.1
Scale-Dependent Dispersivity, Vertical	0.00001	0.002	0.01

Darcy Velocity: Mean of 15 m/yr, Standard deviation of 2

Source Remediation Interface

Parameter	**Minimum Value**	**Likely Value**	**Maximum Value**
Aqueous Phase Source Decay (1/yr)	0	0.002	0.15

Remediation time (yr): Start t = 46.7, End t = 47.0 (corresponds approximately to Oct 2006 and Jan 2007, respectively, the start and end dates of NAPL Area 3 thermal treatment)
Thermal treatment percent of source removed: 96% (deterministic value used)
Unit cost to treat per cubic meter: $184 (deterministic value used)

Plume Decay Rates Interface (matrix format)

Time Period 3 (t > 47.0 yr)	Min Likely Max 0.4 0.8 2.4	Min Likely Max 0.4 0.8 2.4	Min Likely Max 0.4 0.4 2.4
Time Period 2 (t = 46.7-47.0 yr)	Min Likely Max 0.8 1.4 2.4	Min Likely Max 0.8 1.3 2.4	Min Likely Max 0.4 0.4 2.4
Time Period 1 (t = 0-46.7 yr)	Min Likely Max 0.4 0.4 2.4	Min Likely Max 0.4 0.4 2.4	Min Likely Max 0.4 0.4 2.4
	0-50 m Distance From Source	**50-75 m Distance From Source**	**>75 m Distance From Source**

The Sensitivity Analysis Interface and the Optimization Interface are non-operational in the beta version of the model; therefore these interfaces were not evaluated.

To simulate an average area within the shallow thermal treatment zone, an observation location of 5 m was input (X = 5 m, Y& Z = 0). To simulate the approximate location of PW-3, an existing groundwater extraction well downgradient of NAPL Area 3 for which historical chemical data exists, an observation location of 70 m was input. To smooth some of the plotted output, the number of stream tubes was set to 175.

Results.
After all parameter values were input into their respective fields, the Run Model button was selected and the probabilistic model ran all 100 realizations. The run time on the computer utilized was approximately 11 seconds. Model execution time appeared to mainly be a function of the number of realizations and number of stream tubes chosen.

Total Concentration Tab. The graphical output shows yearly time series concentration history since DNAPL emplacement at t = 0 yr, in this case t = 0 corresponds to the year 1960. The probability history shows the statistics including the lower bound, 5% percentile, 25% percentile, median, 75% percentile, 95% percentile, and the upper bound. The view can be toggled between graphical view and tabular data view. A summary of notable years/dates and corresponding dissolved-phase TCE concentrations from both within the treatment area (X = 5 m) and downgradient (X = 70 m) are summarized below.

Simulation Time (yr)	Year	Within Treatment Area		70 m Downgradient of Treatment	
		Mean (ug/L)	95% Percentile (ug/L)	Mean (ug/L)	95% Percentile (ug/L)

1	1961[A]	469,000	720,000	15,500	105,000
46	2006[B]	2,320	10,600	1,180	6,750
49	2009[C]	126	662	784	4,550
77	2037[D]	4.9	23.9	3.9	25.6
100	2060[E]	3.1	12.6	1.2	6.7

Notes:
[A]Estimated time of initial NAPL emplacement at EGDY, plus one year.
[B]Prior to thermal treatment
[C]Present time, approximately 2 years post-treatment
[D]30 years after treatment
[E]End of modeled simulation

Simulated mean TCE concentrations reasonably conformed to analytical data from just prior to thermal treatment of NAPL Area 3 (t = 46 yr) and about 2 years after treatment (t = 49 yr). The mean concentration within the treatment area before treatment was 322 ug/L compared to the simulated mean of 2,320. Although these results are quite dissimilar, the model does not take into account a bioenhancement project which occurred within a portion of NAPL Area 3 just prior to thermal treatment. The effect of the biodemonstration project conducted before thermal treatment within NAPL Area 3 was to reduce chlorinated organics concentrations considerably; pre-biodemonstration concentrations were as high as 13,000 ug/L (no mean determined at that time) which is close to the 95% percentile value of 10,600 ug/L. The latest mean concentration within the treatment area data available (7 months after treatment complete) was 187 ug/L compared to the simulated mean of 126 ug/L. The mean concentration 70 m downgradient of the uppermost point of the treatment area (X = 0 m), at extraction well PW-3, before treatment was 518 ug/L compared to the simulated mean of 1,180 ug/L. The mean concentration at this downgradient point about two years after treatment was 117 ug/L compared to the simulated mean of 784 ug/L. The model does not take into account groundwater extraction and treatment which has occurred within the model domain both before and after thermal treatment, which has acted to reduce contaminant concentrations. Another factor not incorporated into the model is the presence of TCE in groundwater upgradient of NAPL Area 3 treatment zone at concentrations of at least 120 ug/L.

Total Discharge Tab. The graphical and tabular output shows mass discharge in kg/yr over the period of simulation for each year simulated. A summary of notable years/dates and corresponding TCE mass discharge from both within the treatment area (X= 5m) and downgradient (X = 70 m) are summarized below.

Simulation Time (yr)	Year	Within Treatment Area		70 m Downgradient of Treatment	
		Mean (kg/yr)	95% Percentile (kg/yr)	Mean (kg/yr)	95% Percentile (kg/yr)
1	1961[A]	3,410	5,520	339	2230
46	2006[B]	14.2	66.0	13.3	62.7

49	2009[C]	0.2	1.0	7.8	48.6
77	2037[D]	0.03	0.2	0.03	0.14
100	2060[E]	0.02	0.1	0.01	0.08

Notes:
[A]Estimated time of initial NAPL emplacement at EGDY, plus one year.
[B]Prior to thermal treatment
[C]Present time, approximately 2 years post-treatment
[D]30 years after treatment
[E]End of modeled simulation

For comparison, mass flux calculated from integrated pumping tests prior to thermal treatment considering the source area only (downgradient minus upgradient flux) ranged from 32 to 48 kg/yr. No post-treatment testing was conducted for NAPL Area 3; however, assuming the same percentage reduction in mass between pre- and post-treatment as was calculated for NAPL Area 1 (99.8%), a post-treatment mass flux of about 0.1 kg/yr would be expected. In all, the modeled results agree reasonably well with the calculated mass flux values.

It does not appear that either of the Total Concentration Tab or Total Discharge Tab results for breakdown products (Components 2, 3, and 4 in Plume Decay Rates Interface) can be shown in the display. For this reason cis-DCE and vinyl chloride, the two principal daughter products of TCE, were not tested.

Overall, the model is believed to reasonably represent the original contaminant system with respect to TCE and the effects of chlorinated solvent source remediation by electrical resistance heating thermal treatment at NAPL Area 3. The 95% percentile TCE concentrations and mass discharge appear to bound the range of most available site data quite well. Once the modeler becomes familiar with the functionality and operation of REMChlor, the GoldSim Player add-on is quite intuitive. Future versions of the REMChlor/ GoldSim Player probabilistic model may benefit from a library containing typical ranges of parameters encountered based on actual sites. This library could be included as an appendix in the user's manual.

Feedback on PREMChlor from James Henderson, DuPont, 01/07/2010.

General Feedback
In utilizing the model here in DuPont, I have encountered some resistance to this type of screening level approach. Some practitioners prefer to remove a vast majority of uncertainty from the site conceptual model before they undertake remedial decision-making. This can only be done with many years of investigation. For these people, and those who are less familiar with the screening level approach, it is thus important to make clear what the limitations of the model, and how best to apply it.

I continue to receive questions about back diffusion. The fact that the model does not currently account for this process, which may or may not be active at sites, is deemed as being increasingly important. In a few cases, practitioners have opted not to use the model for this reason.

Specific Feedback

It would be helpful if users were able to view results over time or distance (Hailian, you've already taken care of this one).

There are times when the GoldSim controller disappears from my screen. I'm not sure why this happens, but it requires the model be closed and restarted.

People find it difficult to interpret the default color flood. In my experience, it takes some time to understand the way the results are displayed. It might be good to have more description of how to interpret the color floods (similar to that included with the REMChlor User's Manual).

Some confusion results from the multitude of different plume decay rates that can be use. A note of caution should be included in the User's Manaual to be vigilent about this. Where no operative ranges of rates are needed, the deterministic box should be used as necessary.

REMChlor/Goldsim (R/G)
Model Review
Linda Bond, Noblis
July 31, 2009

1. General

Abbreviations: Review all the abbreviations and acronyms used in the text including unit abbreviations and provide definitions in the text. It is also helpful to include a list of all abbreviations used in the text. For example, SERDP and DNAPL do not appear to be have been defined.

a. Comment on referencing key equations or information: The statement in the Background section (page 6) generally referencing REMChlor is insufficient to replace specific references in the text. Any references in the documentation of REMChlor-GoldSim to information that is not included in the test and is, instead, presented in any other document, including the documentation of REMChlor, must be explicit. For example, the Tutorial 1 (page 30), first paragraph, third sentence states, "*The source is assumed to behavior according to Equation (2), with an exponent, Γ, of 1*." This statement does not indicate that this equation is provided in the documentation of REMChlor, not REMChlor-GoldSim.

   If any information, such as Equation (2) is essential to the description of REMChlor-GoldSim, it should be included in the text or explicitly referenced. Noblis recommends that if such information cannot be included in the text, the documentation of REMChlor should be included as an appendix to REMChlor-GoldSim.

2. Introductory Description of REMChlor-GoldSim

a. Structure of RemChlor-GoldSim: The structure of RemChlor-GoldSim and its relationship to the pre-existing RemChlor and GoldSim programs is somewhat confusing. It would assist the user to understand how to use REMChlor-GoldSim if the user's manual structure of REMChlor-GoldSim were clarified.

   The use of the term "model" is often ambiguous. Model is used to refer to both source codes that are used to perform modeling and the input and output files that represent a specific physical system. It would reduce potential ambiguity if the text explicitly differentiated between source codes and input/output files. The text makes references to a REMChlor-GoldSim model. The text also refers to the REMChlor-GoldSim GSP files, the REMChlor source code and the GoldSim Player as models. However, it appears that REMChlor-GoldSim is not a model in the same sense as REMChlor or GoldSim.

Initially, a new user might assume that the REMChlor-GoldSim model is a new application (with an executable *.exe file). It appears that sourceplume_risk4.dll, a Fortran Dynamic Link Library, is the new computer coding that creates the capability to run REMChlor and GoldSim simultaneously to perform probabilistic modeling. The REMChlor-GoldSim GSP illustration and tutorial files appear to be input files for GoldSim, which provide templates or examples of data needed to represent groundwater transport of solvents (for REMChlor).

Some of this information is provided in the section entitled *Software Installation and Computer Requirements* (page 5). Documentation on software installation and computer requirements is often limited to a discussion of RAM, disk-space requirements and the mechanics of loading a program. Noblis suggests that the section might be renamed and the information in the section be expanded to fully explain the structure of REMChlor-GoldSim.

b. Additional information on structure would clarify how to launch REMChlor-GoldSim. It would be evident that GoldSim must be executed prior to running REMChlor-GoldSim. However, the documentation should still explain REMChlor-GoldSim runs can be launched thereafter without re-executing GoldSim by simply double-clicking on a GSP file.

3. Graphical User Interface

a. Step 1 of the Basic Operation instructions should identify the first figure as the **Main Interface**. Consider replacing the second sentence of the instructions which states "You will see the following screen," with "The program will first open the **Main Interface** screen."

b. Suggest implementing a convention for naming and highlighting the component of the graphical user interface and use these conventions consistently throughout the document. For example, in many cases, the document capitalizes and bolds the names of the interface tabs. Apply this convention throughout the document.

c. Suggest using repetition to assist the user in assimilating information. In the description of each interface, rather than describing interfaces as "this interface," use the name. For example, in the **Explore Model** section, state "The **Explore Model** interface tab directs the user to the model structure" rather than "This tab directs the user to the model structure."

d. To the extent possible, the instructions should be accurate and precise. The documentation should differentiate between describing what is actually seen and what actions can be taken at any point in the process.

For example, Step 2 of the Basic Operation instructions states "Click on **Simulation Settings** tab and you will see the basic time settings and the Monte Carlo settings screens. Under **Time** tab, you will see the simulation duration and time steps

window." In fact, when the **Simulation Settings** tab is selected, the user will see the **Time** setting screen, but not the **Monte Carlo** setting screen.

The Step 2 instructions would be clearer and more accurate if they stated "Click on **Simulation Settings** tab and you will see the **Time** interface. You will also see tabs for the **Monte Carlo**, **Globals** and **Information**. The **Time** interface will allow the user to modify basic time settings, including simulation duration and time phase settings, including time steps:"

e. A discussion of the **Monte Carlo** options should be provided in the documentation or the user should be directed to information provided in GoldSim documentation or some other appropriate reference document.

f. The information that can be accessed through the **Explore Model** interface is quite complex. It would be helpful to the user if either the section description of the **Explore Model** interface and Step 3 of the Basic Operation section provided more information on this interface or directed the user to information presumably provided in GoldSim documentation.

g. Review the names of user interface tabs on the Main interface and the names that appear on the interface windows for consistency. For example, Step 4 addresses the Source Zone Parameters tab. However, the interface window is labeled "Source Parameters." For consistency, re-title either the tab or the interface window.

h. There are numerous options to select a "deterministic value," including the interfaces for the **Source Zone Parameters**, **Transport Parameters**, **Source Remediation**, and **Plume Decay Rates**. The section on Model Input Variables of the User's Manual states that the model will use probabilistic values unless deterministic values are specified, but the documentation does not appear to provide any other information. Information explaining the implications of this choice and a description of how the probabilistic values are calculated is needed. Clarify how the minimum, maximum and likely values input to the model (presumably) are used to calculate the probabilistic values. Clarify how the standard deviation for the Darcy Velocity, entered in the **Transport Parameters** interface, is used to calculate the probabilistic value.

i. In the **Source Remediation** interface, the remediation time is specified in units of years [("Remediation Time (yr)"]. It appears that the model may only operate in units of years. If this is correct, the documentation should state this explicitly and clarify that units of years must be specified in the **Simulation Setting** interface. Because GoldSim appears to allow a number of different time units (including days, minutes, seconds), the relation between the units specified in the **Simulation Setting** interface and the **Source Remediation** interface must be clarified. In addition, it does not appear that GoldSim requires a correlation between the units specified for "Time Display Units" and the units specified for the "Duration" input. (However, the

units for the "Time Phase Setting" appear to be hardwired to correspond to the units input for the "Time Display Units.")

j. The interface identified in the documentation as the **Plume Decay Rate** interface does not correspond to the name on the interface window. The window is currently entitled "source plume function – Component #." Consider renaming the interface **Source Plume Function** or changing the name of the window to **Plume Decay Rate** or at least adding this name above the component name shown at the top of the window.

k. In Step 7 of the Basic Operation section, which describes the **Plume Decay Rate** interface, it would be helpful to the user to note that the first screen displayed shows the input for the parent compound, identified as Component 1, and that Components 2 - 4 represent daughter products. Although this information is explained later in the text, it would helpful to orient the user at this juncture. If possible, you might consider relabeling the components, currently identified as Components 1 - 4 as "Parent Compound," "Daughter Product 1," "Daughter Product 2" and "Daughter Product 3," respectively to clarify the relationships.

l. Please clarify if the model does have the capability to simulate a compound that has less than three daughter products?

m. In the **Plume Decay Rate** interface, the first three input windows of the Period 3 Decay Rate for all three zones are not labeled. Add labels (presumably "Min, Likely and Max") to avoid potential input error.

n. In the **Plume Decay Rate** interface, the fourth input window of the Period 1 Decay Rate for all three zones is not labeled. Add labels (presumably "If checked, use Determinist Value") to avoid potential input error.

o. In Step 8 of the Basic Operation section, clarify that the **Treatment Rate** tab is located on the **Plume Decay Rate** interface.

p. The interface identified in the documentation as the **Treatment Rate** does not correspond to the name on the interface window. The window is currently entitled "source plume function – Component #_Rem." Consider changing the name of the window to **Treatment Rate – Component #_Rem** or at least adding this name above the current title "Component #" at the top of the window.

q. In Step 9 of the Basic Operation section, clarify that the **Treatment Dimension/Cost** tab is located on the **Treatment Rate** interface.

r. The interface identified in the documentation as the **Treatment Dimension/Cost** does not correspond to the name on the interface window. The window is currently entitled "source plume function – Plume_Treatment." Consider changing the name of

the window to **Treatment Dimension/Cost** or at least adding this name above the current title "Plume Treatment" at the top of the window.

s. Step 9 of the Basic Operation section, sentence 2, states "As you move the mouse over the input field, a simple explanation of the input is provided in pop-up boxes." This instruction is out of place. It should be provided in the introduction of the Basic Operation section, before Step 1. The pop-ups appear to be provided for most input fields, with the exception of the deterministic value input field. All of the input fields should be systematically checked.

t. In Step 11 of the Basic Operation section, the definition of total concentration is unclear. For example, does concentration refer to the concentration of the parent compound or a composite of the parent and all three daughter compounds?

4. Model Input Variables

a. Provide an introductory paragraph to explain that the purpose, organization and content of the section. It appears that the documentation steps through each of the user interfaces providing definitions and instructions for each of the data inputs. If this is correct, the introduction should include this explanation, plus anything else covered in the section.
b. Definitions and instructions for data input to the Main Interface and the Simulation Setting Interface should be included. This section should also note that no input is required for the "Explain Model" Interface.
c. Be sure to name and organize each of the Model Input Variables sections with the same titles that are used in the actual model interfaces (the names you see on the Main Interface tabs) and in the Basic Operation section of the documentation. Consistency in naming, organization and terms is an important aid to the user's ability to quickly learn and operate the model and will avoid unnecessary confusion. For example, the subsection titled "DNAPL Source Parameters and Dimensions" should be renamed "Source Zone Parameters." Additional information can be provided in an introduction to the section or the subsection.
d. It would be helpful to preface the definitions of parameters for each interface with an introductory paragraph that describes the organization of, and relationship between, the input parameters. Develop a consistent convention for discussing parameters that have multiple options or multiple components. Be sure that documentation uses the same wording and names that are used in each user interface window.
e. For most of the parameters, the distribution of model input variables are described as triangular. Provide a definition or example of a triangular distribution.
f. Consider providing a brief definition or description, a figure, and an equation to describe and provide a context for the Source Zone Parameters. Also reference RemChlor (include a section or page reference), if appropriate.
g. The Source Remediation interface for the illustration example (REMChlorGoldSim_illustration.gsp) shows a "Source Contaminant" option with three parameters (t_f, n and Q_{in}) that are grayed out. Explain why this option is grayed

out and whether it is ever used. If it can be used, explain how to activate the option and provide definitions.

h. In the Source Remediation interface, provide an introductory discussion describing the structure of this interface, including a sentence that identifies each remediation technology by name. Clarify the definition of the Aqueous Phase Source Decay input. It is not clear whether input to this parameter is independent of the selection of a technology option. The difference between Aqueous Phase Source Decay and Enhanced Aqueous Phase Source Decay is not clear. If these parameters are defined and discussed in more detail in the RemChlor documentation, provide an explicit reference.
i. Describe the structure of the inputs to the Transport Parameter's interface in the text by noting that three Scale-Dependent Dispersivity is three dimensional. Identify the three parameters - Longitudinal, Traverse and Vertical.
j. It appears that the transport parameter, Number of Streamtubes, is not specified in the Transport Parameter interface, but rather in the Main Interface. If so, note this incongruity in this Transport Parameter section and insert an additional section that describes the parameter inputs to Main interface, including this parameter.
k. The description of the inputs for the Plume Decay Rates and its sub-interfaces is difficult to follow. The documentation needs to provide an overview of the purpose and organization of each interface. This section should be reorganized and rewritten. The documentation should provide clearly delineated, step-by-step instructions for the inputs to each interface, one at a time and include examples showing the user interface windows. It is very important to use the same titles and terms in the text and in the interface windows. For example, it is confusing that the titles of the interfaces windows [Component 1, Component 1 (Remediation), Plume Treatment] do not correspond to the subsections of the documentation (Yield Coefficients, Plume Reaction Zones, Plume Species First Order Decay Rates, and Plume Treatment Dimensions and Costs).
l. The first sentence of description of inputs for the Plume Decay Rates interface refers to a "distance-time reaction graph." However, no such graph appears to be provided in the documentation.
m. The second sentence of description of inputs for the Plume Decay Rates interface directs the user to note the start time and start location of the model. However, it is unclear where the user would note this fact. Nothing in the Plume Decay Rates interface indicates the start time or start location.
n. The third sentence of description of inputs for the Plume Decay Rates interface discusses the entry of nine different reaction rates. Presumably, this direction is referring to the seven inputs labeled "Decay Rate" in the interface. Also it appears that two of the rates are not entered in the Plume Decay Rates interface but rather must be entered in the sub-interface accessed by selecting either of the tabs labeled "Treatment Rate." The user does not find the rest of this explanation of rates until the end of the next page under the heading of Plume Species First Order Decay Rates.
o. The function of the two Treatment Rate tabs is unclear. It is unclear whether selection of either of these tabs opens the same window. It is also unclear why the Treatment Zones are restricted to the Period 2 and Zones 1 and 2.

p. Although the text discusses yield coefficients, there is no reference to this term in the interface windows. It is unclear how the discussion of yield coefficients relates to the specification of inputs.

5. Tutorials

a. Tutorial 1 (page 30), first paragraph, last sentence states "initial source concentration was 10mg/l, leading to an initial source discharge of 30 kg of PCE per year." Explain how a discharge of 30 kg/year is derived. Provide a simple equation and a description.
b. In viewing the Total Concentration results, the probability results would be clearer if the color coding was unique. For example, the results would be easier to read if the upper bound and the five percentile were color coded in different colors or patterns.
c. It is not clear how the Total Concentration plot of the second probabilistic run shows that the remediation effort is predicted to meet the goal only about 50% of the time.
d. The tutorial should be expanded to discuss the rest of the model results (Cancer Risk, Total Discharge, Plume Cost and Source Cost).

MEMORANDUM FOR RECORD

SUBJECT: REMChlor/GoldSim Sensitivity Analysis and Source Reduction Evaluation for Site Well 12A in Tacoma, Washington

PREPARED BY: Jefferey Powers, Seattle District, U.S. Army Corps of Engineers

Date: 2 February 2010

Introduction and Purpose.
The Seattle District, U.S. Army Corps of Engineers (USACE Seattle) utilized the calibrated REMChlor/GoldSim model for Site Well 12A developed by CDM to evaluate the sensitivity of the model to 1) initial contaminant source concentration, and 2) initial contaminant source mass. USACE Seattle also tested the source remediation required to achieve a 90 percent reduction in downgradient mass flux. The third objective was to use the results of the sensitivity analysis to develop a source remediation reduction range necessary to reach the 90 percent downgradient reduction goal.

Software Tested.
GoldSim Player model beta version 1.0, utilizing GoldSim version 9.6 SP4
REMChlor version 1.0 is called and run from within the GoldSim Player model

Computer Specifications on which Software Installed.
Dell Latitude D600
Pentium processor, 1.50 GHz
1.00 GB of RAM
Microsoft Windows XP operating system

Model Input Parameters.
The input parameters were identical to those utilized and reported by CDM (See Table 1 from the attached *Evaluation of Remchlor for Remediation Assessment at Site Well 12A, Tacoma, Washington*), with only a few exceptions as noted in the following paragraphs.

SENSITIVITY ANALYSIS

A sensitivity analysis was run owing to uncertainty in original contaminant mass and dissolved-phase concentrations in the source area. USACE Seattle ran three sensitivity simulations each for variations in A) source concentration, B) source mass, and C) source concentration *and* mass. The three assumptions were: 1) source was 50 percent less than values used, 2) source was 50 percent greater than values used, and 3) source was 100 percent greater than values used.

Since the deterministic, calibrated model input parameters in the model developed by CDM were 190 ug/L source concentration, and 1,500 kg source mass, the actual values used to test sensitivity were as shown in the following table.

Initial Source Concentration (ug/L)	50% lower (ug/L)	50% greater (ug/L)	100% greater (ug/L)
190	95	285	380
Initial Source Mass (kg)	50% lower (ug/L)	50% greater (ug/L)	100% greater (ug/L)
1,500	750	2,250	3,000

SOURCE REMEDIATION REQUIRED USING DETERMINISTIC SOURCE CONCENTRATION AND MASS

The model was used to determine what percentage reduction in source was required to achieve a 90 percent reduction in downgradient mass flux. The downgradient location modeled was Well CWB-10, 250 meters (820 ft) downgradient from the source area. For these model runs it was necessary to extend the simulation duration from 45 to 65 years, and to activate a source remediation with a start time of year 47 and an end time of year 48. Since the approximate year of source zone contamination was 1963 (based on CDM memo), this places the treatment in the current timeframe (2010-2011 time frame) with the simulation running until the year 2028 (although the assumed dates ultimately have no bearing on the actual results). The same deterministic values for source concentration and mass (190 ug/L and 1,500 kg, respectively) as those used in the original CDM model were also used. The results appeared to indicate a linear relationship between source reduction and downgradient mass flux reduction because a 90 percent reduction in source was required to achieve 90 percent reduction at Well CWB-10 (concentration reduction from about 50 to 5 ug/L or mass reduction from about 2.8 to 0.25 kg). Most reduction in both mass and concentration at Well CWB-10 was seen by about 8 years after the end of active treatment, although comparisons were made at the end of the simulations (i.e., year 2028).

SOURCE REMEDIATION REQUIREMENTS CONSIDERING PROBABILISTIC SOURCE CONCENTRATION AND MASS

The third step in the modeling process was to combine the uncertainty in the original concentration and mass estimates as brought forward by the sensitivity analysis with the source remediation requirements to attain 90 percent downgradient mass flux reduction. Since the deterministic source values indicated a 90 percent source reduction would be required, we would expect lower actual original source concentrations to require less source remediation (so <90 percent) and higher original source concentrations to require remediation to a higher level (>90 percent). The following table summarizes the results at the 95 percent confidence level.

Source Reduction Required for 90% Downgradient Mass Flux Decrease			
	50% lower source	50% greater source	100% greater source
By concentration	87%	92%	93%
By mass	88%	91%	92%
Both concentration and mass	85%	92%	94%

For example, the first data cell in the table indicates that if the source concentration were 50% lower than that estimated by CDM in their calibrated model (i.e., 95 instead of 180 ug/L), then an 87% source reduction would be required to achieve a 90% reduction in downgradient concentration.

It is noted by the lower percentages with respect to mass compared to concentration in the table above that there is less sensitivity to source mass than source concentration in the REMChlor/GoldSim model. The greatest level of source treatment is required (94 percent reduction) when both source mass and concentration were underestimated.

Evaluation of Remchlor for Remediation Assessment at Site Well 12A
Tacoma, Washington

Introduction

Trichloroethene (TCE) and its associated daughter products have been detected in the Well 12A contamination site in Tacoma, WA since the early 1980s. Various remedial activities have been put in place since that time, but contamination is still present. In order to assess the impacts of future remedial activities, the Remchlor transport model is being applied to the site. This report has two objectives:

- Evaluate the applicability of the recently developed Remchlor software to model the Trichloroethene (TCE) plume at the Well 12A Site
- Provide recommendations that can be used by the Remchlor developers to improve the software functionality

Computational Domain and Data Selection for Calibration – Well 12A Transport

The Remchlor model was prepared and calibrated to reproduce the time history of VOCs at wells along prevailing pathways modeled. The indicator wells selected for this calibration process are EW-1, CBW-10, and CBW-11. These wells were chosen based on data history and proximity to the straight path line connecting well 12A to the source, identified as the Time Oil Building. Distances from the source to each well were approximated by projecting the well locations onto the path line. Well locations, the model path line, assumed source location and Well 12A are shown in Figure 1. Also shown in Figure 1 are a path line and calibration well set used to verify the calibrated model.

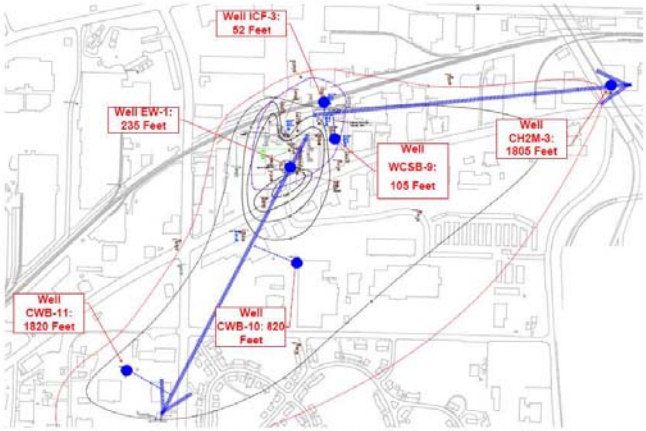

Figure 1: Schematic of modeled contaminant source and transport path line, and calibration wells. Wells EW-1, CWB-10 and CWB-11 were used to calibrate the south-pointing path line, while wells ICF-3, WCSB and CH2M-3 were used to verify the calibrated model as applied to the eastern-pointing path line.

Calibration Process and Assumptions

Initial conjectures for parameter values were based on published literature values and formulas, and also on collected field data. All parameters are listed in Table 1, with their appropriate ranges and the values used in the final calibrated model. Parameter values that differ from original estimates are highlighted in the table and discussed below. Chemical decay original estimates are median published values, and ranges in parentheses are the 25-75 percentile bounds. All parameters are listed in Table 1 as they are inserted into Remchlor. Dispersivity is entered into the model as a unitless parameter; is it multiplied by the plume length in the model to obtain dispersivity.

Table 1
GoldSim Model Calibration Parameters

	Parameter	Calibrated Model Value	Estimate based on Literature or Data
Simulation Settings	simulation length	45.5 years	
	Number of Stream Tubes	100	
	Time Step	1 year	
Source Parameters	C(t=0)	190 ug/L	2500 ug/L
	M(t=0)	1500 kg	5500 kg
	Gamma	1	1
	Width	220 ft	220 ft
	Depth	70 ft	70 ft
	Length	220 ft	220 ft
Transport Parameters	Darcy Velocity	115 ft/yr	115 ft/yr
	porosity (n)	0.21	0.21
	R	3.5	3.5
	D_x (Longitudinal Dispersivity)	0.0136	0.0136
	D_y (Lateral Dispersivity)	0.00136	0.00136
	D_z (Vertical Dispersivity)	3.79×10^{-5}	3.79×10^{-5}
Remediation Settings	none		
TCE decay rate	Decay constant (0-250 feet from source)	1.46 $year^{-1}$	1.46 (0.55-2.92) $year^{-1}$
	Decay constant (250-5000 feet from source)	0.6 $year^{-1}$	1.46 (0.55-2.92) $year^{-1}$
	yield 2 from 1	0.74	0.74
DCE decay rate	Decay constant (0-250 feet from source)	1.46 $year^{-1}$	1.46 (0.913-2.56) $year^{-1}$
	Decay constant (250-5000 feet from source)	3 $year^{-1}$	1.46 (0.913-2.56) $year^{-1}$
	yield 2 from 1	0.64	0.64
Vinyl Chloride decay rate	Decay constant (0-250 feet from source)	1.825	1.825 (0.73-5.48) $year^{-1}$
	Decay constant (250-	5.5	1.825 (0.73-

	5000 feet from source)		5.48) year^{-1}

Confidence in Initial Estimates

Confidence in initial estimates for the source configuration was low based on available data, requiring calibration of these variables. Confidence in transport parameters was higher: velocity, porosity and retardation estimates were based on data analysis. Dispersivity values were based on the literature formula from Xu and Eckstein (1995). There is some degree of uncertainty associated with this estimate, due to both the model's treatment of dispersivity and the nature of the velocity field at Site Well 12A. These uncertainties are discussed below. Although remediation has taken place at the source over the course of the time history simulated, we are not able to represent remediation at the source in the calibrated model. This is because Remchlor simulations only allow a single remediation activity. If we intend to apply remedial activities to the model for evaluation of future activities, we are not able to also model past remediation. Decay rate estimates are based decay rates published in Aziz et al (2000). While initial estimates are taken from the reported median decay rate values, a range of possible values allows for calibration of this parameter. Figures 2-4 show calibrated model results plotted with historical data at the three indicator wells. A discussion of calibration results follows.

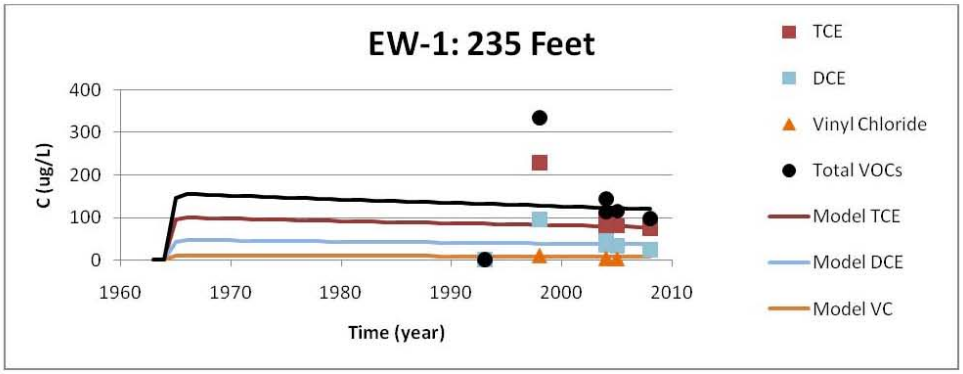

Figure 2: Modeled TCE, DCE, Vinyl Chloride and Total VOC's plotted against historical data at well EW-1.

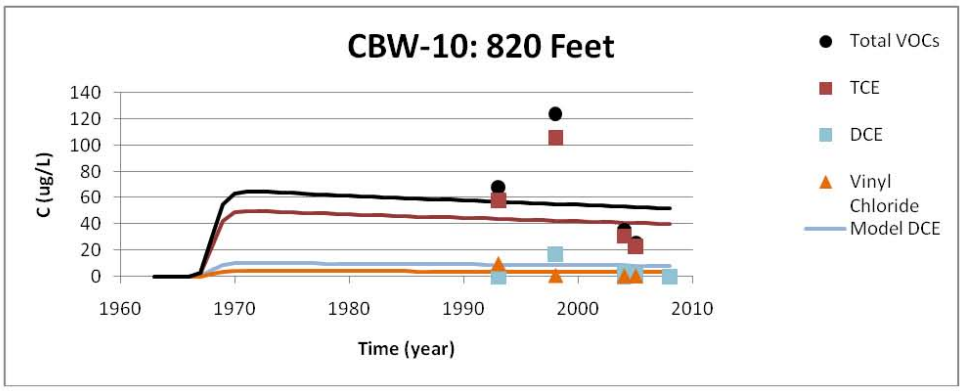

Figure 3: Modeled TCE, DCE, Vinyl Chloride and Total VOC's plotted against historical data at well CBW-10.

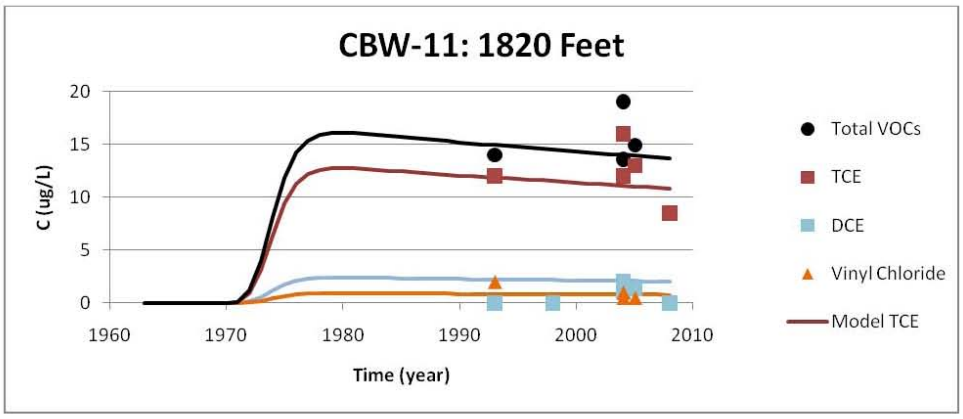

Figure 4: Modeled TCE, DCE, Vinyl Chloride and Total VOC's plotted against historical data at well CBW-11.

Source Conditions

Remchlor treats sources as one-time releases of a source mass into a system. The Time Oil contaminant site was therefore approximated as a source that was released into the soil in 1963. For calibration, all subsequent source releases were neglected, as were all remedial activities.

Initial source mass and concentration are parameters with high levels of uncertainty. The initial estimates for source mass (5500 kg) and concentration (2500 ug/L) were determined from analysis of field data representing the existing plume to estimate a mass and concentration in

1963. Unknowns associated with this process included remediation activities that removed unknown quantities of VOCs, and an unknown history of source release.
For the calibration process, the source initial concentration was calibrated to achieve a level of contamination consistent with well data close to the source. The initial mass was calibrated to achieve a decay of concentration over time that was consistent with well data. Because data were only available from the 1990s on (30 years after the initiation of the plume), several combinations of initial concentrations and initial mass may exist that qualitatively represent available well data.

The calibrated initial mass was 1500 kg, which is almost four times smaller than the initial mass that was estimated from field data. In addition, the calibrated initial concentration was 190 ug/L, which is more than an order of magnitude smaller then the initial estimate. The discrepancy between estimated and calibrated source parameters may be attributable to the unknowns related to the contaminant source, and may also imply some uncertainty in the model's ability to respond to source remediation appropriately.

Darcy Velocity

Darcy velocity is calculated in the model as a function of hydraulic conductivity (550 ft/day) and head gradient (0.0023). When Well 12A is not pumping, the prevailing groundwater flow direction is to the east, perpendicular to the model axis. Because Well 12A operation is intermittent, the gradient along the model axis is assumed to be near zero when Well 12A is not pumping. The modeled velocity is calculated by taking the weighted average of the gradient over a typical year, in which the well is not operating for 9 months. Both pumping and non pumping gradients were calculated based on data collected when GETS was not operating.

Dispersivity

The model was calibrated to the estimated literature vales. However, a time-varying velocity field at the Well 12A Site raises some uncertainty regarding the applicability of this estimate. When Well 12A is not operating (which is the case for ¾ of the calendar year), groundwater flow moves in an eastward direction. During this time the primary direction of groundwater flow is not in the direction of the model's axis (which is toward Well 12A), and significant dispersion is occurring in the model's lateral direction. To account for the dispersive effects of the intermittent flow field, dispersion should potentially be calibrated by increasing the lateral dispersion beyond conventional ranges. However, this was not done with the present model calibration. The model was calibrated using the convention of lateral dispersion being 1/10 of the longitudinal dispersion.

Remchlor calculates dispersivity by multiplying a dimensionless parameter with the plume length. This creates a linear relationship between plume length and dispersivity. However, the relationship used to calculate the initial estimate of dispersion at Well 12A uses a logarithmic relationship:

$$D_x = 0.83(\log(x))^{2.414}$$

where x is plume length in meters. Figure 5 shows the relationship between the dispersivity calculated using Xu and Eckstein (1995) and calculated by the model as calibrated in Table 1. Therefore while the model is calibrated using the dispersivity as described in Table 1, uncertainty in dispersion associated with both the variable flow field may limit the model's applicability to the Well 12A Site, and the discrepancy between the model's treatment of dispersivity along the model axis and the method used to calculate an initial estimate of dispersivity is also a source of uncertainty.

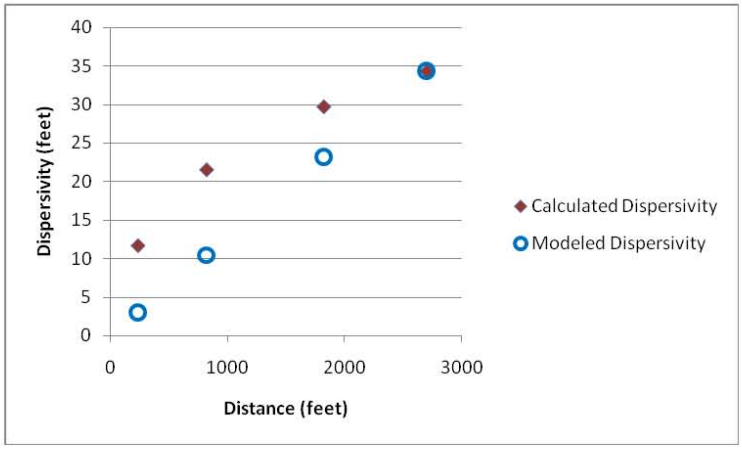

Figure 5: Modeled vs Calculated Dispersivity.

Decay Rates

The model was calibrated to the literature values of chemical decay. However, obtaining model-data agreement required changing decay rates significantly between the initial 250 feet of the plume and the remaining sections. This change in decay signal showed an increase in DCE and VC decay, and a decrease in TCE decay. While the calibrated DCE decay rate farther from the source, 3/year, is outside of the range in Table 1 (which ranges up to 2.55/year), it is still lower than the published maximum value of 3.65/year.

Model Evaluation

The calibrated model was applied to the path line headed east in Figure 1 as a means of verifying the model. As shown in the figure, wells ICF-3, WCSB-9 and CH2M3 were used for model-data comparison. For this application, all parameters were set as in Table 1 with the exception of velocity.

Velocity Estimate

Velocity for the eastern gradient was approximated based on observed water table measurements from 1999 in wells ICF-3 and CH2M-3 and other near-by wells. A head gradient of 0.004 was used. Conductivity for the path line was based on conductivity measurements in the source area. These values ranged between 40 and 400 ft/day, so a range of velocities reflecting this variability were applied for the verification study.

The best model-data fit for the verification study was achieved using a Darcy velocity of 590 ft/year, which corresponds to the maximum observed conductivity. The conductivity of 400 ft/day is near the conductivity used to calibrate the southern path line, which is 550 ft/day. Figures 6-8 show comparisons of historical data with model results at the three indicator wells used for comparison.

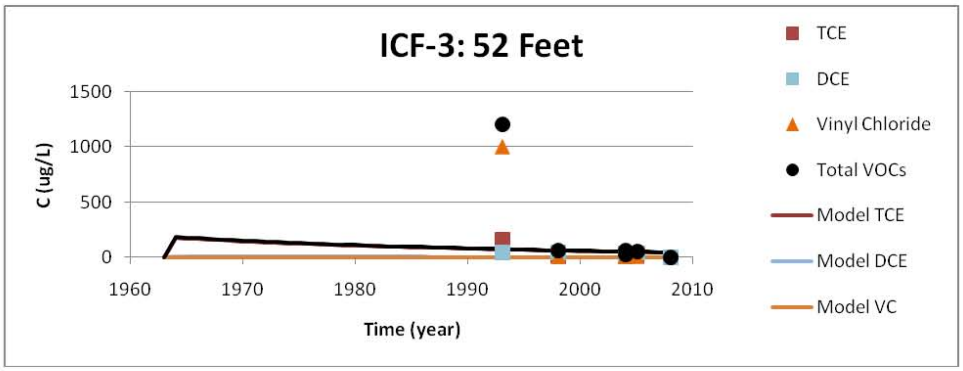

Figure 5: Modeled TCE, DCE, Vinyl Chloride and Total VOC's plotted against historical data at well ICF-3.

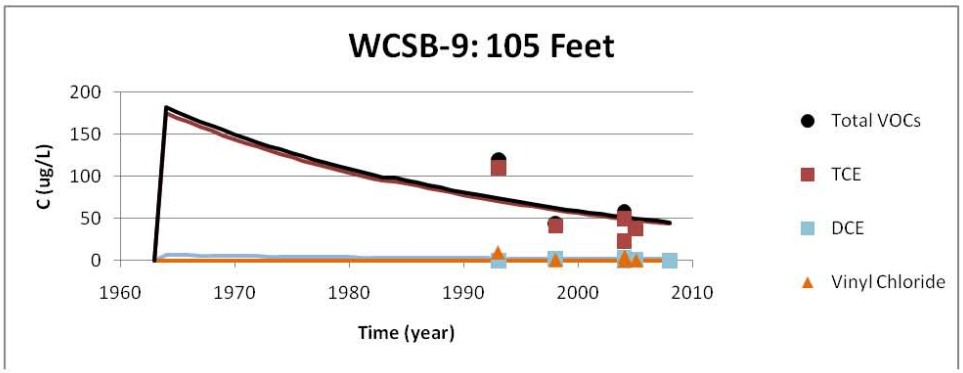

Figure 6: Modeled TCE, DCE, Vinyl Chloride and Total VOC's plotted against historical data at well WCSB-9.

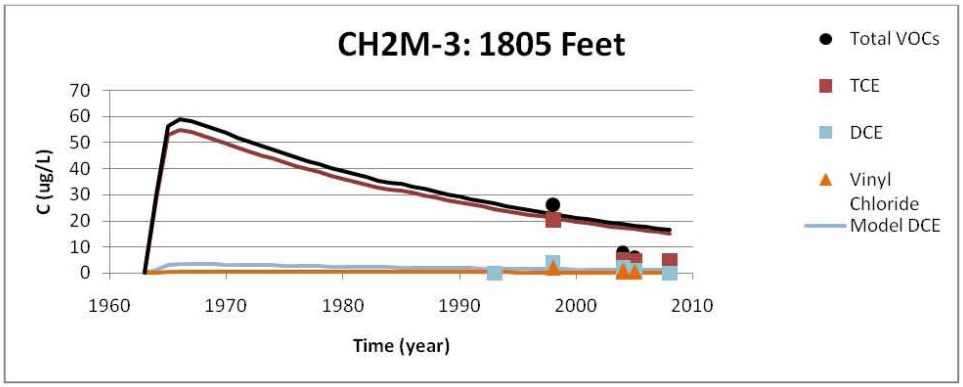

Figure 7: Modeled TCE, DCE, Vinyl Chloride and Total VOC's plotted against historical data at well CH2M-3.

Model results compare well with field data for the two near wells, ICF-3 and WCSB-9. Model results are slightly higher than data at wells WCSB-9 and CH2M-3. This variance implies that longitudinal disperison in the eastern pathline may be higher than in the southern path line.

Applicability of Remchlor to the Well 12A Site

The calibrated model appears to apply reasonably well to both the southern and eastern gradient path lines, with some limitations. Model parameters were, with the exception of source values, within the range of initial estimates postulated from data and literature values. Some concerns regarding the applicability to a complex site such as Well 12A are listed below.

Source Treatment: Field data for the Well 12A site suggests that there may be an unidentified source near well ICF-2. Because Remchlor only allows a single contaminant source to be introduced per simulation, this information was disregardarded during the model calibration.

The source remediation in Remchlor also only allows for a single remedial activity per simulation. Because of this feature, the source properties in the calibrated model do not reflect any remediation; as such, the source mass and concentration in the calibrated model may accurately represent the actual source at the Well 12A site. This mis-representation may create complications if the model is used to evaluate future source remediation.

Velocity: The model only allows velocity to be treated as a constant in both space and time. This limitation may be particularly inapplicable to the Well 12A site, because the gradient is known to vary greatly between pumping and non-pumping periods. Because of this limitation and the variable gradient at the site, the velocity used in the model for the Well 12A site is one fourth the magnitude of the actual velocity. The "average" velocity used in the model may have an impact on modeled dispersion and chemical decay.

Dispersivity: Because of the variable flow field at the Well 12A Site, it is possible that the simple relationship between plume length and dispersivity is not adequate to capture the physical processes taking place. This may contribute to the widely varying chemical decay rates observed in the calibrated model.

General Concerns and Recommendations for Remchlor

User Interface: It may help users to include units for all parameters in the user interface. The decay rate constants do not have units associated with them, and this was a source of confusion in the calibration process

Source Treatment: The model would be applicable to more sites if the source treatment were more flexible. For example, allowing multiple releases along the pathline would be useful for the Well 12A site. Time varying source release would also be useful for many sites where industrial activities introduce new chemical releases.

Model Output: There is no option within GoldSim to view output at a given time as a function of distance from the source. This would aid in the calibration process.

Velocity Treatment: Well activity and other environmental variables can change flow fields over the time scales that are appropriate for the GoldSim model. In the case of the Well 12A site, the capability to model a time-varying velocity would increase the model's applicability. For other sites with spatially varying gradients, a spatially varying velocity would also increase the model's applicability.

Conclusions

The Remchlor model has been calibrated to the Well 12A site. While simulation results match field data well, it is uncertain whether the model will accurately respond to simulated remediation treatment at the Well 12A Site. This uncertainty is partially due to the discrepancy between calibrated source mass and concentration and the values estimated from field data; if the source term does not reflect the actual source at the Site, then the model may not respond appropriately to remediation. Uncertainty is also due to the temporal variability of the flow field at the Well 12A Site, which may alter the appropriate representation of both velocity and dispersivity.

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14. ABSTRACT

A new probabilistic remediation model, Probabilistic Remediation Evaluation Model for Chlorinated solvents (PREMChlor), has been developed for simultaneously evaluating the effectiveness of source and plume remediation considering the uncertainties in all major parameters. PREMChlor is developed by linking the analytical model REMChlor to a Monte Carlo modeling package GoldSim via a FORTRAN Dynamic Link Library (DLL) application. In PREMChlor, all of the uncertain input parameters are treated as stochastic parameters represented by probability density functions (PDFs). The outputs from PREMChlor are probability distributions and summary statistics of the distributions. Cost analysis of common technologies for dense, non-aqueous phase liquid (DNAPL) source removal and dissolved plume treatment are included. PREMChlor gives users a single platform where cost, source treatment, plume management, monitored natural attenuation, and risk assessment can all be evaluated together, and where uncertainty can be incorporated into the site decision making process.

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DNAPL, groundwater remediation, probabilistic simulation

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