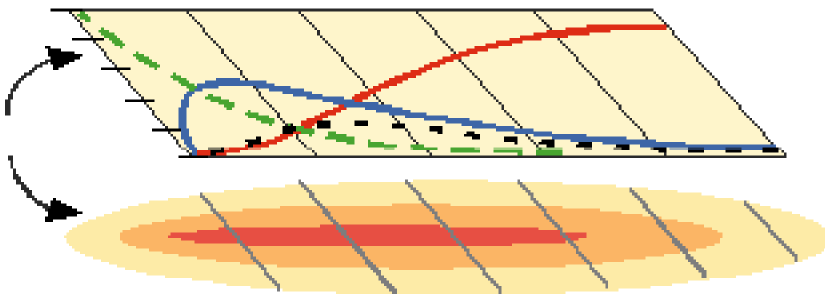
BIOCHLOR

Chlorinated Solvent Plume Database Report



June, 2000

AIR FORCE CENTER FOR ENVIRONMENTAL EXCELLENCE (AFCEE)

BIOCHLOR
CHLORINATED SOLVENT PLUME DATABASE

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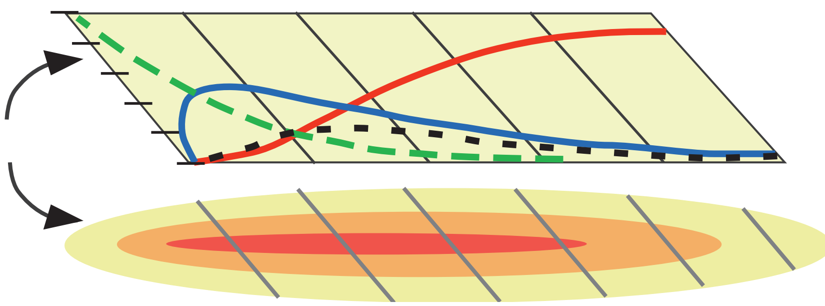

by

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EXECUTIVE SUMMARY

This database of chlorinated solvent plume characteristics was compiled for the Technology Transfer Division at the Air Force Center of Environmental Excellence. The primary objective of this study was to identify key characteristics of parent and daughter chlorinated solvent plumes and to determine important relationships between plume characteristics and hydrogeologic and environmental variables. The results are intended to aid site managers by providing them with general plume length information, which they can use to estimate the likelihood of off-site migration and the potential effectiveness of natural attenuation for plume management. This information also helps engineers focus on collecting plume and site characterization data that are most important for estimating plume lengths.

A secondary objective of the study was to estimate field-scale biodegradation rate constants by calibrating the BIOCHLOR model (Aziz *et al*., 2000) to plume centerline data from the database. Unlike other methods of rate constant estimation, this method accounts for daughter product formation and degradation and yields a biodegradation rate constant rather than a gross attenuation rate constant. Biodegradation rate constants were correlated with site variables when sufficient data were present. These rate constants and correlations provide site managers with literature rate constant values to be used in the BIOCHLOR model for natural attenuation screening purposes.

Chlorinated ethenes (i.e., perchloroethylene (PCE), trichloroethylene (TCE), cis-1,2-dichloroethylene (cDCE), vinyl chloride (VC)) and chlorinated ethanes (i.e., 1,1,1-trichloroethane (TCA) and 1,1-dichloroethane (1,1-DCA)) were the constituents of interest in this study. Mean hydrogeologic property values and chlorinated solvent concentration data were extracted from site reports for the most contaminated unit. Plume lengths were determined using isopleths for each chlorinated ethene or chlorinated ethane constituent included in the site report. Plume lengths were delineated to the 1 ppb contour, in most cases, by measuring from the upgradient to the downgradient edge of the plume. Plume length information for BTEX found in association with the chlorinated solvents was also tabulated. Data from a total of 24 sites and 93 individual chlorinated solvent plumes are included in the database. Approximately half the site data were from Air Force Bases, with the remainder from industrial sites where solvents had been released. The sites were widely distributed across the country. Most of the sites contaminated with chlorinated ethenes had TCE or TCE and PCE as the parent compounds. Only one site had PCE as the sole parent compound.

The following are the key results of the study. These findings should be viewed as general trends and may not necessarily apply to a given site. However, the results presented below should prove useful for site managers evaluating the potential impact of dissolved chlorinated solvent and BTEX plumes at chlorinated solvent release sites.

Chlorinated Solvent Plume Characteristics

- At sites contaminated with chlorinated ethenes only, TCE or c-DCE was the most likely constituent to have the longest plume at the site. TCE and c-DCE had median plume lengths of 1215 ft and 1205 ft, respectively.
- VC had the shortest median plume length of 860 ft. Because the daughter product plumes were coincident or almost coincident with the parent plumes, these results indicate that vinyl chloride is unlikely to be the longest plume at a site. This is an encouraging result given the relatively high associated carcinogenicity of vinyl chloride. Because laboratory

studies report that VC degrades slowly via reductive dechlorination, these results suggest that other degradation mechanisms are at work in degrading vinyl chloride.

- Of the chlorinated ethanes, TCA had a shorter median plume length (865 ft) than 1,1-DCA (1650 ft) and 1,1-DCE (1470 ft). TCA's shorter median plume length is likely due to its degradation by both abiotic and biotic mechanisms.
- cDCE, VC, and ethene, daughter products of reductive dechlorination, were found at 92%, 79%, and 58% of the sites, indicating that reductive dechlorination is widespread at the sites in this database. The presence of BTEX at 75% of the sites may explain the high incidence of reductive dechlorination.
- Large increases in chloride concentrations within the plume relative to background levels are further evidence of significant reductive dechlorination.

BTEX Plumes at Chlorinated Solvent Release Sites

- BTEX plumes had a median length of 750 ft, much longer than the 101-180 ft median BTEX plume lengths reported at retail UST sites by other investigators.
- Longer BTEX plumes may be linked to larger source areas or spills or more anaerobic conditions than those typically found at retail UST sites.

Factors Impacting Dissolved Solvent Plume Length

- The plume width in the source area (or source area width) was used to represent the size of the NAPL-affected source area. The product of the source area width and the maximum dissolved phase solvent concentration was strongly correlated with plume length. This finding indicates that source characteristics, including the extent of DNAPL migration, are the most important factors impacting the maximum dissolved chlorinated solvent plume length.
- Chlorinated ethene plume lengths were moderately correlated with seepage velocity and groundwater travel distance, indicating that advection is also an important factor impacting chlorinated solvent plumes. Therefore, the seepage velocity should be accurately determined to predict plume lengths.
- Environmental factors, such as temperature, pH, dissolved oxygen, and redox potential were not strongly correlated with chlorinated ethene plume length. However, there was a strong trend of increasing PCE plume length with increasing redox potential, once the PCE plume length was normalized to remove the effects of advection. These results suggest that source width, source strength, and seepage velocity are more important factors impacting overall plume length than environmental conditions that are conducive to reductive dechlorination.

Biodegradation Rate Constants and Factors Impacting Rate Constants

- Field-scale biodegradation rate constants were estimated for 35 plumes using the BIOCHLOR model. BIOCHLOR is an analytical model that assumes first order sequential kinetics for reductive dechlorination, thereby accounting for daughter product generation and degradation. The resulting median rate constants and half-lives are shown below for the chlorinated ethenes and chlorinated ethanes. Note that the majority of sites in this database had significant BTEX contamination (an indirect electron donor). These rate constants can be used as literature values in model simulations for anaerobic plumes that are not electron donor-limited.

Constituent	Rate Constant (1/yr)	Half Life (yr)
PCE	1.1	0.63
TCE	1.2	0.58
cDCE	1.2	0.58
VC	1.7	0.40
1,1,1-TCA	2.4	0.29
1,1-DCA	0.3	2.3

- TCE, cDCE and VC rate constants were strongly correlated with biodegradation capacity (i.e., expressed assimilative capacity). TCE rate constants increased with increasing temperature and hydrogen concentration.

1.0 INTRODUCTION

The ultimate goal of this study was to further the understanding of solvent plume characteristics to enable better management of chlorinated solvent plumes. By understanding key factors influencing solvent plumes, engineers and decision-makers can more effectively prioritize sites requiring remediation and identify conditions where natural attenuation is likely to be a viable plume management strategy. Knowledge of typical plume lengths and the effects of hydrogeologic and environmental conditions on plume length also provide the site manager with valuable information about the likelihood of off-site migration and impact to sensitive receptors.

It has been shown in previous studies that the nature of plume behavior can be better understood by analyzing a population of plumes. Studies, such as the Lawrence Livermore National Laboratory study of benzene plumes at 271 underground storage tank sites in California (Rice *et al*., 1997) and a subsequent study of 605 underground storage tank sites in Texas (Mace *et al*., 1997), led to greater insight and understanding of benzene plume behavior, risks, and the potential for natural attenuation as a plume management strategy.

Another study, based on plume dimension data collected in the Hydrogeologic Database (HGDB) (Newell and Connor, 1998; Newell et al., 1990), indicated that dissolved chlorinated solvent plumes were much longer and wider than BTEX plumes at retail UST sites (i.e. gas stations) as shown in Figure 1.

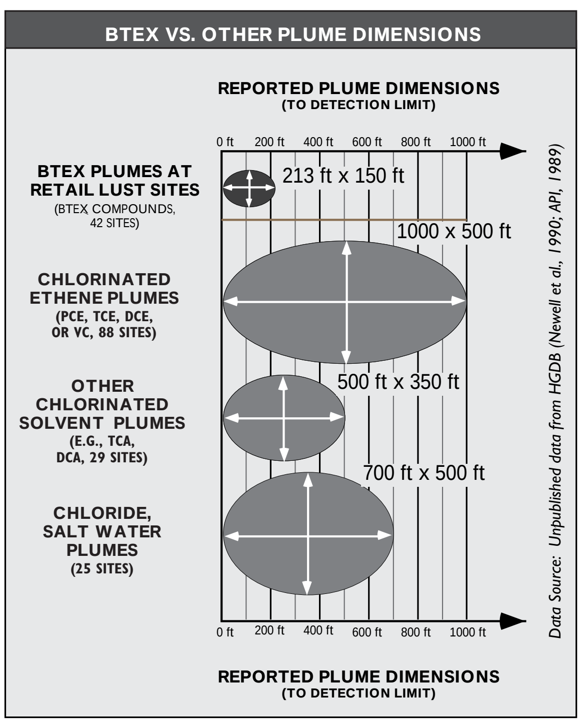


Figure 1. Plume Length Comparison

Recently, a chlorinated solvent plume study was released by Lawrence Livermore National Laboratory (LLNL) (McNab et al., 1999). The LLNL study focused on the effects of hydrogeological parameters on plume length and investigated temporal trends of chlorinated solvent plumes. All chlorinated solvent plumes were lumped together because no statistical difference existed between the plume lengths of the various constituents. The LLNL study found no evidence of reductive dechlorination at one third of the sites investigated and found reductive dechlorination had a relatively subtle effect on plume lengths. The most important factors impacting plume length were advection and source strength.

To gain further insight into the characteristics and behavior of chlorinated solvent plumes, the Technology Transfer Division of the Air Force Center for Environmental Excellence embarked on the BIOCHLOR database project. In the BIOCHLOR study, key characteristics of individual chlorinated solvent and daughter product plumes were identified and the effect of hydrogeologic and environmental factors on the plume lengths were investigated. The constituents of interest were the chlorinated ethenes (i.e., perchloroethylene (PCE), trichloroethylene (TCE), cis-1,2-dichloroethylene (cDCE), vinyl chloride (VC)) and the chlorinated ethanes (i.e., 1,1,1-trichloroethane (TCA) and 1,1-dichloroethane (1,1-DCA)). In addition, data on BTEX, ethene, and ethane plumes at chlorinated solvent release sites were collected and analyzed. Chlorinated solvent data were used also to calibrate the BIOCHLOR model to generate field-scale biodegradation rate constants. Emphasis was placed on chlorinated solvent plumes found at Air Force Bases; however, solvent plumes from a number of industrial sites were also included in the study. Almost all the sites in the database showed evidence of reductive dechlorination.

1.1 Objectives

This study addressed the following two general areas related to chlorinated solvent plumes:

- Typical dimensions for chlorinated solvent plumes and key factors that are correlated to plume length
- Typical biodegradation rate constants for dissolved chlorinated solvent constituents in groundwater and factors correlated to biodegradation rate constants

The first objective of this study was to determine plume lengths for chlorinated ethenes and ethanes for the sites in the database. Median plume lengths were determined using data extracted from existing site investigation and feasibility reports and information on other site variables were compiled. Plume lengths for each identified chlorinated ethene were correlated with hydrogeologic and environmental variables to understand which hydrogeologic or environmental variables have the most pronounced impact on plume length.

The second objective of this study was to determine field-scale rate constants using the BIOCHLOR model (Aziz *et al*., 2000) and plume centerline data from the database. BIOCHLOR is an analytical model, developed for the Air Force Center of Environmental Excellence, which simulates the reactive transport of chlorinated solvents in the subsurface. An important attenuation mechanism of chlorinated solvent plume migration is biodegradation. However, the biodegradation rate constants reported in the literature vary by over 4 orders of magnitude, making it difficult to choose a reasonable rate constant value for modeling purposes. Furthermore, many of the rate constants reported in the literature do not account for daughter product formation. In this study, the BIOCHLOR model is calibrated to data from the database to determine field-scale rate constants that can be used in the

BIOCHLOR and other transport models. The rate constants estimated from the database span a smaller range and are correlated to site variables to assist the site manager or modeler to select an appropriate literature value for modeling purposes.

1.2 Background

Chlorinated solvent plumes are often found at Air Force Bases because solvents were widely used as degreasing agents and as chemicals in fire protection training. Chlorinated solvents, such as TCE, PCE, and 1,1,1-TCA, are predominantly released to the subsurface as Dense Non-Aqueous Phase Liquids (DNAPLs) that can penetrate an aquifer below the water table (Pankow and Cherry, 1996; Wiedemeier et al., 1999; Schwille, 1988). The mobile DNAPL becomes trapped as a residual DNAPL in the pores and fractures of the aquifer and, being sparingly soluble in water, acts as a long-term continuing source of dissolved constituents in the groundwater. Once dissolved, solvents may sorb to the soil phase, especially where organic matter is present. The plume is attenuated by sorption to the aquifer material, dispersion, dilution, abiotic reactions (for some constituents), and biodegradation.

Biodegradation can be an important process in the natural attenuation of chlorinated solvents. At chlorinated solvent contaminated sites, the majority of solvent biodegradation occurs by reductive dechlorination (Wiedemeier *et al.*, 1996). Reductive dechlorination is a microbially-mediated reaction whereby a chlorine atom on the chlorinated solvent is replaced by a hydrogen atom (Vogel and McCarty, 1987). During reductive dechlorination, hydrogen acts as the *electron donor* and the chlorinated solvent acts as an *electron acceptor* and thus becomes reduced. Typical pathways for the chlorinated ethenes are as follows:

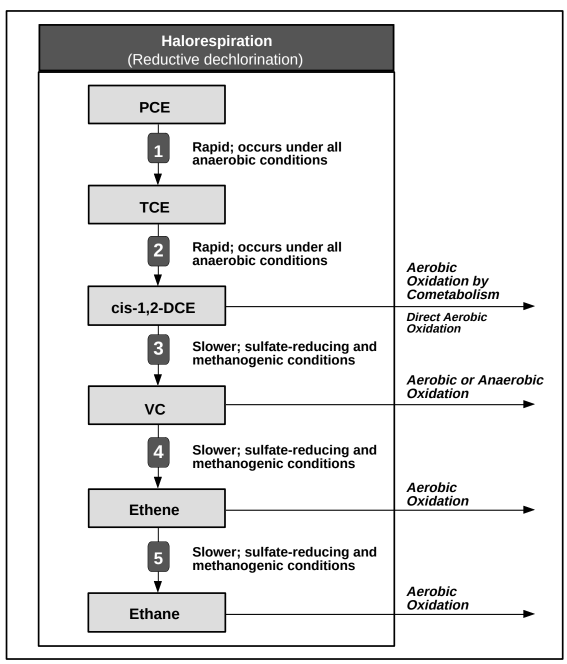


Figure 2. Reaction Sequence and Relative Rates for Halorespiration of Chlorinated Ethenes, with other reactions shown (Adapted from Wiedemeier et al., 1999).

For chlorinated ethanes, reductive dechlorination pathways are shown in Figure 3. 1,1,1-TCA also undergoes abiotic degradation to form either 1,1-DCE or acetic acid (Vogel and McCarty, 1987).

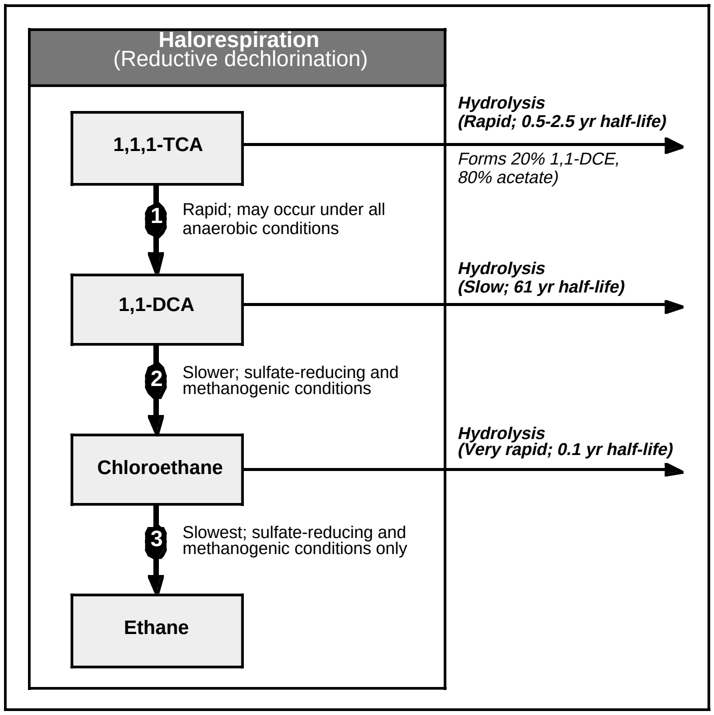


Figure 3. Reaction Sequence and Relative Rates for Halorespiration of Chlorinated Ethanes Associated with 1,1,1-TCA Degradation, with other reactions shown. (Wiedemeier et al., 1999)

The environmental chemistry and the oxidation-reduction potential of a site play an important role in determining whether reductive dechlorination will occur. Based on thermodynamic considerations, reductive dechlorination will occur only after both oxygen and nitrate have been depleted from the aquifer, because oxygen and nitrate are more energetically favorable electron acceptors than chlorinated solvents when hydrogen is the electron donor (Wiedemeier *et al.*, 1999). A detailed flow diagram outlining redox reactions in the subsurface can be found in Appendix C.

Hydrogen is recognized as a key electron donor during reductive dechlorination (Gossett and Zinder, 1996; Holliger et al., 1993; Carr and Hughes, 1998). Hydrogen is produced in the subsurface by the fermentation of a wide variety of organic compounds including anthropogenic compounds, such as petroleum hydrocarbons, and natural organic matter. Dechlorinating bacteria then use hydrogen as an electron donor to facilitate dechlorination of the solvents.

In summary, if biodegradation is occurring, daughter products will be evident and the plume is expected to be shorter than predicted by considering only dissolution, dispersion, sorption, and volatilization.

2.0 METHODOLOGY

2.1 Site Selection and Data Collection

For a site to be included in the database, sufficient chlorinated solvent concentrations, electron acceptor concentrations, and water quality information were required. If chlorinated solvent concentrations were too low (i.e., close to the detection limit), the plumes were ill defined, or significant commingling of plumes was evident, the site was excluded.

Data from site investigation, treatability, and natural attenuation reports were used to compile the database. Questionnaires were completed using mean hydrogeologic property values extracted from the site reports for the most contaminated unit (see Appendix A for sample questionnaire). Seepage velocities were calculated from mean hydraulic conductivity, hydraulic gradient, and porosity values. Plume lengths were determined using concentration isopleths for each chlorinated ethene or chlorinated ethane constituent included in the site report. The plume lengths and widths were delineated to the detection limit reported on the isopleth maps, which in most cases was 1 ppb for the chlorinated solvents. The plume length was measured from the upgradient edge to the downgradient edge of each plume, as illustrated in Figure 4. The source was assumed to be the center of the confirmed or suspected NAPL zone or the area of highest dissolved contamination. Chlorinated ethene and chlorinated ethane concentrations near the plume source and centerline were included, along with concentrations of electron acceptor/metabolic by-products and potential fermentation substrates, and water quality parameter values.

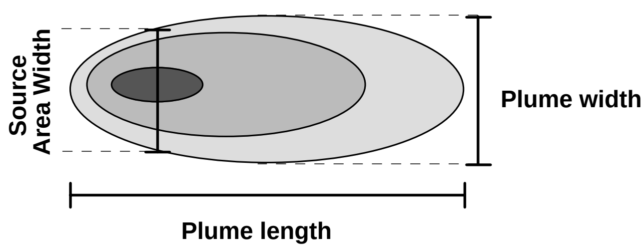


Figure 4. Plume Length and Width Delineation

Site and plume characteristics were summarized using quartiles. Quartiles consist of the 25th percentile, the 50th percentile (median), and the 75th percentile. Each quartile has the same number of data points. A number at the 25th quartile indicates that 75% of the measured values are greater than that value and 25% are lower. Minimum and maximum values were also calculated to determine the range of plume or site characteristics.

Plume lengths were correlated with various hydrogeologic and environmental variables. R^2 values were calculated to estimate the correlations for the sample of plumes in this database.

2.2 Biodegradation Rate Constant Estimation

Field-scale biodegradation rate constants were estimated using the BIOCHLOR model and plume centerline data from the database. BIOCHLOR is an analytical model, which simulates the reactive transport of chlorinated solvents in the subsurface and assumes sequential first order reductive dechlorination (Aziz *et al*., 2000). An overview of the model's governing equations, boundary conditions, solution technique, and assumptions is presented in Appendix D. Other approaches for estimating field-scale rate constants do not take into consideration the effect of daughter production formation, and some methods lump all attenuation processes together to generate an attenuation rate constant. The strength of using the BIOCHLOR model for biodegradation rate constant estimation is that daughter product formation and degradation are incorporated in the model and the resulting biodegradation rate constant will reflect this. Although the effects of advection, dispersion, and retardation are also accounted for in the model, the resulting rate constant is a biodegradation rate constant (not a lumped attenuation rate constant). The limitation of this approach is that the model will permit only one retardation factor for all of the constituents. However, in aquifer matrices with low amounts of organic carbon or plumes near steady-state, the choice of retardation factor becomes less important and will not impact the magnitude of the rate constant.

Rate constants were estimated by calibrating the BIOCHLOR model to chlorinated solvent concentration data near the plume centerline. Only chlorinated solvent data taken from wells screened at similar intervals were employed. Furthermore, data were used only from wells in the part of the plume deemed to be anaerobic (i.e., D.O. less than 1 mg/L). The mean hydraulic conductivity, hydraulic gradient, and porosity were used as inputs to the model to determine seepage velocity. A fixed value of longitudinal dispersivity, based on data reported by Gelhar *et al.* (1992) and summarized in Aziz *et al.* (2000), was employed. Transverse dispersivity was assumed to be one tenth of the longitudinal dispersivity and vertical dispersivity was set to zero because the depth of the plume usually approached the depth of the saturated zone. The simulation time was taken to be the amount of time elapsed from the date of first solvent release to the date of chlorinated solvent data collection. Initial concentration data were based on the dissolved concentrations of solvent in the source zone, with the assumption that these concentrations are similar to those in the source zone shortly after the start of the release. To calculate a common retardation factor, the retardation factors for the compounds present at the site were averaged. Rate constants were estimated by adjusting the rate constants until the BIOCHLOR concentration predictions best matched the field data, as determined by minimizing the sum of squares of the residuals.

Rate constants were correlated with various hydrogeologic and environmental variables. R^2 values were calculated to estimate the correlations.

3.0 RESULTS

3.1 Site Characteristics

Air Force Bases were the primary focus of this investigation, but a large number of industrial sites were also included as shown in Figure 5. FTA refers to Fire Training Area sites, where solvents were typically mixed with fuels and set ablaze for fire training purposes with the unintended release of both contaminant types to the subsurface. In total, the database comprises 24 sites, with widespread representation across the country as shown in Table 1 and Figure 6. Most of the sites had TCE as a parent compound (either alone or together with PCE), as shown in Figure 7. Only one site had PCE as the sole parent compound.

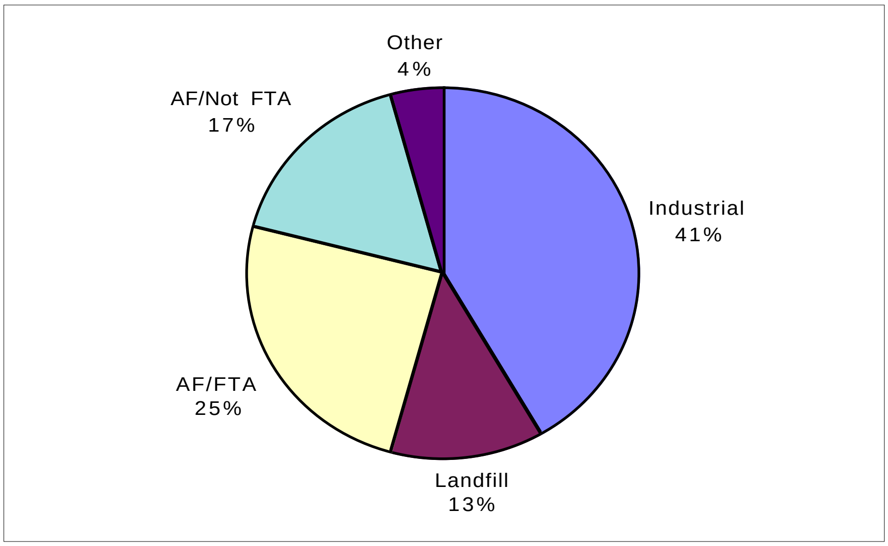


Figure 5. Breakdown of Site Type in BIOCHLOR Database

Table 1
Facility Information for Sites in BIOCHLOR Database

Facility/Site Name	State	Site Process	Chemicals Used in Process	Chemical Release Date Initial	Chemical Release Date Final	Time Since Release (yrs)
1. Aerojet Superfund Site	California	Septic Waste	Solvents/Degreasers/Septage	1960	1977	34
2. Altus AFB/LF-04	Oklahoma	Landfill	Paint Wastes	1956	1983	41
3. Cape Canaveral AS/CCFTA-2	Florida	Fire Training Area	Solvents/Degreasers/JP Fuels	1965	1985	31
4. Cape Canaveral AS/Facility 1381	Florida	Missile Technology	Solvents/Degreasers/Waste Acids	1968	1989	28
5. Chemical Distribution Facility	Oregon	Chem Distribution	Solvents/Degreasers/TEX	1979	1985	17
6. Chemical Manufacturer/Waste Site	Michigan	Chemical Refining/Incineration	Solvents/Degreasers/Chemical Waste	1969	1980	27
7. Chlorinated Site #1/Hanger	Alaska	FTA Hanger	Solvents/Degreasers/JP Fuels/Gasoline	1940	1980	53
8. Chlorinated Site #2/Tank Farm	Alabama	Refueling Tank Farm	Solvents/Degreasers/JP Fuels	1961	1983	34
9. Chlorinated Site #3/Junkyard	Alabama	Junkyard	Solvents/Degreasers/Gasoline			
10. Eielson AFB/Site 45/57	Alaska	Fire Training and Photo Lab	Solvents/Degreasers/Photo Chemicals			
11. Hill AFB/OU-5	Utah	Engine service/repair	Solvents/Degreasers/Gasoline/Sodium Cyanide	1942	1979	54
12. Industrial Facility/Plume 1	Ontario	Metal Manufacturing	Solvents/Degreasers	1940	1989	56
13. Industrial Facility/Plume 2	Ontario	Metal Manufacturing	Solvents/Degreasers	1940	1989	56
14. Kelly AFB/MP Site	Texas	Metal Plating Shop	Solvents/Degreasers/Metals	1970	1981	27
15. Landfill #1	New Hampshire	Waste Disposal	Solvents/Degreasers/TEX	1969	1984	27
16. Landfill #2/VC Site	Maryland	Landfill	Ag/Munic/Ind Wastes, PVC	1960	1981	37
17. Offutt AFB/Bldg. 301	Nebraska	Acid Pit & Manufacturing	Solvents/Acids	1942	1965	54
18. Offutt AFB/FPTA3	Nebraska	Fire Training Area	Solvents/Degreasers/JP Fuels	1960	1990	34
19. Plattsburgh AFB/FT-002	New York	Fire Training Area	Solvents/Degreasers/JP Fuels/waste oil	1955	1989	41
20. Sterling/OW-31/OW-41	Texas	Pond/Sewer	Solvents/Degreasers/Gasoline/Diesel/VC	1950	1960	41
21. Sterling/Unit K	Texas	Solid Waste Management Unit	Solvents/Degreasers/Gasoline/Diesel	1950	1982	46
22. USCG Site	North Carolina	Solvent Disposal	Solvents/Degreasers/Ind. Wastes	1958		39
23. Westover ARB/FT-03	Massachusetts	Fire Training Area	Solvents/Degreasers/JP Fuels	1940	1964	55
24. Westover ARB/FT-08	Massachusetts	Fire Training Area	Solvents/Degreasers/JP Fuels	1964	1986	31

Note:
1. Data on Sites 1, 5, 12, 13, and 15 provided by Beak International Incorporated. Data on Sites 7, 8, and 9 provided by Radian International LLC. Data on Sites 6, 16, and 22 provided by USEPA. Data on remaining sites provided by Air Force Center for Environmental Excellence (AFCEE).
2. The time since release is the year the data were collected minus the initial release date.

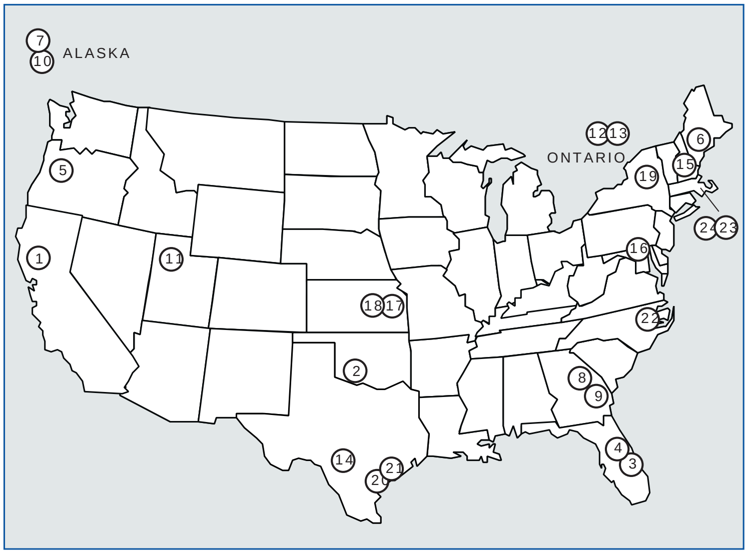


Figure 6. Map Showing Location of Sites in the BIOCHLOR Database
(Numbers Correspond to Sites Listed in Table 1)

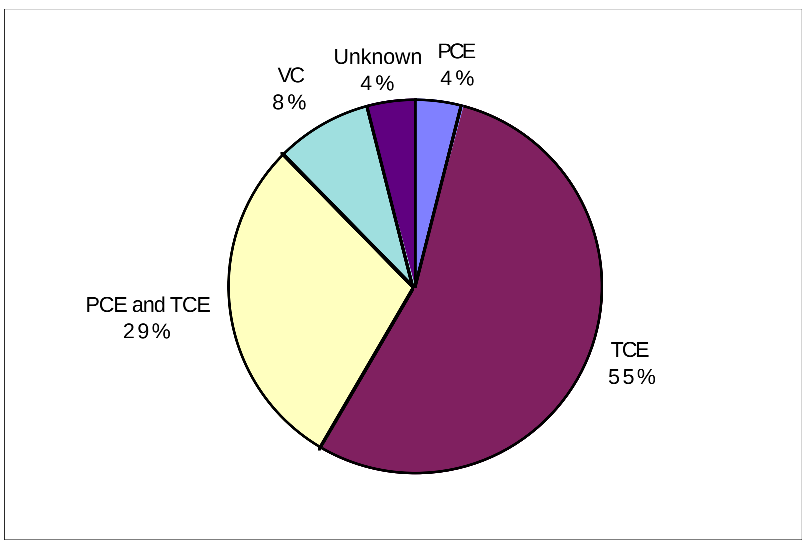


Figure 7. Breakdown of Chlorinated Ethene Parent Compounds at 24 Sites

3.2 Site Hydrogeologic Conditions

The sites in the BIOCHLOR database encompass a wide range of soil classifications, but 62% of the sites had silty sands. Table 2 presents a summary of the hydrogeology for the major contaminated unit for the sites in the database. The median seepage velocity was 60 ft/yr, the median hydraulic conductivity was $4x10^{-3}$ cm/s, the median gradient was 0.002 ft/ft, the median effective porosity was 0.25, and the median fraction of organic carbon was 0.0018. These hydrogeologic conditions are representative of nationwide groundwater flow conditions, where a median seepage velocity from 290 sites of 88 ft/yr and a median hydraulic conductivity of $5x10^{-3}$ cm/sec from 287 sites, as reported by Newell et al. (1990).

TABLE 2
SUMMARY OF SITE HYDROGEOLOGIC CHARACTERISTICS

	Units	Minimum	25th Percentile	Median	75th Percentile	Maximum	Mean	n
Avg. Depth to GW	(ft; BGS)	2.0	6.4	**15.0**	29.5	52.5	20.2	24
Seepage Velocity	(ft/yr)	2.9	16.8	**60.3**	152.2	1287.5	229.9	24
Hydraulic Conductivity	(cm/s)	7.00E-05	1.54E-03	**4.10E-03**	1.78E-02	2.00E-01	2.61E-02	23
Hydraulic Gradient	(ft/ft)	0.001	0.001	**0.002**	0.015	0.040	0.010	24
Effective Porosity	(dim.)	0.03	0.20	**0.25**	0.30	0.38	0.25	21
Saturated Thickness	(ft)	10	27	**40**	55	390	55	24
Soil Bulk Density	(kg/L)	1.40	1.60	**1.65**	1.65	1.81	1.64	13
Fraction Organic Carbon	(dim.)	1.00E-06	7.68E-04	**1.85E-03**	4.79E-03	3.00E-02	4.40E-03	16

Note:
1. Soil and aquifer characteristics identified for major contaminated unit.

3.3 Presence of Observed NAPL

Information regarding NAPL contamination was collected whenever possible; however, the data were scant (see Table B.1 in Appendix B). This undoubtedly stems from the difficulty associated with delineating the extent of NAPL contamination (Pankow and Cherry, 1995; USEPA, 1993). DNAPL was observed at 6 out of the 24 sites and LNAPL was observed at 7 out of 24 sites. Using dissolved phase concentrations that exceed 1% of the aqueous solubility as an indicator of NAPL (Newell and Ross, 1992), 12 out of 24 sites had NAPL. Although the presence or absence of observable NAPL did not appear to be correlated with chlorinated solvent plume length, a relationship between plume length and source width, which is related to NAPL migration processes, was noted (see Section 4.2).

3.4 Chlorinated Solvent Plume Lengths

Plume lengths are of particular interest because this information provides an indication of the likelihood of off-site migration and impact to downgradient. The dissolved plume length quartiles for chlorinated ethenes, chlorinated ethanes, and chloride are presented in Tables 3 and the detailed table showing data from individual sites can be found in Appendix B. In addition, Figure 8 summarizes all the chlorinated ethene parent and daughter constituent plume data.

Table 3
Plume Length Summary

Plume Lengths (ft)

	Minimum	25th Percentile	Median	75th Percentile	Maximum	Mean	n
PCE	100	228	**970**	1335	13700	1933	11
TCE	250	450	**1215**	2600	11900	2137	21
cis-DCE	200	540	**1205**	3100	9400	2046	20
trans-DCE	440	1190	**1200**	1890	2750	1494	5
VC	180	398	**860**	1310	3300	1084	15
Ethene	120	320	**600**	1045	1500	675	11
Chloride	270	863	**1418**	2900	4520	1848	14
BTEX	60	595	**750**	1270	3600	1183	15
TCA	130	365	**865**	2183	2700	1230	6
1,1-DCA	1040	1370	**1650**	1925	2500	1675	8
1,1-DCE	1000	1245	**1470**	1643	1820	1438	6

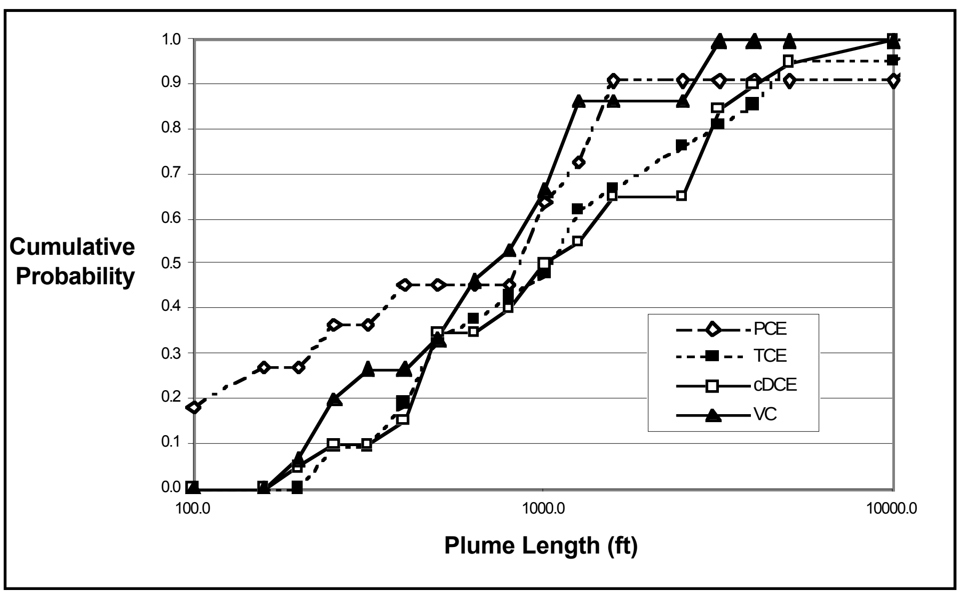


Figure 8. Cumulative Probability Plot for Chlorinated Ethene Plume Lengths

When comparing the chlorinated ethenes (i.e., PCE, TCE, c-DCE, t-DCE, and vinyl chloride), TCE and the DCE isomers have the longest median plume lengths, all in the 1200 ft range, as shown in Table 3. Vinyl chloride has the shortest median plume length of 860 ft, followed by PCE with a plume length of 970 ft.

The relatively short median VC plume length is encouraging given that VC has a higher associated carcinogenicity than the other chlorinated ethenes. Because VC has a shorter median plume length than c-DCE, this implies that VC is being degraded more rapidly than c-DCE, possibly by mechanisms other than reductive dechlorination. Laboratory studies have shown VC to undergo reductive dechlorination at the slowest rates relative to PCE, TCE, and c-DCE (Vogel and McCarty, 1985). However, other studies have shown that VC is oxidized under iron reducing conditions (Bradley and Chapelle, 1996), acts as a primary growth substrate under aerobic conditions (Davis and Carpenter, 1990) and is cometabolized under both anaerobic and aerobic conditions (Gossett and Zinder, 1996; Dolan and McCarty, 1995). Therefore, VC's shorter median plume length may be attributed, in part, to its degradability under a variety of redox conditions. Because VC plumes are usually coincident or nearly coincident with the parent compound plumes (see section 3.6), they are less likely to reach downgradient receptors than TCE and c-DCE.

Ethene plumes lengths (median length of 640 ft) are shorter than those of VC, likely because of the volatilization and biodegradation of ethene. Conversely, chloride plumes are the longest (median length of 1418 ft), stemming from the conservative nature of chloride in the subsurface. The presence of ethene and chloride plumes, both products of dechlorination, provide another line of evidence that reductive dechlorination is occurring. Furthermore, ethene is evidence of complete dechlorination (rather than incomplete dechlorination where the process stops at c-DCE or VC).

The plume length trends are different for the chlorinated ethanes. TCA's median plume length of 865 ft is shorter than that of its daughter product, 1,1-DCA (median plume length of 1650 ft). This result may be explained by the fact that TCA is rapidly degraded by both reductive dechlorination and by abiotic mechanisms (abiotic half-life of 0.5-2.5 yr) (Vogel and McCarty, 1987). The presence of a long 1,1-DCE plume (median length of 1470 ft) is further evidence that 1,1,1-TCA is degraded abiotically (see Figure 3). 1,1-DCA has the longest median plume length of the chlorinated ethanes and is longer than that of the chlorinated ethenes.

3.5 Relative Plume Lengths

The longest plume at a site is of interest from the standpoint of impacting adjacent sites and downgradient receptors. Figure 9 shows the proportion of the longest plumes at the sites in the BIOCHLOR database when only chlorinated ethenes are considered. c-DCE or TCE have the longest plume at 79% of the sites and occur at almost equal frequency. The remaining 21% of sites have VC and PCE as the longest plume. Note that vinyl chloride was the longest plume at 3/24 or 13% of the sites. However, two of these sites had VC as the parent compound.

When both chlorinated ethenes and ethanes are present at a site, TCE and c-DCE tend to be the longest plumes as shown in Figure 10. However, approximately a third of the sites had either 1,1-DCA or 1,1-DCE as the longest plume.

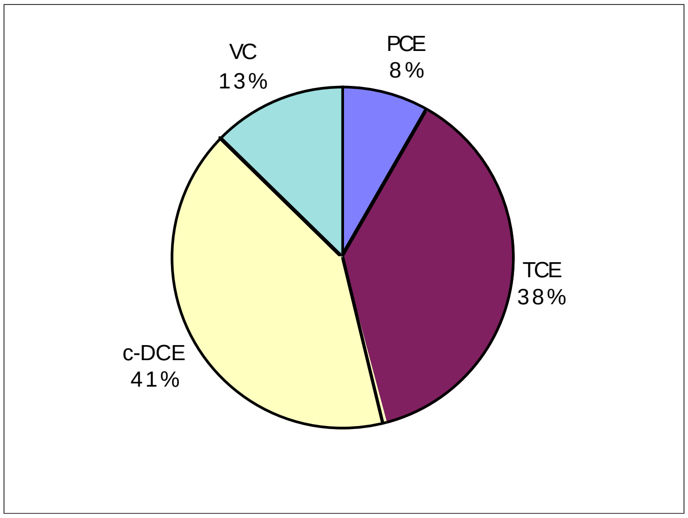


Figure 9. Relative Proportion of Chlorinated Solvents Yielding Longest Plumes (Chlorinated Ethenes Only)

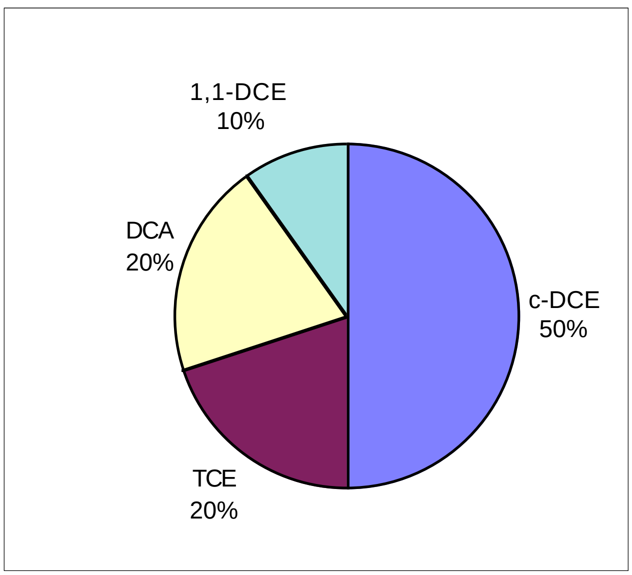


Figure 10. Relative Proportion of Chlorinated Solvents Yielding Longest Plumes (Chlorinated Ethenes and Ethanes)

3.6 Plume Coincidence

Coincidence means that the maximum concentrations of the parent and daughter products occur at the same well, as illustrated in Figure 11. Figure 12 shows that 88% of the sites in the database had plumes that are coincident. The remaining 12% of the sites had plumes whose maximum daughter concentrations occurred downgradient of the maximum parent compound concentration, but only by less than 20% of the parent plume length. Similar results were reported in the Lawrence Livermore chlorinated solvent plume study, which reported that daughter product plumes are contained within or roughly coincide with the respective parent plume (McNab *et al.*, 1999).

Because all the plumes in this study were coincident or almost coincident, some conclusions can be drawn regarding potential impacts to downstream receptors. Because VC has the shortest median plume length and its highest concentration is usually coincident with that of the parent compound, VC should be less likely to reach downstream receptors than TCE and cDCE. This is encouraging in light of the high carcinogenicity associated with VC. Its shorter plume length is attributed either to faster rates of reductive dechlorination or, more likely, its ability to be degraded by a variety of mechanisms including aerobic metabolism, cometabolism under both aerobic and anaerobic conditions, and oxidation by ferric iron reduction.

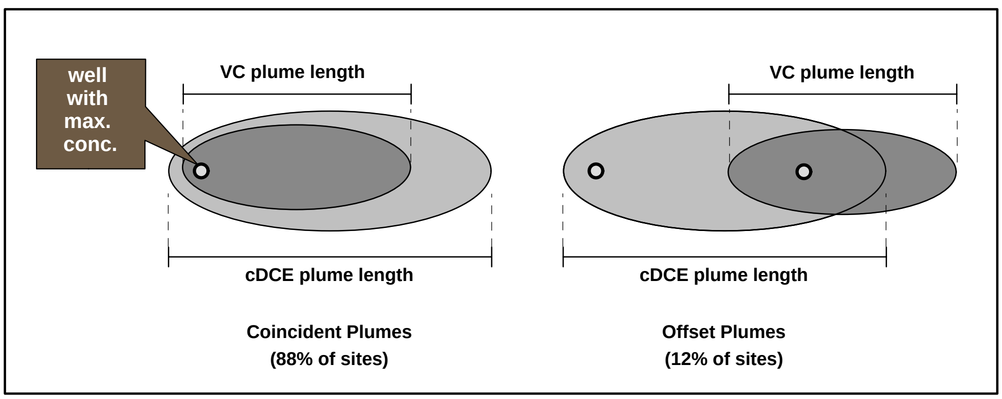


Figure 11. Coincident and Offset Plumes

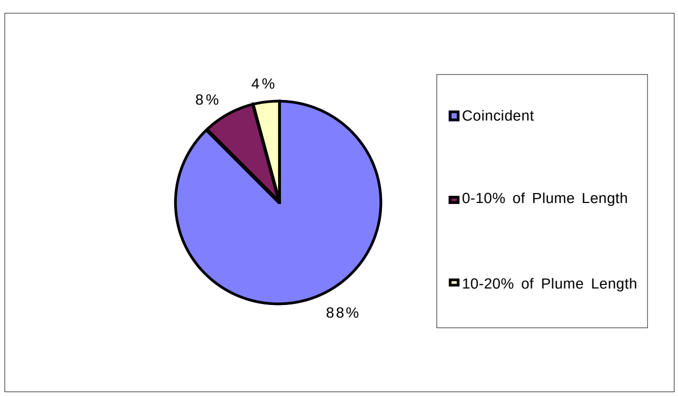


Figure 12. Degree of Coincidence of Parent and Daughter Plumes

3.7 Plume Widths

Median maximum plume widths and the width of the widest chlorinated solvent plume in the source area are shown in Table 4. Median maximum plume widths range from 300 to 750 ft. Because lateral dispersion is typically weak (Pankow and Cherry, 1996), the width of the plume is dependent largely on the width of the source area. For the sites in this database, the median source area width is 555 ft.

Table 4
Maximum Plume Widths Summary

Plume Width (ft)

	Minimum	25th Percentile	Median	75th Percentile	Maximum	Mean	n
PCE	90	205	**750**	1138	10100	1493	11
TCE	140	350	**610**	1400	9100	1208	21
cis-DCE	85	258	**668**	1025	8300	1172	20
trans-DCE	110	140	**300**	875	1320	549	5
VC	90	240	**540**	1030	1800	683	15
Ethene	100	150	**400**	585	730	382	11
Chloride	240	400	**480**	840	2950	854	13
BTEX	40	345	**480**	550	1400	495	15
TCA	170	236	**365**	659	1200	508	6
1,1-DCA	301	335	**483**	763	2000	685	8
1,1-DCE	200	343	**385**	574	800	456	6
Source Area Width	75	313	**555**	777	1300	585	20

3.8 Dissolved Chlorinated Solvent Concentrations

The statistics for the maximum chlorinated constituent concentrations are provided in Table 5 and a detailed table can be found in Appendix B. The highest maximum concentrations were associated with TCE (i.e., median concentration of 3.255 mg/L). This relatively high concentration may be due to solubilization of free phase TCE and the relatively high solubility of TCE (about 1100 mg/L). In contrast, PCE has the lowest median maximum concentration, which is likely linked to its low aqueous solubility (about 150 mg/L at 25 °C) and relatively rapid degradation rates (Haston and McCarty, 1999).

Table 5
Summary of Maximum Chlorinated Solvent Concentrations

Chlorinated Solvent Concentrations (mg/L)

	Minimum	25th Percentile	Median	75th Percentile	Maximum	Mean	n
PCE	0.001	0.002	**0.056**	2.330	60.000	8.317	15
TCE	0.002	0.362	**3.255**	15.050	570.000	34.736	22
cis-DCE	0.004	0.191	**1.240**	10.825	300.000	22.428	22
trans-DCE	0.002	0.009	**0.025**	0.084	0.389	0.075	13
VC	0.001	0.071	**1.300**	2.700	6.520	1.840	16
TCA	0.002	0.120	**0.180**	0.258	30.000	3.855	9
DCA	0.001	0.005	**0.059**	0.441	11.150	1.145	12
1,1-DCE	0.002	0.016	**0.039**	0.249	3.800	0.479	11

The presence of high concentrations of c-DCE relative to t-DCE is indicative of reductive dechlorination. c-DCE is the DCE isomer produced most frequently as a result of the reductive dechlorination of TCE, while commercially manufactured DCE is composed largely of t-DCE. Therefore, a high percentage (i.e., greater than 80%) of c-DCE relative to t-DCE indicates reductive dechlorination (Wiedemeier *et al*., 1996). With the exception of one site, c-DCE is present at concentrations one or more orders of magnitude greater than t-DCE concentrations, indicating widespread reductive dechlorination.

Chlorinated ethanes (1,1,1-TCA and 1,1-DCA) are present at about one tenth the concentration of the chlorinated ethenes. TCA is degraded under both abiotic and biotic conditions, which may result in its lower concentration. Also, if TCA is degraded largely under abiotic conditions, less TCA is converted to DCA. Both TCA and DCA are degraded under both anaerobic and aerobic conditions, increasing the likelihood of their degradation and lower groundwater concentrations.

3.9 BTEX Plume Characteristics

An interesting finding from analysis of this database is the long length of BTEX plumes at chlorinated solvent release sites as shown in Table 6. BTEX plume lengths range from 60 to 3600 ft with a median plume length of 750 ft, and BTEX plume widths range from 40 to 1400 ft with a median width of 480 ft.

Table 6
Summary of BTEX Plume Dimensions at Chlorinated Solvent Sites

BTEX Plume Dimensions (ft)

	Minimum	25th Percentile	Median	75th Percentile	Maximum	Mean	n
Length	60	595	**750**	1270	3600	1183	15
Width	40	345	**480**	550	1400	495	15

The median length of BTEX plumes in this database is considerably longer than the median BTEX plume length of 132 ft reported in a compilation of four fuel hydrocarbon plume studies focusing on gas station releases (Newell and Connor, 1998) and slightly longer than the median plume dimensions reported for Air Force Bases contaminated with fuel hydrocarbons (Wiedemeier *et al.*, 1999) as shown in Figure 13.

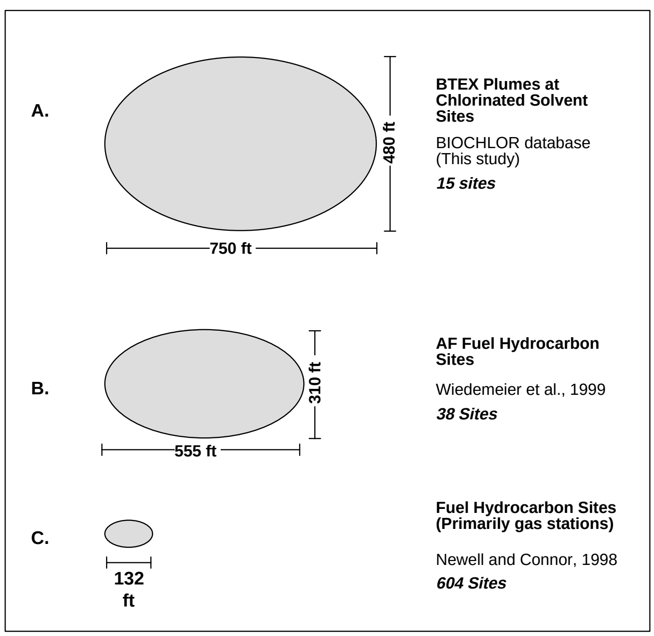


Figure 13. Comparison of Median BTEX Plume Dimensions

One explanation to account for the differing BTEX plume lengths is the spill size. By examining the width of the plumes, it is possible that larger and/or more disperse spills occurred in the case of Plumes A and B relative to plumes typically found at retail UST sites (Plume C). Larger spills would result in larger plumes.

Another explanation to account for the longer BTEX plume lengths at chlorinated solvent sites is the nature of the NAPL. At sites with mixed fuel and chlorinated solvents, some BTEX will dissolve in the DNAPL and travel downward through the saturated zone under the force of gravity. As the DNAPL travels downward, lateral movement attributed to differences in permeability in the subsurface stratigraphy can occur (Pankow and Cherry, 1996). This vertical and lateral spreading of the DNAPL, coupled with the enhanced dissolution of BTEX from the DNAPL because of the increased surface area, may account for the longer BTEX plumes found at chlorinated solvent release sites relative to retail UST sites. More importantly, the BTEX has the potential to migrate to areas of the aquifer that are anaerobic. Because BTEX generally degrades more slowly under anaerobic conditions than under aerobic conditions, the presence of DNAPL and the increased likelihood of anaerobic conditions may contribute to longer BTEX plumes.

3.10 Electron Acceptor/Metabolic By-Product and Electron Donor Data

Electron acceptor data, shown in Table 7 and Appendix B, give an indirect indication of redox conditions in the aquifer. At 16/18 sites, the dissolved oxygen decreased in locations upgradient of the source to those downgradient. Sulfate decreased at 17/19 sites, indicating a high frequency of sulfate-reducing conditions. Nitrate reduction was evident at 15/19 sites, iron reduction was evident at 14/17 sites, and methanogenesis occurred at 13/16 sites. Reductive dechlorination of chlorinated solvents has been demonstrated under nitrate- and iron-reducing conditions, but the most rapid biodegradation rates, affecting the widest range of chlorinated aliphatic hydrocarbons occurs under sulfate-reducing and methanogenic conditions (Bouwer, 1994). The electron acceptor data support the chlorinated solvent concentration data, which showed widespread reductive dechlorination.

Highly reducing conditions are driven by the oxidation of substrates such as natural organic matter and anthropogenic compounds, such as BTEX in gasoline. After these substances are degraded under aerobic, nitrate-reducing, iron-reducing, and sulfate-reducing conditions, they are fermented to produce hydrogen (see Appendix C for a flowchart of redox reactions). At 10/18 sites, BTEX concentrations are greater than 1% of the solubility of at least one BTEX constituent, indicating ample supply of fermentation substrate. At the six sites where hydrogen was measured, the median value was 4 ng/L and the hydrogen concentration ranged from 0.6 to 12.3 ng/L.

A high percentage of sites (i.e., 58%) had detectable ethene concentrations. This value is considered an underestimate of the occurrence of ethene because ethene was not measured at every site in the database. The presence of ethene and ethane are evidence of complete reductive dechlorination. Incomplete reductive dechlorination occurs when dechlorination stops at c-DCE or VC. Only 6/24 (25%) of the sites showed incomplete dechlorination. These results differ from those reported in the LLNL chlorinated solvent plume study (McNab *et al.*, 1999), where one third of the sites did not proceed beyond TCE and one third did not proceed beyond c-DCE. However, the population of sites differed between the two studies, with most of the LLNL sites being in California and Oregon and the BIOCHLOR sites being distributed around the country. Different amounts of native organic matter and fuel co-contaminants in the groundwater may be responsible for the difference in the incidence of complete reductive dechlorination between the two studies.

Table 7
Electron Acceptor/Metabolic By-Product Data Summary

	Units	Minimum	25th Percentile	Median	75th Percentile	Maximum	Mean	n
Δ Dissolved Oxygen	(DO, mg/L)	-1.867	0.372	**1.945**	4.404	8.500	2.628	18
Δ Sulfate	(SO_4^{2-}, mg/L)	-710.000	7.345	**18.850**	52.700	201.000	5.097	19
Δ Nitrate	(NO_3^-, mg/L)	-1.180	0.065	**0.170**	1.254	5.645	1.013	19
Δ Ferrous Iron	(Fe II, mg/L)	-15.950	3.250	**6.620**	31.600	600.000	84.059	17
Δ Methane	(mg/L)	-9.510	0.183	**1.477**	4.584	22.399	3.264	16
Max. Ethene	(mg/L)	0.001	0.008	**0.257**	0.903	7.750	1.473	14
Max. Ethane	(mg/L)	0.004	0.027	**0.173**	2.923	3.850	1.336	6
Max. Dissolved H2	(mg/L)	6.05E-07	2.09E-06	**3.98E-06**	4.45E-06	1.23E-05	4.49E-06	6
Max. Total BTEX	(mg/L)	0.006	0.096	**1.676**	8.924	75.800	11.125	18

Note:
1. Values for ΔDO, ΔSO_4, and ΔNO_3 calculated as average background concentration minus minimum plume concentration. Values for ΔFe and Δmethane calculated as maximum plume concentration minus average background concentration.

3.11 Water Quality Parameters

Water quality parameters were also examined for the sites in this database. Summary statistics are shown in Table 8 and the detailed data can be found in Appendix B. A highly negative redox potential of less than -100 mV has been linked to reductive dechlorination under field conditions (Wiedemeier *et al*., 1996). In this database, the median minimum redox potential was -116 mV, a value conducive to reductive dechlorination.

Table 8
Water Quality Parameters Summary

	Units	Minimum	25th Percentile	Median	75th Percentile	Maximum	Mean	n
Δ Chloride	(mg/L)	-235.9	11.5	**77.0**	181.9	5097.7	443.1	19
Δ Chloride	(mmol/L)	-6.6	0.3	**2.2**	5.1	143.6	12.5	19
Min. Redox Potential	(mV)	-340	-170	**-116**	-60	158	-104	17
Background Avg. TOC	(mg/L)	0.5	4.8	**8.6**	18.4	34.9	12.1	11
Δ Total TOC	(mg/L)	-27.1	-1.5	**10.3**	19.6	299.5	35.5	12
Avg. pH	(-)	5.6	6.6	**7**	7.2	7.5	6.8	22
Minimum Alkalinity	(mg/L)	10	82	**207**	315	520	204	21
Maximum Alkalinity	(mg/L)	260	320	**354**	500	940	439	21
Avg. Temperature	(°C)	5.7	10.8	**15.4**	20.75	26.2	15.7	22

Note:
1. Values for Δchloride and Δtotal TOC calculated as maximum plume concentration minus average background concentration.

Nine out of twelve sites where TOC was measured showed higher TOC within the plume compared to background, an indication that TOC (in the form of fuel or other hydrocarbons) was co-contaminating the aquifer. High concentrations of fermentable substrates, such as BTEX, have been linked to higher levels of reductive dechlorination because they ferment to produce hydrogen, an electron donor for reductive dechlorination (Wiedemeier *et al.*, 1996).

Generally, all the sites had pH levels close to neutral, with the median pH being 7.0. The median temperature was 15.4 °C, and the aquifer temperatures ranged from 5.7 to 26.2 °C.

At the 18 sites where chloride concentrations were measured, all but three showed increasing levels of chloride, indicating reductive dechlorination (Table 8). Table 8 also shows the median Δ chloride concentration (i.e., maximum chloride concentration in plume – average background concentration) is 2.2 mmol/L, and Table 9 shows the median maximum VOC concentrations in mmol/L. These data show that the amount of chloride produced (2.2 mmol/L) is much higher than the maximum that could be produced if all the dissolved solvents in the source zone are completely degraded (i.e., 0.122 mmol/L in Table 9). This analysis suggests that the high concentration of chloride is originating from the reductive dechlorination of solvent that is dissolving out of residual or mobile DNAPL.

Because chloride is a by-product of reductive dechlorination, elevated chloride concentrations are indicative of reductive dechlorination. The higher concentration of dissolved solvents in the source area coupled with the availability of larger amounts of electron donor (i.e., hydrogen from the fermentation of BTEX compounds) suggest that the high amounts of chloride are being generated by reductive dechlorination of solvents in the source area. The temporary depression of dissolved concentrations in the source zone will drive the mass transfer of solvents from the residual or mobile phase into the bulk aqueous phase. Therefore, reductive dechlorination can speed the rate of source mass decay, as has been reported elsewhere (Carr and Hughes, 2000).

Table 9
Chloride Concentration vs. VOC Concentrations

Constituent	Concentration (mmol/L)	Conc. of Chloride if Complete Degradation (mmol/L)
PCE	0.0003	0.001
TCE	0.025	0.074
cis-DCE	0.013	0.026
trans-DCE	0.0003	0.001
VC	0.021	0.021
Total Chloride	NA	**0.122**

4.0 PLUME LENGTH CORRELATIONS

Chlorinated ethene (i.e., PCE, TCE, c-DCE, VC) plume lengths were correlated with various hydrogeologic and environmental variables to determine important factors impacting plume length. In general, there were insufficient data to estimate correlations for the chlorinated ethane plume lengths.

4.1 Effect of Advection

One important factor influencing chlorinated solvent plume length was the effect of advection. Logarithmic plots of plume length vs. seepage velocity for the chlorinated ethenes are shown in Figure 14. For each constituent, the plume length increases as the seepage velocity increases (with R^2 ranging from 0.14 to 0.43), indicating that advection is a moderately important factor impacting chlorinated ethene plume lengths.

When plume length was plotted vs. seepage velocity multiplied by time (i.e., the distance groundwater traveled since the release occurred) similar trends were observed. Plume lengths increased with the distance the groundwater had traveled on a logarithmic scale, with R^2 ranging from 0.21 to 0.35 as shown in Figure 15. This result is in agreement with the LLNL chlorinated solvent plume study, which concluded that chlorinated solvent plume lengths correlate with groundwater velocity (McNab *et al*., 1999).

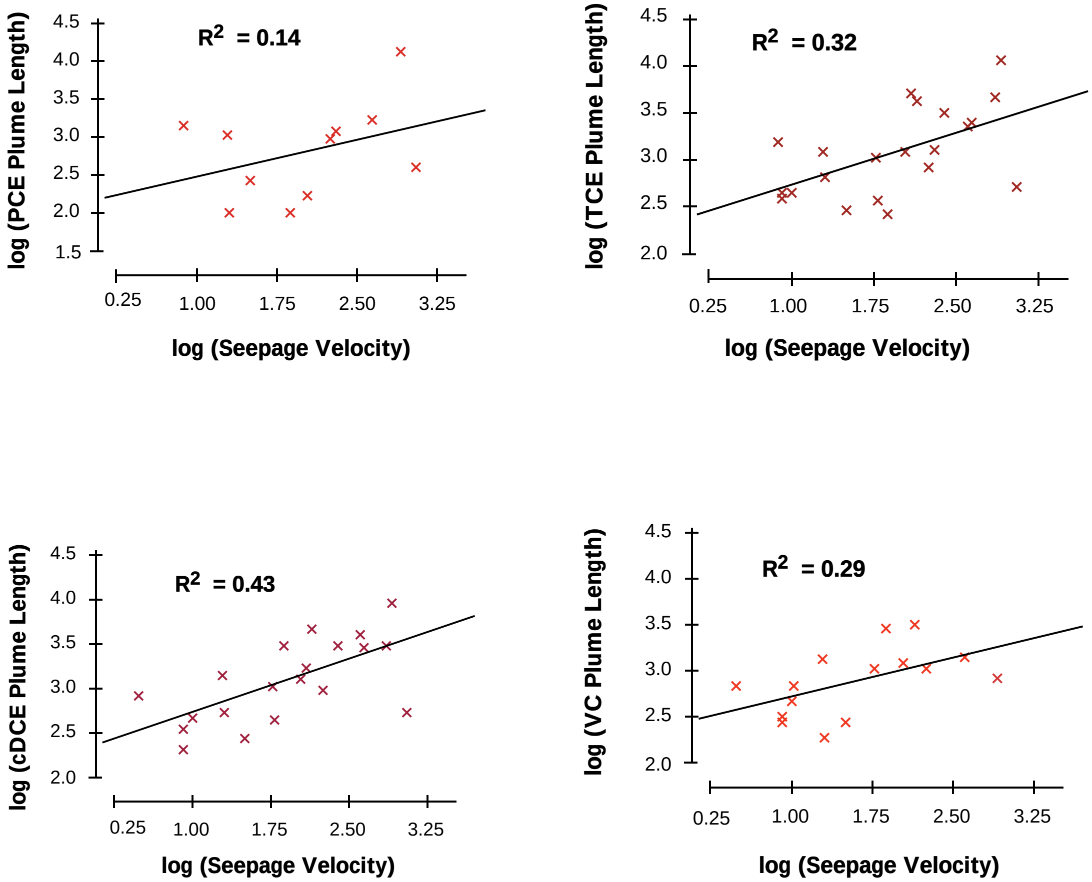


Figure 14. Correlation of Plume Length with Seepage Velocity

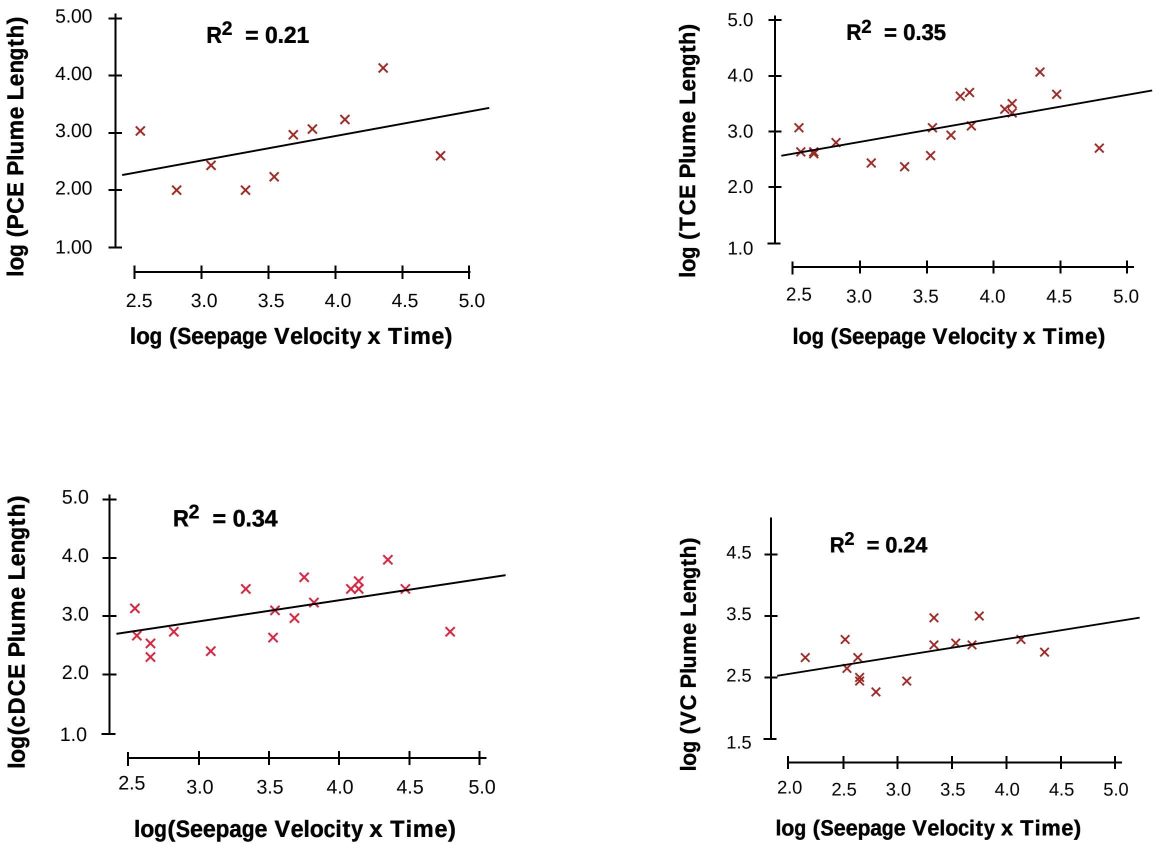


Figure 15. Correlation of Plume Length with Groundwater Travel Distance

4.2 Effect of Source

Previous studies have indicated that the size of the source may be an important factor impacting plume length (Rice *et al*., 1995; Mace *et al*., 1997). Because residual DNAPL is difficult to detect, the extent of the source area is often poorly defined. To represent the effect of the source size, the effect of the source area width was examined. The source area width is the width of the widest plume in the source area. The logarithm of the plume length was plotted vs. the logarithm of source area width and good correlations were obtained for each of the chlorinated ethenes as shown in Figure 16. As the source area width increased, so did the plume length, with R^2 ranging from 0.38 to 0.52.

Poor correlations were obtained when maximum plume length was plotted against maximum concentrations; however, when plume lengths were plotted versus the product of source width and maximum concentrations as shown in Figure 17, good correlations were obtained. R^2 values varied from 0.38 to 0.76, implying that data obtained in the source area alone are useful for estimating maximum plume lengths.

Both Figures 16 and 17 indicate that the size of the source is a key factor impacting chlorinated solvent plume length. Source areas at chlorinated solvent release sites may be larger than those found at retail UST sites, for example, possibly because of larger or more dispersed historical releases and/or the dense non-aqueous phase nature of chlorinated solvents. During the active period of the release, the solvent or DNAPL travels vertically downward through the saturated zone. As the DNAPL travels downward, considerable lateral movement, attributed to differences in permeability in the subsurface stratigraphy, can occur (Pankow and Cherry, 1996). The DNAPL migration has the effect of increasing the surface area of the DNAPL and the size of the source zone, resulting in higher rates of dissolution and longer dissolved plumes. Pankow and Cherry (1996) provide a detailed discussion of source zone characteristics and dissolution.

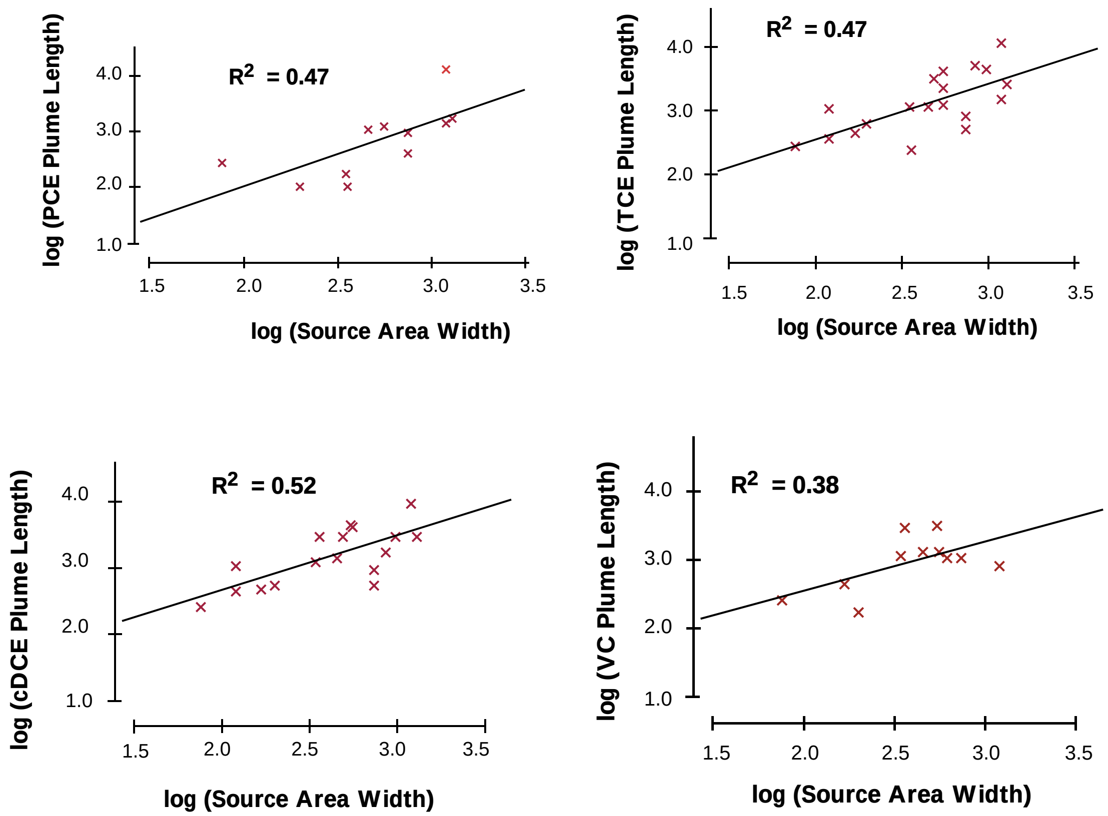


Figure 16. Correlation of Log of Plume Length with Log of Source Area Width

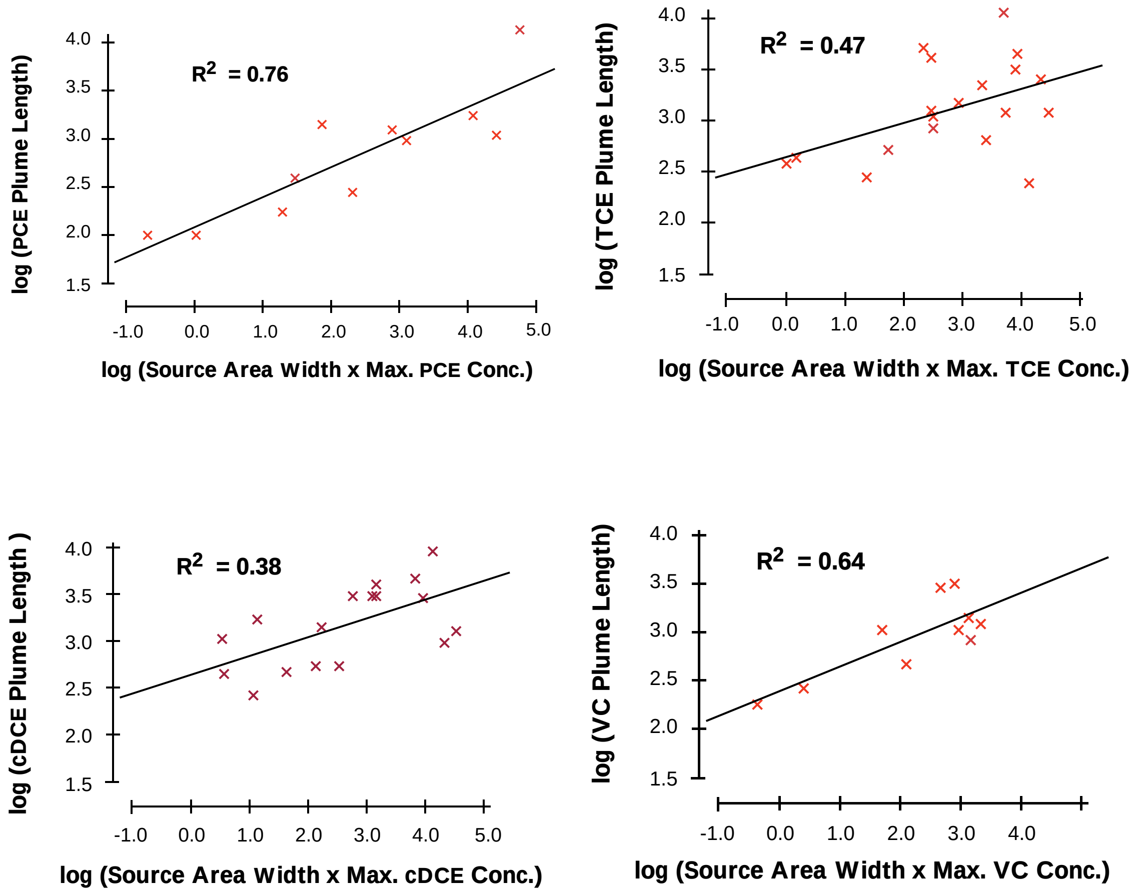


Figure 17. Correlation of Plume Length with Source Area Width x Maximum Concentration

The effect of both source size and seepage velocity on plume length is shown in Figure 18. In this figure, each grouping depicts dissolved plume lengths and widths for chlorinated ethenes, ethene, chloride, and BTEX at a particular site along with time since release and the site type. The plumes are drawn to reflect plume length and width but not actual shapes, and all plumes are assumed to be coincident.

The source area width (used as an indicator of the size of the DNAPL source zone) and seepage velocity of that site are plotted on the graph using black circles with crosses. Longer plume lengths for the chlorinated ethenes are correlated to higher seepage velocities (right hand side of the chart) and larger estimated source sizes (top of the chart). Chloride and BTEX plumes are also shown for comparison where these data are available.

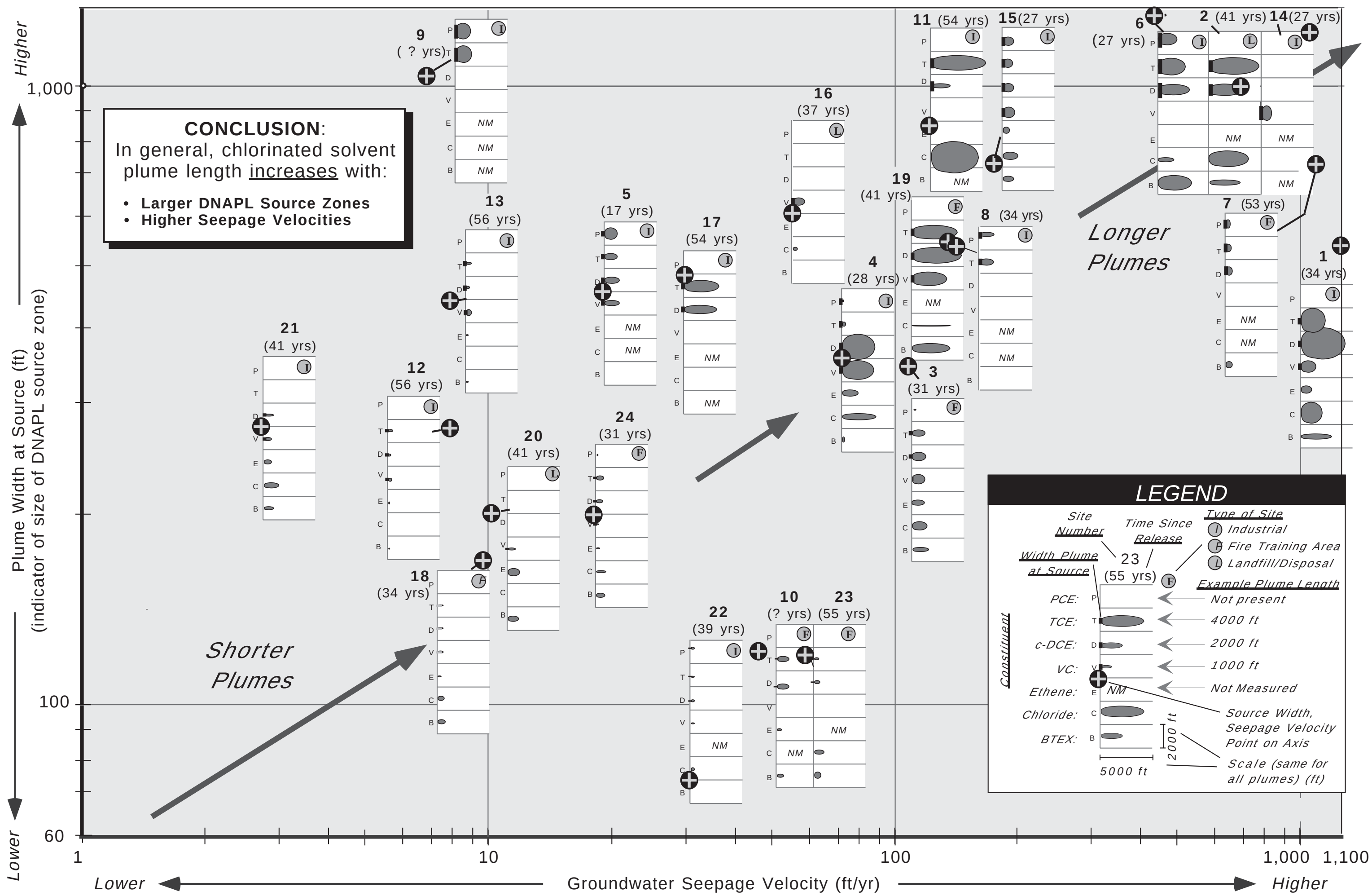


Figure 18. Effect of Estimated Source Size and Groundwater Seepage Velocity on Plume Length. Each grouping depicts dissolved plume lengths and widths for chlorinated ethenes, ethene, chloride, and BTEX at a particular site along with time since release and the site type. The plume width at the source (used as an indicator of the size of the DNAPL source zone) and seepage velocity of that site are plotted on the graph using the ⊕ symbol. Longer plumes are associated with larger DNAPL source zones (approximated by the width of the source zone perpendicular to groundwater flow) and higher seepage velocities. Note that plumes are drawn as coincident ellipses, and reflect plume length and width but not actual shapes.

4.3 Effect of Electron Donors

During reductive dechlorination, chlorinated solvents act as electron acceptors and become reduced. An electron donor, such as hydrogen, is required to complete the reaction (see Appendix C). Many natural organic compounds or anthropogenic compounds, including BTEX, can also ferment to produce hydrogen in the subsurface. To test the effect of electron donors on plume length, chlorinated solvent plume length was plotted vs. maximum BTEX concentration and also versus hydrogen concentration. There was no apparent correlation with chlorinated ethene plume lengths and the maximum BTEX concentration. A trend of shorter plumes was observed as the hydrogen concentration increased but the data set was not sufficiently large to generate reliable correlations. As shown in Figure 19, there was a marked difference between chlorinated ethene plumes at sites with and without BTEX. The plumes at sites with BTEX were considerably shorter, because the BTEX can serve as a source of electron donor needed for the reductive dechlorination of the chlorinated solvents.

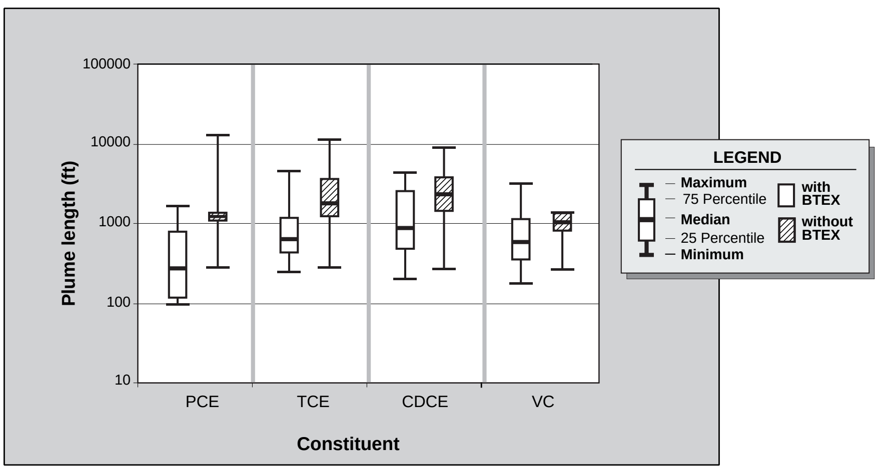


Figure 19. Chlorinated Ethene Plume Lengths at Sites With and Without BTEX

A good correlation between solvent plume length and the BTEX plume length exists (with the exception of one outlier) as shown in Figure 20, which is likely attributed to the effect of advection and/or the size of the source on both plumes. Figure 21 demonstrates the effect of advection on BTEX plumes. Here BTEX plume length is strongly correlated to groundwater travel distance (i.e., seepage velocity multiplied by time since release), suggesting that advection is an important factor impacting plume length. This result contrasts with both the California and Texas UST studies (Rice *et al*., 1995; Mace *et al*., 1997) that showed BTEX plumes to be short (with median plume lengths of 101 ft and 181 ft, respectively). In addition, the California study found that the hydrogeologic parameters had little relationship to plume length.

The BTEX plume length is also positively correlated to the source width (a proxy for extent of NAPL migration), as shown in Figure 22. The assumption that is made is that the larger the source area width, the further the NAPL migration and the more surface area that is available for dissolution. More available surface area will lead to higher mass fluxes of dissolved solvent from the NAPL and the consequence will be longer plumes. This relationship may explain, in part, the long BTEX plumes found at chlorinated solvent sites versus those found at retail UST sites.

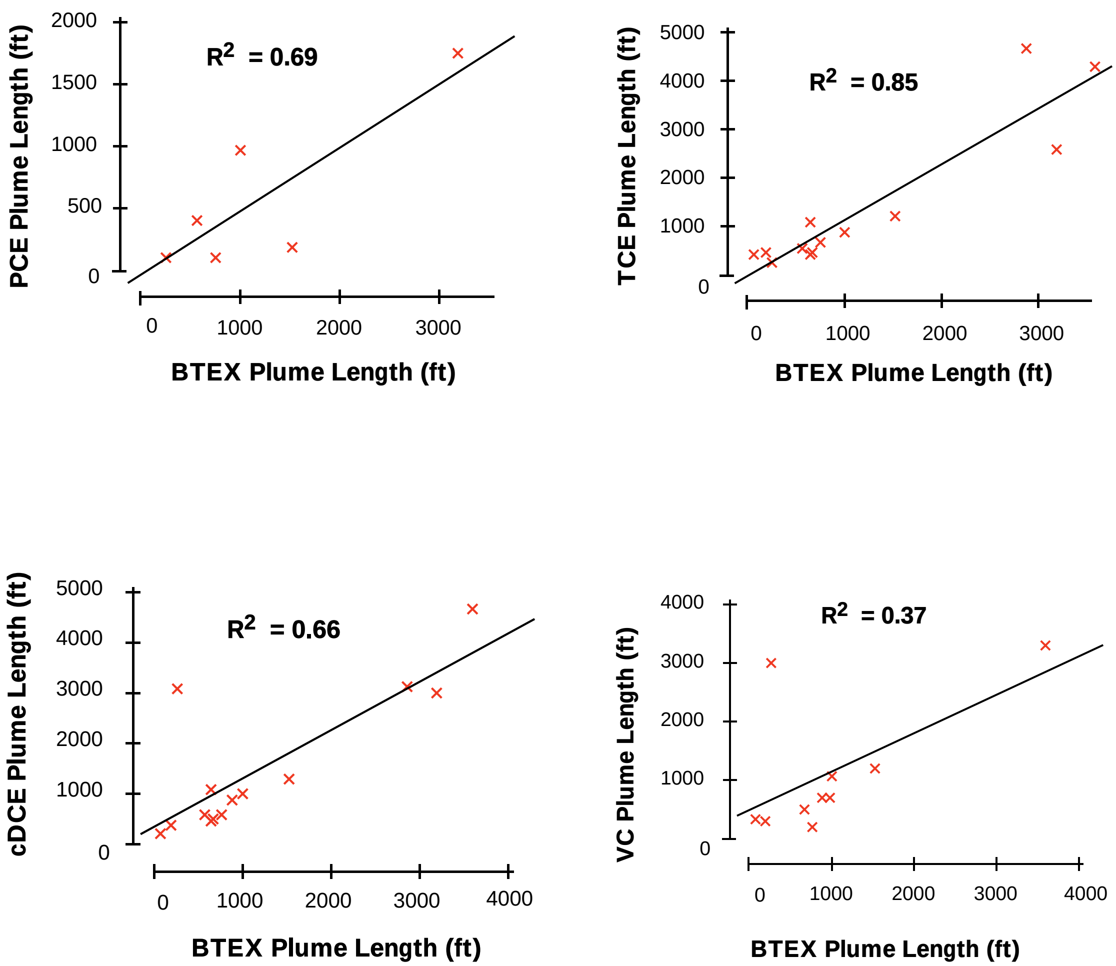


Figure 20. Correlation of Chlorinated Solvent Plume Length with BTEX Plume Length

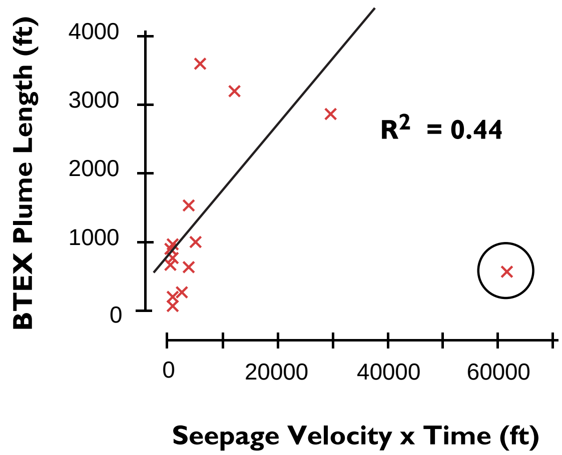


Figure 21. Correlation of BTEX Plume Length with Groundwater Travel Distance

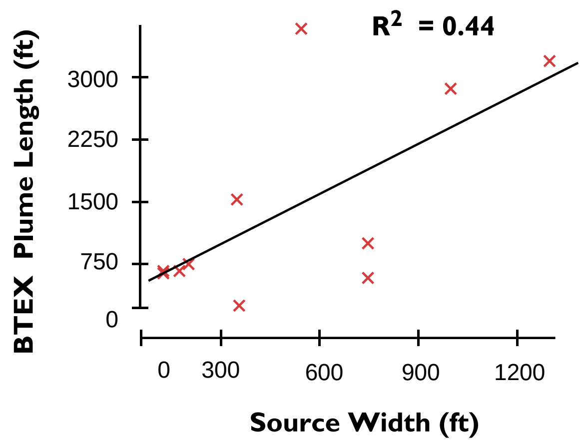
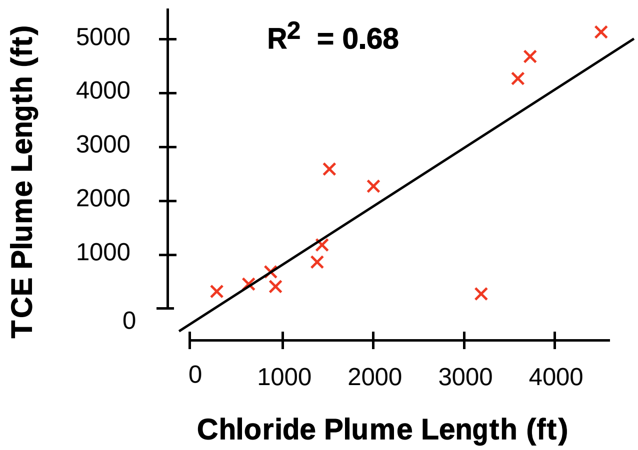
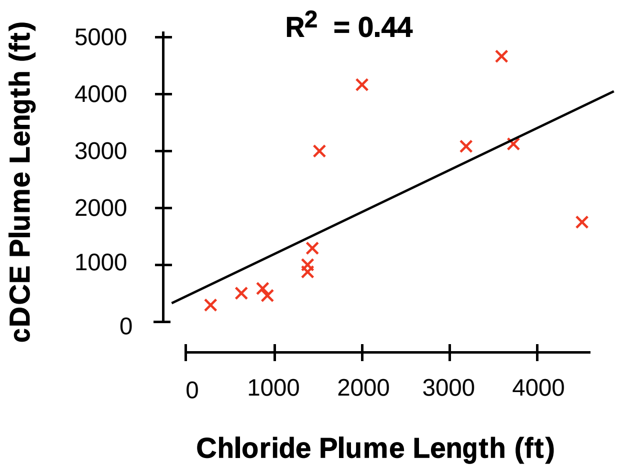


Figure 22. Correlation of BTEX Plume Length with Source Width

4.4 Correlations with Chloride

During reductive dechlorination, chloride ions are released in succession. Thus, elevated levels of chloride ions are indicators of reductive dechlorination. To investigate how chloride plumes compare to chlorinated solvent plumes, chlorinated ethene plume length was plotted vs. chloride plume length as shown in Figure 23. As the solvent plume length increased so did the chloride plume length. However, the chloride plume length was almost always greater than the solvent plume length, as anticipated. Chloride is not retarded and is conservative and thus is expected to be longer than the solvent plume. The chloride plumes are actually longer than the numbers suggest because the detection limit for chloride is higher than for the solvents (e.g., 0.2 mg/L vs. 1 µg/L). The trend of increasing chloride plume length with increasing solvent plume length is linked to advection and plume age.





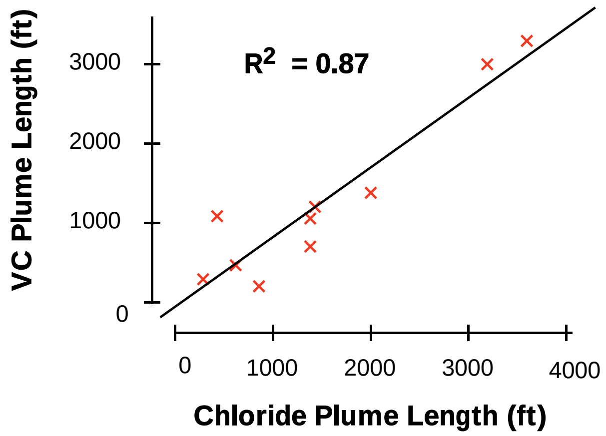


Figure 23. Correlation of Plume Length vs. Chloride Plume Length

4.5 Environmental Effects

Various environmental parameters, such as average groundwater temperature, pH, dissolved oxygen concentrations, and redox potential were plotted versus chlorinated plume length and normalized plume length. Plume length normalization was conducted to remove the effects of groundwater water velocity and plume age. The only environmental factor that was strongly correlated to normalized plume length was the redox potential as shown in Figure 24. As the redox potential decreased, the normalized PCE plume length decreased. This result indicates that redox potential is an important factor for predicting PCE plume lengths, once the effect of advection has been factored out. The normalized TCE plume length was only weakly correlated to redox potential (i.e., R^2=0.14), and VC and cDCE normalized plume lengths were poorly correlated to redox potential, likely because they are degraded under a variety of redox conditions.

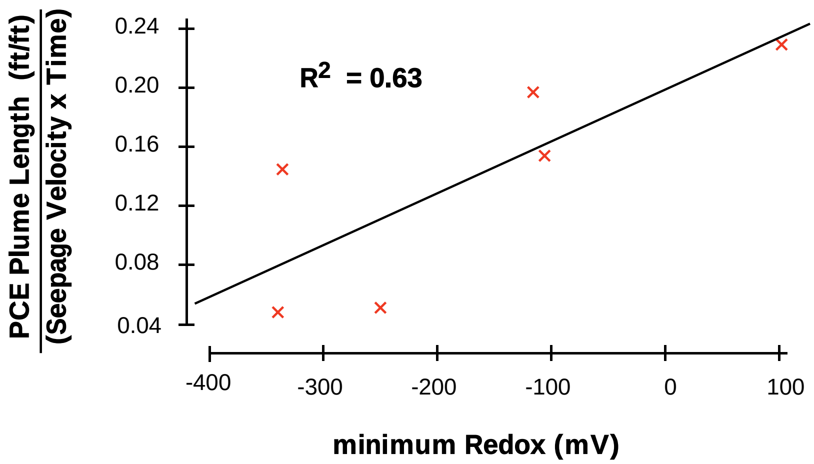


Figure 24. Normalized PCE Plume Length vs. Redox Potential

5.0 RATE CONSTANT ESTIMATION

The analytical model, BIOCHLOR, was used to estimate rate constants for plumes in the BIOCHLOR database. The BIOCHLOR model accounts for the sequential first order decay of chlorinated solvents and accounts for daughter product generation. Rate constants were estimated only for plumes with sufficient centerline concentration data, site data, and information about the original solvent release. Only data from wells with dissolved oxygen concentrations of less than 1 mg/L (i.e., wells deemed anaerobic) were used. A summary of the estimated rate constants can be found in Table 10 and Figure 25. Half-life data can be found in Table 11. For the chlorinated ethenes (i.e., PCE through VC) the median values of the rate constants ranged from 1.1 1/yr to 1.7 1/yr. VC had a slightly higher median rate constant than the other chlorinated ethenes. This result might be attributable to the variety of mechanisms by which VC is degraded (Bradley and Chapelle, 1996; Wiedemeier *et al*., 1999). As a result, the estimated VC reductive dechlorination rate constant may actually be a gross biodegradation rate constant. Table 12 presents laboratory and field-derived rate constants for comparison. Rate constants estimated with the BIOCHLOR model were of similar magnitude to rate constants determined using field data, but were considerably smaller than laboratory derived values with the exception of the VC rate constant (Wiedemeier et al., 1999).

Only a limited number of rate constants could be estimated for TCA and DCA. Rate constants for DCA were estimated where there was no parent TCA present. The reported rate constant for TCA represents a lumped rate constant, incorporating the effects of both abiotic degradation and biodegradation, because of the difficulty in isolating the effect of reductive dechlorination. From the limited data set, it appears that TCA degrades faster than DCA. This result is likely due to both the abiotic and biological degradation of TCA.

Table 10
Rate Constants Summary

Rate Constants (1/yr)

	Minimum	25th Percentile	Median	75th Percentile	Maximum	Mean	n
PCE	0.8	--	**1.1**	--	2.4	1.4	3
TCE	0.3	0.5	**1.2**	2.4	3.2	1.5	10
cDCE	0.1	0.7	**1.2**	2.2	20.9	3.5	9
VC	0.4	0.6	**1.7**	4.9	12.2	3.6	7
TCA	1.6	--	**2.4**	--	3.2	2.4	2
DCA	0.2	--	**0.3**	--	1.2	0.5	3

-- : Insufficent data to calculate

Table 11
Half-Lives Summary

Half Lives (yr)

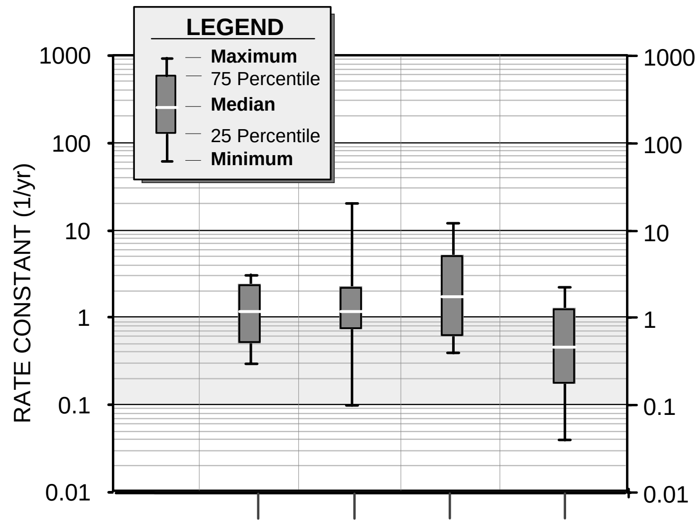
	Minimum	25th Percentile	Median	75th Percentile	Maximum	Mean	n
PCE	0.29	--	**0.63**	--	0.87	0.50	3
TCE	0.22	0.29	**0.58**	1.4	2.3	0.46	10
cDCE	0.03	0.32	**0.58**	1.0	6.9	0.20	9
VC	0.06	0.14	**0.42**	1.1	1.7	0.19	7
TCA	0.22	--	**0.29**	--	0.45	0.29	2
DCA	0.60	--	**2.3**	--	3.9	1.28	3

-- : Insufficent data to calculate

Table 12
Rate Constants Reported in the Literature
(from Wiedemeier et al., 1999)

Rate Constants (1/yr)

	Range of Laboratory-Derived Values	Median Field-Derived Values
PCE	13.9	1.1
TCE	0.04-126	1.1
cDCE	3.15-9.36	
VC	0.01	2.9
TCA	3.6	5.8
DCA	1.6-3.5	



Contaminant	TCE	cDCE	VC	BTEX
Source	This study	This study	This study	Rifai et al., 1998
Number of Sites	10	9	7	23

Figure 25. Biodegradation Rate Constants for Chlorinated Solvents and BTEX

Figure 25 compares the rate constants for dissolved chlorinated solvents estimated in this study to BTEX rate constants estimated by Rifai et al. (1998) in another study. This figure shows that the BTEX rate constants are within the same order of magnitude as the chlorinated solvent rate constants. Although this is a small sample set, it implies that chlorinated solvents may degrade at a similar rate to BTEX compounds under anaerobic conditions. If sufficient electron donor is present, relatively high chlorinated solvent biodegradation rate constants are possible.

6.0 BIODEGRADATION RATE CONSTANT CORRELATIONS

This section reports factors influencing the magnitude of chlorinated ethene first order reductive dechlorination rate constants. These correlations should be viewed as preliminary in nature due to the limited data set available.

6.1 Biodegradation Capacity

The reductive dechlorination rate constants for TCE, c-DCE, and VC correlated well with biodegradation capacity (also known as expressed assimilative capacity). Biodegradation capacity is an estimate of the amount of electron acceptors consumed in the biodegradation of organic compounds (such as BTEX). Higher biodegradation capacity values imply the consumption of large amounts of electron acceptors and suggest more highly reduced conditions. In Figure 26, R^2 values of 0.20 to 0.64 were obtained when correlating solvent rate constants with biodegradation capacity. Higher rate constants were obtained at higher biodegradation capacity values or under more highly reduced conditions. This result is consistent with other studies that have shown chlorinated solvent degradation to be optimum under sulfate-reducing or methanogenic conditions (Bouwer, 1994).

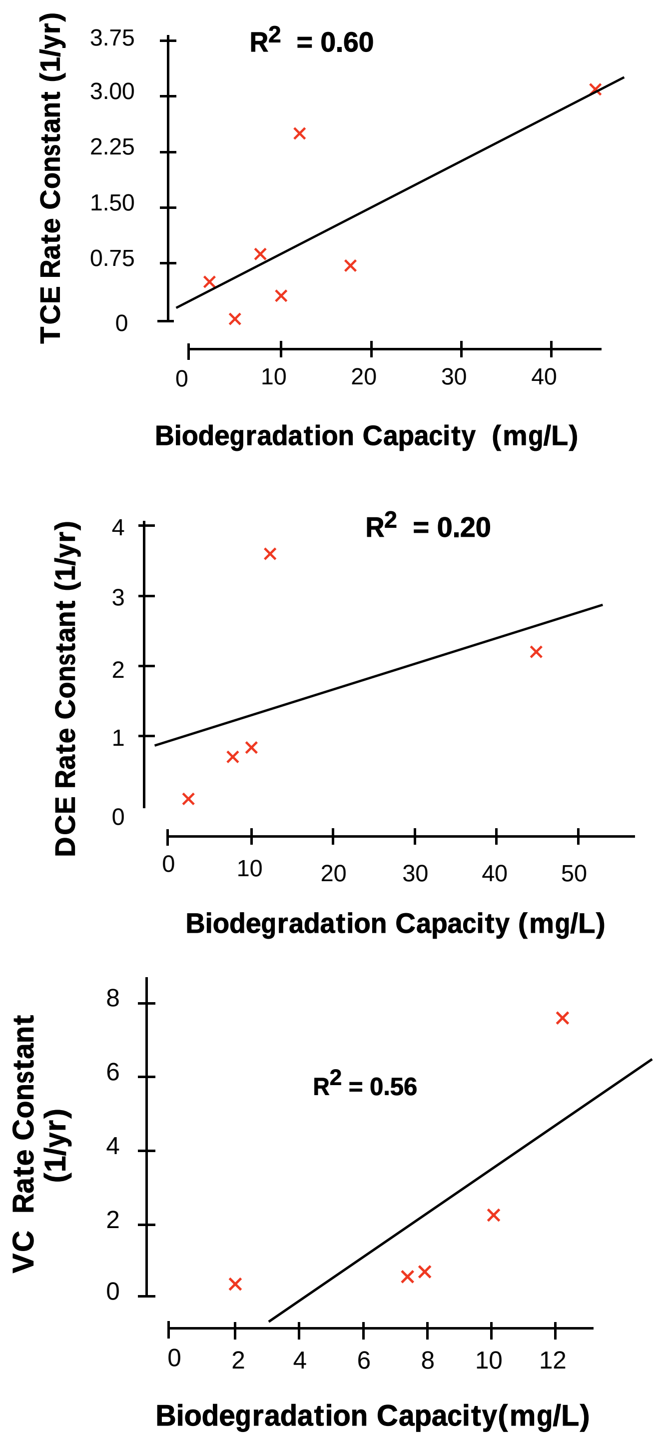


Figure 26. Impact of Biodegradation Capacity on Rate Constants

6.2 Effects of Temperature and Hydrogen Concentration on TCE Rate Constant

Both temperature and dissolved hydrogen concentration were found to have a large impact on the magnitude of the TCE rate constant. As temperature increased, the TCE rate constant increased, with a R^2 of 0.70, as shown in Figure 27. This result suggests that reductive dechlorination may occur more rapidly in warmer climates. However, when the normalized TCE plume length was plotted versus temperature, there was only a weak trend of decreasing normalized plume length with increasing temperature (R^2 of 0.14).

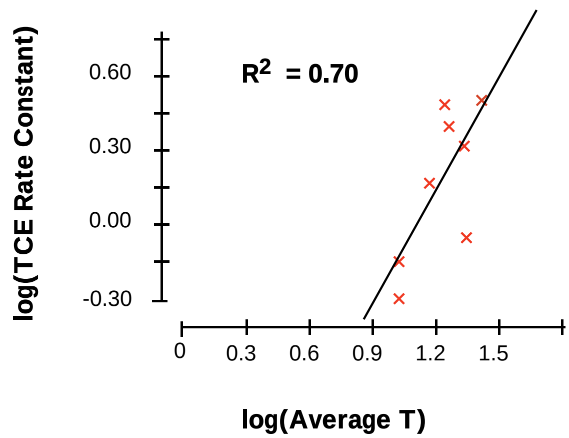


Figure 27. Effect of Temperature on TCE Rate Constant

Another important factor impacting the TCE rate constant is the hydrogen concentration. Hydrogen is used as the electron donor by many dechlorinating bacteria, and the magnitude of the hydrogen concentration has been linked to different redox conditions (Chapelle *et al.*, 1996). In Figure 28, higher hydrogen concentrations are correlated with higher TCE rate constants. One explanation for this trend is that when the hydrogen concentration is higher, the rate constant is larger because the number of dechlorinating bacteria is higher and/or the availability of hydrogen is not limiting the reaction. Due to the limited data available (only 3 points), more information is required to empirically verify this relationship.

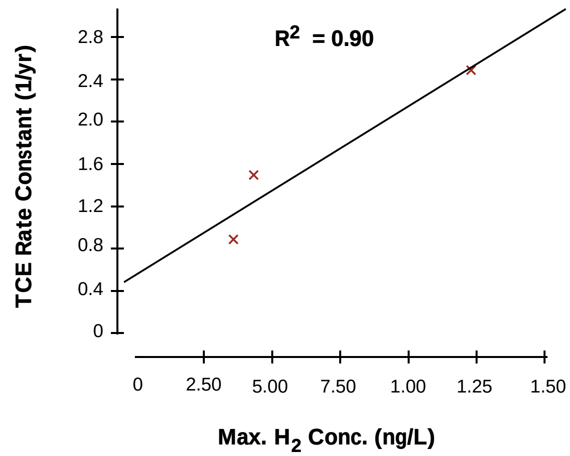


Figure 28. Effect of Hydrogen Concentration on TCE Rate Constant

7.0 OVERALL CONCLUSIONS

Chlorinated Solvent Plume Characteristics

- At sites contaminated with chlorinated ethenes only, TCE or c-DCE was the most likely constituent to have the longest plume at the site. TCE and c-DCE had median plume lengths of 1215 ft and 1205 ft, respectively.
- VC had the shortest median plume length of 860 ft. Because the daughter product plumes were coincident or almost coincident with the parent plumes, these results indicate that vinyl chloride is unlikely to be the longest plume at a site. This is an encouraging result given the relatively high associated carcinogenicity of vinyl chloride. Because laboratory studies report that VC degrades slowly via reductive dechlorination, these results suggest that other degradation mechanisms are at work in degrading vinyl chloride.
- Of the chlorinated ethanes, TCA had a shorter median plume length (865 ft) than 1,1-DCA (1650 ft) and 1,1-DCE (1470 ft). TCA's shorter median plume length is likely due to its degradation by both abiotic and biotic mechanisms.
- C-DCE, VC, and ethene, daughter products of reductive dechlorination, were found at 92%, 79%, and 58% of the sites, indicating that reductive dechlorination is widespread at the sites in this database. The presence of BTEX at 75% of the sites may explain the high incidence of reductive dechlorination.
- Large increases in chloride concentrations within the plume relative to background levels at are further evidence of significant reductive dechlorination.

BTEX Plumes at Chlorinated Solvent Release Sites

- BTEX plumes had a median length of 750 ft, much longer than the 101-180 ft median BTEX plume lengths reported at retail UST sites by other investigators.
- Longer BTEX plumes may be linked to larger source areas or spills or more anaerobic conditions than those typically found at retail UST sites.

Factors Impacting Dissolved Solvent Plume Length

- The plume width in the source area (or source area width) was used to represent the size of the NAPL-affected source area. The product of the source area width and the maximum dissolved phase solvent concentration was strongly correlated with plume length. This finding indicates that source characteristics, including the extent of DNAPL migration, are the most important factors impacting the maximum dissolved chlorinated solvent plume length.
- Chlorinated ethene plume lengths were moderately correlated with seepage velocity and groundwater travel distance, indicating that advection is also an important factor impacting chlorinated solvent plumes. Therefore, the seepage velocity should be accurately determined to predict plume lengths.
- Environmental factors, such as temperature, pH, dissolved oxygen, and redox potential were not strongly correlated with chlorinated ethene plume length. However, there was a strong trend of increasing PCE plume length with increasing redox potential, once the PCE plume length was normalized to remove the effects of advection. These results suggest that source width, source strength, and seepage velocity are more important factors impacting

overall plume length than environmental conditions that are conducive to reductive dechlorination.

Biodegradation Rate Constants and Factors Impacting Rate Constants

- Field-scale biodegradation rate constants were estimated for 35 plumes using the BIOCHLOR model. BIOCHLOR is an analytical model that assumes first order sequential kinetics for reductive dechlorination, thereby accounting for daughter product generation and degradation. The resulting median rate constants and half-lives are shown below for the chlorinated ethenes and chlorinated ethanes. Note that the majority of sites in this database had significant BTEX contamination (an indirect electron donor). These rate constants can be used as literature values in model simulations for anaerobic plumes that are not electron donor-limited.

Constituent	Rate Constant (1/yr)	Half Life (yr)
PCE	1.1	0.63
TCE	1.2	0.58
cDCE	1.2	0.58
VC	1.7	0.40
1,1,1-TCA	2.4	0.29
1,1-DCA	0.3	2.3

- TCE, cDCE and VC rate constants were strongly correlated with biodegradation capacity (i.e., expressed assimilative capacity). TCE rate constants increased with increasing temperature and hydrogen concentration.

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8.0 ACKNOWLEGDMENTS

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- Ms. Ann Smith, formerly of Groundwater Services, Inc. and currently with Radian International, collected data for all Air Force sites.
- Dr. Robert LeGrand of Radian International provided information on 3 sites (sites 7, 8, and 9).
- Mr. Evan Cox, currently with GeoSyntec Consultants, provided information on 5 sites (sites 1, 5, 12, 13, and 15).
- Dr. John Wilson of the USEPA provided data on 3 sites (sites 6, 16, and 22).

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APPENDIX A - SAMPLE QUESTIONNAIRE

CHLORINATED SOLVENT DATA SUMMARY FORM

BIOCHLOR: Intrinsic Remediation Decision Support Tool for Chlorinated Solvents
Air Force Center for Environmental Excellence (AFCEE)

Optimal Criteria for Chlorinated Database Sites

This data questionnaire was developed to evaluate sites contaminated with chlorinated ethenes and ethanes in order to develop predictive biodegradation relationships for the BIOCHLOR Natural Attenuation model. Optimal sites have a single, homogeneous contaminated unit, well characterized in terms of parent compounds, daughter products, electron acceptors/metabolic by-products, and fermentation substrates.

A. SITE INFORMATION

1. Facility *(optional)* : Private Landfill #1
2. City: Farmington
3. State: NH
4. Site Name *(optional)* :

References: Cox et al., 1996 and 1997; Edwards and Cox 1997

B. SOURCE INFORMATION

Provide source information on principal release associated with major contaminant plume(s):

5. Site Process (e.g., fire training, refueling, impoundment): Waste Disposal
6. Chemicals Used in Process: (mark with x)
   - Solvents/Degreasers: X
   - JP - Jet Fuels:
   - Gasoline:
   - Diesel:
   - Other: X
   - Describe "other": TEX
7. Initial Chemical Release Date (yr): 1969
8. Chemical Release Conclusion Date (yr): 1984
9. Chemical Volume Released (gal): Unknown

C. SITE CHARACTERIZATION

Geologic and Hydrogeologic Conditions

Identify Geologic characteristics of aquifer with affected groundwater plume.

10. Using USCS Letter Symbols, identify geologic characteristics of major contaminated unit:

Depth Interval (ft; BGS): From: 0 To: 75

USCS Classification: SM
(or other descriptor such as fractured bedrock)

11. Depth to Groundwater (BGS, ft): Average: 25

Provide hydrogeologic information on aquifer with affected groundwater plume.

12. Seepage Velocity (*Vs*; ft/yr): 182.0
13. Hydraulic Conductivity (*K*; cm/s):
14. Hydraulic Gradient (*i*; ft/ft): 0.020
15. Effective Porosity (*n*; dim.):
16. Saturated Thickness (*b*; ft): <50
17. Soil Bulk Density (ρ ; kg/L):
18. Fraction Organic Carbon (*foc*; dim.): <0.03
19. Retardation Factor (*R* , dim):

Unified Soil Classification System

MAJOR DIVISIONS	GRAPHIC SYMBOL	LETTER SYMBOL	TYPICAL DESCRIPTIONS
CLEAN GRAVEL (LITTLE OR NO FINES)		GW	Well-graded gravels, gravel-sand mixtures, little or no fines
		GP	Poorly-graded gravels, gravel-sand mixtures, little or no fines
GRAVELS WITH FINES (APPRECIABLE AMOUNT OF FINES)		GM	Silty gravels, gravel-sand-silt mixtures
		GC	Clayey gravels, gravel-sand-clay mixtures
CLEAN SAND (LITTLE OR NO FINES)		SW	Well-graded sands, gravelly sands, little or no fines
		SP	Poorly-graded sands, gravelly sands, little or no fines
SANDS WITH FINES (APPRECIABLE AMOUNT OF FINES)		SM	Silty sands, sand-silt mixtures
		SC	Clayey sands, sand-clay mixtures
SILTS AND CLAYS LIQUID LIMIT LESS THAN 50%		ML	Inorganic silts and very fine sands, rock flour, silty or clayey fine sands or clayey silts with slight plasticity
		CL	Inorganic clays of low to medium plasticity, gravelly clays, sandy clays, silty clays, lean clays
		OL	Organic silts and organic silty clays of low plasticity
SILTS AND CLAYS LIQUID LIMIT GREATER THAN 50%		MH	Inorganic silts, micaceous or diatomaceous fine sand or silty soils
		CH	Inorganic clays or high plasticity, fat clays
		OH	Organic clays of medium to high plasticity, organic silts
HIGHLY ORGANIC SOILS		PT	Peat, humus, swamp soils with high organic contents

CHLORINATED SOLVENT DATA SUMMARY FORM

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Air Force Center for Environmental Excellence (AFCEE)

Affected Groundwater

Characterize extent of LNAPL and DNAPL zones (if present), and indicate whether recovery efforts have been implemented.

20. Identify whether LNAPL or DNAPL is present:	both	(Indicate "LNAPL", "DNAPL", or "NA")
Provide dimensions of LNAPL/DNAPL zone (if present):		
Affected length, parallel to groundwater flow (ft):		difficult to assess distribution given disposal nature, multi-sourc
Affected width, perpendicular to groundwater flow (ft):		
Affected thickness (ft):		
21. Maximum plume width in source zone (ft):		(325'@ 1 mg/L, 750' at max width)
22. Has NAPL recovery effort been implemented? Yes/No	No	
Date recovery commenced:		
Date recovery ended:		(Indicate if operation is "ongoing")
23. Has groundwater remediation system been installed? Yes/No	No	
Date system operation commenced:		
Date system operation ended:		(Indicate if operation is "ongoing")
Groundwater remediation method: (mark with an x)		
• Pump & treat		
• Air sparging		
• Air sparging w/SVE		
• Other		
• Describe "other"		

Characterize extent of affected plume for the following chlorinated ethenes and ethanes and their respective daughter products.

	PCE	TCA
Plume maximum length, parallel to gw flow (ft):	970	
Plume maximum width, perpendicular to gw flow (ft):	770	
Plume maximum thickness (ft):	50	

	TCE	1,1 - DCA
Plume maximum length, parallel to gw flow (ft):	860	
Plume maximum width, perpendicular to gw flow (ft):	820	
Plume maximum thickness (ft):	50	

	cis-DCE	1,1 - DCE
Plume maximum length, parallel to gw flow (ft):	990	
Plume maximum width, perpendicular to gw flow (ft):	840	
Plume maximum thickness (ft):	50	

	trans-DCE	Chloroethane
Plume maximum length, parallel to gw flow (ft):		
Plume maximum width, perpendicular to gw flow (ft):		
Plume maximum thickness (ft):		

	Vinyl Chloride	Ethane
Plume maximum length, parallel to gw flow (ft):	1080	
Plume maximum width, perpendicular to gw flow (ft):	960	
Plume maximum thickness (ft):	50	

	Ethene	Dichloromethane	Acetic Acid
Plume maximum length, parallel to gw flow (ft):	600	880	950
Plume maximum width, perpendicular to gw flow (ft):	600	920	600
Plume maximum thickness (ft):	50	50	50

	Chloride
Plume maximum length, parallel to gw flow (ft):	1400
Plume maximum width, perpendicular to gw flow (ft):	650
Plume maximum thickness (ft):	

	BTEX
Plume maximum length, parallel to gw flow (ft):	1000
Plume maximum width, perpendicular to gw flow (ft):	500
Plume maximum thickness (ft):	50

PCE = Tetrachloroethene
TCE = Trichloroethene
cis-DCE = cis-1,2-Dichloroethene
trans-DCE = trans-1,2-Dichloroethene

TCA = Trichloroethane
DCA = Dichloroethane
BTEX = Total benzene, toluene, ethylbenzene, xylenes
Other fermentation substrates = acetone, methanol, etc.

CHLORINATED SOLVENT DATA SUMMARY FORM

BIOCHLOR: Intrinsic Remediation Decision Support Tool for Chlorinated Solvents
Air Force Center for Environmental Excellence (AFCEE)

D. SITE SPECIFIC GROUNDWATER PARAMETERS

Observed Groundwater Concentrations

Provide concentrations for constituents of concern along the plume centerline for i) a minimum of 1 and a maximum of 3 background well locations, and ii) a minimum of 5 and a maximum of 10 monitoring well locations.
Alternativ ely, include all well location maps, concentration isopleths and data tables for chlorinated solvents, electron donors and acceptors, metabolic by-products, and water quality parameters associated with the groundwater contaminant plume area.

	Observed Constituent Concentration				
	First Background Well	First Observation Well	Second Observation Well	Third Observation Well	Fourth Observation Well
Well No.:	SW106A	OW101	SW103	MW6	SW104S
Sample Date (mo/yr):	11/95	1/96	11/95	1/96	1/96
Distance from Source* (ft):	-750	0	85	250	320
Distance off Plume Centerline (ft):	0	0	100	30	130
Depth to Center of Screened Interval (ft BGS):	18	44	68	27	46
Observed LNAPL or DNAPL? Yes/No	No	No	No	No	No
DNAPL or LNAPL?					
Thickness (ft)					
Chlorinated Compounds					
Tetrachoroethene (PCE, mg/L):	<0.005	<0.025	<1	0.034	1.8
Trichloroethene (TCE, mg/L):	<0.005	0.17	<1	0.45	<0.025
cis-1,2-Dichloroethene (cis-DCE, mg/L):	<0.005	22	29	5.2	7.75
trans-1,2-Dichloroethene (trans-DCE, mg/L):					
Vinyl Chloride (VC, mg/L):	<0.01	0.23	<2	<0.05	0.19
Trichloroethane (TCA, mg/L):	<0.005	0.061	<1	0.03	0.12
Dichloroethane (DCA, mg/L):	<0.005	<0.025	<1	0.44	0.086
1,1-Dichloroethene (1,1-DCE, mg/L):	<0.005	<0.025	<1	<0.025	<0.025
Chloroethane (CA, mg/L):	<0.01	<0.05	<2	0.068	<0.05
Electron Acceptors/Metabolic By-Products					
Dissolved Oxygen (DO, mg/L):	8.8	0.5	0.6	0.5	3.3
Sulfate (SO_4^{2-}, mg/L):	5	ND	7	5	8
Nitrate (NO_3-, mg/L):	0.16	0.04	0.05	<0.01	ND
Ferrous/Total Iron (Fe II, mg/L):	0.02	248	210	310	168
Methane (mg/L):	<0.0001	1.452	NA	7.323	0.7567
Ethene (mg/L):	<0.0001	<0.0001	NA	<0.0001	<0.0001
Ethane (mg/L):	<0.0001	<0.0001	NA	<0.0001	<0.0001
Potential Fermentation Substrates					
Acetic Acid (mg/L):	18	210	82	280	160
Benzene (mg/L):	<0.005	<0.025	<1	<0.025	<0.025
Toluene (mg/L):	<0.005	1.7	5	0.96	1.8
Ethylbenzene (mg/L):	<0.005	0.16	1	0.12	0.445
Xylenes (mg/L):	<0.005	0.57	3.7	0.64	1.7
Acetone (mg/L):	<0.01	0.43	<4	0.59	0.335
Dichloromethane (mg/L)	<0.005	1.3	<1	7.6	0.075
Water Quality Parameters					
Chloride (mg/L):	1.7	157	150	78.2	82.2
Redox Potential (mV):	282	22	-56.9	-43.1	-52
Total Organic Carbon (TOC, mg/L):	0.5	70.2	176	300	178
pH:	6.9	6.4	6.4	6.1	6.1
Alkalinity (mg/L):	24	355	288	424	284
Temperature (°C):	8	9.5	10.4	12	10
TPH (mg/L):					
Dissolved H_2 (mg/L):					

** Assume "Source" is center of confirmed or suspected NAPL zone or area of highest dissolved contamination.*

CHLORINATED SOLVENT DATA SUMMARY FORM

BIOCHLOR: Intrinsic Remediation Decision Support Tool for Chlorinated Solvents
Air Force Center for Environmental Excellence (AFCEE)

Observed Groundwater Concentrations cont'd

Observed Constituent Concentration *(cont'd from previous page)*

	Fifth Observation Well	Sixth Observation Well	Seventh Observation Well	Seventh Observation Well	Eighth Observation Well
Well No.:	MW2A	MW303D	MW5	MW304D	MW301D
Sample Date (mo/yr):	1/96	12/95	1/96	12/95	12/95
Distance from Source* (ft):	360	480	680	850	1060
Distance off Plume Centerline (ft):	230	150	40	140	0
Depth to Center of Screened Interval (ft BGS):	48	72	36	59	50
Observed LNAPL or DNAPL? Yes/No	No	No	No	No	No
DNAPL or LNAPL?					
Thickness (ft)					
Chlorinated Compounds					
Tetrachoroethene (PCE, mg/L):	ND	<0.042	<0.025	0.011	<0.005
Trichloroethene (TCE, mg/L):	ND	<0.042	<0.025	<0.007	0.008
cis-1,2-Dichloroethene (cis-DCE, mg/L):	3	1.1	0.95	0.12	0.16
trans-1,2-Dichloroethene (trans-DCE, mg/L):					
Vinyl Chloride (VC, mg/L):	ND	1.3	0.21	0.14	<0.01
Trichloroethane (TCA, mg/L):	ND	<0.042	0.11	<0.007	<0.005
Dichloroethane (DCA, mg/L):	ND	<0.042	<0.025	<0.007	<0.005
1,1-Dichloroethene (1,1-DCE, mg/L):	ND	<0.042	<0.025	<0.007	<0.005
Chloroethane (CA, mg/L):	ND	<0.083	<0.05	<0.014	<0.01
Electron Acceptors/Metabolic By-Products					
Dissolved Oxygen (DO, mg/L):	5	0.3	3.6	9.2	6
Sulfate (SO_4^{2-}, mg/L):	6	NA	ND	ND	10
Nitrate (NO_3^-, mg/L):	ND	NA	ND	0.01	4.2
Ferrous/Total Iron (Fe II, mg/L):	203	NA	73.9	88	<0.1
Methane (mg/L):	8.269	1.2654	0.662	NA	0.0004
Ethene (mg/L):	0.025	0.9058	0.0044	NA	<0.0001
Ethane (mg/L):	<0.0001	<0.0001	<0.0001	NA	<0.0001
Potential Fermentation Substrates					
Acetic Acid (mg/L):	150	NA	33	NA	<1
Benzene (mg/L):	ND	<0.042	<0.025	<0.007	<0.005
Toluene (mg/L):	1.1	0.96	0.35	0.16	<0.005
Ethylbenzene (mg/L):	ND	0.2	0.061	0.02	<0.005
Xylenes (mg/L):	0.32	0.81	0.25	0.06	<0.005
Acetone (mg/L):	0.45	0.12	0.11	<0.014	<0.01
Dichloromethane (mg/L):	<0.025	<0.042	<0.025	<0.005	<0.005
Water Quality Parameters					
Chloride (mg/L):	72.7	NA	26.5	16.9	17.6
Redox Potential (mV):	-112.5	-97.3	-116	-82	257
Total Organic Carbon (TOC, mg/L):	133	NA	28.8	28.1	1.2
pH:	6.6	6.3	6.5	6.6	7.6
Alkalinity (mg/L):	249	NA	124	122	42
Temperature (°C):	14.2	8.8	10.4	9.9	8.3
TPH (mg/L):					
Dissolved H_2 (mg/L):					

** Assume "Source" is center of confirmed or suspected NAPL zone or area of highest dissolved contamination.*

APPENDIX B – DETAILED SUMMARY OF BIOCHLOR DATABASE

TABLE B-1
STATISTICAL ANALYSIS OF CHLORINATED SITE DATA

BIOCHLOR: Chlorinated Solvent Plume Database
Air Force Center for Environmental Excellence (AFCEE)

FACILITY INFORMATION

Facility/Site Name	State	Site Process	Chemicals Used in Process	Chemical Release Date Initial	Chemical Release Date Final	Time Since Release (yrs)
1. Aerojet Superfund Site	California	Septic Waste	Solvents/Degreasers/Septage	1960	1977	34
2. Altus AFB/LF-04	Oklahoma	Landfill	Paint Wastes	1956	1983	41
3. Cape Canaveral AS/CCFTA-2	Florida	Fire Training Area	Solvents/Degreasers/JP Fuels	1965	1985	31
4. Cape Canaveral AS/Facility 1381	Florida	Missile Technology	Solvents/Degreasers/Waste Acids	1968	1989	28
5. Chemical Distribution Facility	Oregon	Chem Distribution	Solvents/Degreasers/TEX	1979	1985	17
6. Chemical Manufacturer/Waste Site	Michigan	Chemical Refining/Incineration	Solvents/Degreasers/Chemical Waste	1969	1980	27
7. Chlorinated Site #1/Hanger	Alaska	FTA Hanger	Solvents/Degreasers/JP Fuels/Gasoline	1940	1980	53
8. Chlorinated Site #2/Tank Farm	Alabama	Refueling Tank Farm	Solvents/Degreasers/JP Fuels	1961	1983	34
9. Chlorinated Site #3/Junkyard	Alabama	Junkyard	Solvents/Degreasers/Gasoline			
10. Eielson AFB/Site 45/57	Alaska	Fire Training and Photo Lab	Solvents/Degreasers/Photo Chemicals			
11. Hill AFB/OU-5	Utah	Engine service/repair	Solvents/Degreasers/Gasoline/Sodium Cyanide	1942	1979	54
12. Industrial Facility/Plume 1	Ontario	Metal Manufacturing	Solvents/Degreasers	1940	1989	56
13. Industrial Facility/Plume 2	Ontario	Metal Manufacturing	Solvents/Degreasers	1940	1989	56
14. Kelly AFB/MP Site	Texas	Metal Plating Shop	Solvents/Degreasers/Metals	1970	1981	27
15. Landfill #1	New Hampshire	Waste Disposal	Solvents/Degreasers/TEX	1969	1984	27
16. Landfill #2/VC Site	Maryland	Landfill	Ag/Munic/Ind Wastes, PVC	1960	1981	37
17. Offutt AFB/Bldg. 301	Nebraska	Acid Pit & Manufacturing	Solvents/Acids	1942	1965	54
18. Offutt AFB/FPTA3	Nebraska	Fire Training Area	Solvents/Degreasers/JP Fuels	1960	1990	34
19. Plattsburgh AFB/FT-002	New York	Fire Training Area	Solvents/Degreasers/JP Fuels/waste oil	1955	1989	41
20. Sterling/OW-31/OW-41	Texas	Pond/Sewer	Solvents/Degreasers/Gasoline/Diesel/VC	1950	1960	41
21. Sterling/Unit K	Texas	Solid Waste Management Unit	Solvents/Degreasers/Gasoline/Diesel	1950	1982	46
22. USCG Site	North Carolina	Solvent Disposal	Solvents/Degreasers/Ind. Wastes	1958		39
23. Westover ARB/FT-03	Massachusetts	Fire Training Area	Solvents/Degreasers/JP Fuels	1940	1964	55
24. Westover ARB/FT-08	Massachusetts	Fire Training Area	Solvents/Degreasers/JP Fuels	1964	1986	31

Note:

1. Data on Sites 1, 5, 12, 13, and 15 provided by Beak International Incorporated. Data on Sites 7, 8, and 9 provided by Radian International LLC. Data on Sites 6, 16, and 22 provided by USEPA. Data on remaining sites provided by Air Force Center for Environmental Excellence (AFCEE).
2. The time since release is the time the data were collected minus the initial release date.

TABLE B-1
STATISTICAL ANALYSIS OF CHLORINATED SITE DATA

BIOCHLOR: Chlorinated Solvent Plume Database
Air Force Center for Environmental Excellence (AFCEE)

SITE HYDROGEOLOGIC CONDITIONS

	Saturated Unit			**Avg. Depth to GW**	**Seepage**	**Hydraulic**	**Hydraulic**	**Effective**	**Saturated**	**Soil Bulk**	**Fraction Organic**
Facility/Site Name	**From (ft; BGS)**	**To (ft; BGS)**	**USCS Classification**	**(ft; BGS)**	**Velocity (ft/yr)**	**Conductivity (cm/s)**	**Gradient (ft/ft)**	**Porosity (dim.)**	**Thickness (ft)**	**Density (kg/L)**	**Carbon (dim.)**
1. Aerojet Superfund Site	0.0	90.0	SM	50.0	1287.5	2.50E-02	0.015	0.30	40	1.60	1.00E-03
2. Altus AFB/LF-04	5.0	35.0	CL	8.0	731.3	7.10E-03	0.003	0.03	30	1.40	1.50E-03
3. Cape Canaveral AS/CCFTA-2	5.0	60.0	SW	5.0	111.2	1.80E-02	0.001	0.20	55	1.60	1.84E-03
4. Cape Canaveral AS/Facility 1381	0.0	50.0	SW	7.0	76.1	3.13E-02	0.001	0.25	45	1.72	4.55E-03
5. Chemical Distribution Facility	0.0	30.0	SM	10.0	20.0	5.00E-03	0.001		20		
6. Chemical Manufacturer/Waste Site	0.0	40.0	SP	25.0	448.1	8.70E-03	0.015	0.30	15		
7. Chlorinated Site #1/Hanger	0.0	75.0	SM	42.0	1129.7	2.00E-01	0.002	0.31	20	1.81	4.00E-03
8. Chlorinated Site #2/Tank Farm	10.0	24.0	ML	20.5	142.3	5.92E-02	0.001	0.30	55		
9. Chlorinated Site #3/Junkyard	10.0	50.0	GM	26.0	7.4	2.16E-03	0.001	0.30	35		
10. Eielson AFB/Site 45/57	10.0	400.0	SW	6.5	47.8	1.76E-02	0.001	0.38	390	1.60	4.50E-03
11. Hill AFB/OU-5	0.0	80.0	SM	20.0	125.1	8.10E-04	0.030	0.20	60	1.65	7.90E-04
12. Industrial Facility/Plume 1	0.0	16.0	SM	6.0	8.4	7.00E-05	0.035	0.30	10		
13. Industrial Facility/Plume 2	0.0	16.0	SM	6.0	8.4	7.00E-05	0.035	0.30	10		3.00E-04
14. Kelly AFB/MP Site	20.0	40.0	GC	20.0	824.0	2.00E-01	0.001	0.25	40	1.60	
15. Landfill #1	0.0	75.0	SM	25.0	182.0		0.020		50		3.00E-02
16. Landfill #2/VC Site	15.0	90.0	saprolite	40.0	57.7	2.80E-04	0.040	0.20	40		
17. Offutt AFB/Bldg. 301	62.0	92.0	SP/CL	52.5	32.0	3.88E-03	0.002	0.25	30	1.65	2.40E-04
18. Offutt AFB/FPTA3	8.0	21.0	SM	8.0	10.4	3.35E-03	0.001	0.20	100	1.65	7.00E-04
19. Plattsburgh AFB/FT-002	0.0	90.0	SM	45.0	140.8	4.10E-03	0.010	0.30	45	1.60	5.50E-03
20. Sterling/OW-31/OW-41	7.0	31.0	SM/SC/ML	6.0	10.7	1.85E-03	0.001	0.25	24		6.80E-03
21. Sterling/Unit K	15.0	43.0	SM	5.0	2.9	3.46E-04	0.002	0.25	28		6.80E-03
22. USCG Site	0.0	60.0	SM	2.0	32.0	8.00E-03	0.001		58		
23. Westover ARB/FT-03	42.0	80.0	SM	42.0	62.8	1.22E-03	0.010	0.20	38	1.65	1.00E-06
24. Westover ARB/FT-08	0.0	80.0	SM	7.0	18.8	2.54E-03	0.002	0.25	73	1.75	1.85E-03
			max	52.5	1287.5	2.00E-01	0.040	0.38	390	1.81	3.00E-02
			75th percen.	29.5	152.2	1.78E-02	0.015	0.30	55	1.65	4.79E-03
			median	**15.0**	**60.3**	**4.10E-03**	**0.002**	**0.25**	**40**	**1.65**	**1.85E-03**
			25th percen.	6.4	16.8	1.54E-03	0.001	0.20	27	1.60	7.68E-04
			min	2.0	2.9	7.00E-05	0.001	0.03	10	1.40	1.00E-06
			Average	20.2	229.9	2.61E-02	0.010	0.25	55	1.64	4.40E-03
			n	24	24	23	24	21	24	13	16

Note:
1. Soil and aquifer characteristics identified for major contaminated unit.

TABLE B-1
STATISTICAL ANALYSIS OF CHLORINATED SITE DATA

BIOCHLOR: Chlorinated Solvent Plume Database
Air Force Center for Environmental Excellence (AFCEE)

EXTENT OF LNAPL/DNAPL CONTAMINATION, AND NAPL/GROUNDWATER REMEDIATION EFFORTS

	LNAPL or DNAPL				NAPL Recovery Dates		Groundwater Remediation System Operation		
Facility/Site Name	**Observed**	**Length (ft)**	**Width (ft)**	**Max Thickness (ft)**	**Commenced**	**Ended**	**System**	**Commenced**	**Ended**
1. Aerojet Superfund Site	DNAPL								
2. Altus AFB/LF-04	NA								
3. Cape Canaveral AS/CCFTA-2	LNAPL	275	400	1			Air Sparging	1996	Ongoing
4. Cape Canaveral AS/Facility 1381	NA								
5. Chemical Distribution Facility	DNAPL/LNAPL								
6. Chemical Manufacturer/Waste Site	LNAPL	430	125	5					
7. Chlorinated Site #1/Hanger									
8. Chlorinated Site #2/Tank Farm	NA						AS/SVE		
9. Chlorinated Site #3/Junkyard	NA								
10. Eielson AFB/Site 45/57	NA								
11. Hill AFB/OU-5	NA						Air Sparging	1997	
12. Industrial Facility/Plume 1	DNAPL								
13. Industrial Facility/Plume 2	DNAPL								
14. Kelly AFB/MP Site	LNAPL						Pump and Treat	1995	Ongoing
15. Landfill #1	DNAPL/LNAPL								
16. Landfill #2/VC Site	NA								
17. Offutt AFB/Bldg. 301	NA						LVDPE	1996	1996
18. Offutt AFB/FPTA3	res. LNAPL								
19. Plattsburgh AFB/FT-002	LNAPL	1100	400	10	1993	Ongoing	Pump and Treat		
20. Sterling/OW-31/OW-41	NA								
21. Sterling/Unit K	DNAPL	220	270	48					
22. USCG Site	NA								
23. Westover ARB/FT-03	NA								
24. Westover ARB/FT-08	NA								

TABLE B-1
STATISTICAL ANALYSIS OF CHLORINATED SITE DATA

BIOCHLOR: Chlorinated Solvent Plume Database
Air Force Center for Environmental Excellence (AFCEE)

AFFECTED GROUNDWATER PLUME CHARACTERISTICS

Facility/Site Name	Chlorinated Plume Width at Source (ft)	PCE Plume Characteristics			TCE Plume Characteristics			cis-DCE Plume Characteristics		
		Length (ft)	**Width (ft)**	**Thickness (ft)**	**Length (ft)**	**Width (ft)**	**Thickness (ft)**	**Length (ft)**	**Width (ft)**	**Thickness (ft)**
1. Aerojet Superfund Site	560				2300	2300	25	4200	3000	25
2. Altus AFB/LF-04	1000				4700	1625		3125	1100	
Cape Canaveral AS/CCFTA-2	350	175 3.	140	20	1225	610	56	1310	750	56
4. Cape Canaveral AS/Facility 1381	360	100	200		250	350		3100	2350	10
5. Chemical Distribution Facility	460	1110	1215	20	1215	570	20	1440	585	20
6. Chemical Manufacturer/Waste Site	1300	1760	1060		2600	1600		3000	1000	
7. Chlorinated Site #1/Hanger	750	400	750	30	520	700	30	560	790	30
8. Chlorinated Site #2/Tank Farm	560	1250	370		1275	600				
9. Chlorinated Site #3/Junkyard	1200	1420	1520		1540	1620				
10. Eielson AFB/Site 45/57	122				1100	480		1100	480	
11. Hill AFB/OU-5	858				5180	1400	55	1750	420	36
12. Industrial Facility/Plume 1					400	220	10	200	225	10
13. Industrial Facility/Plume 2					450	185	10	360	260	10
14. Kelly AFB/MP Site	1200	13700	10100	35	11900	9100	35	9400	8300	35
15. Landfill #1	750	970	770	50	860	820	50	990	840	50
16. Landfill #2/VC Site	620									
17. Offutt AFB/Bldg. 301	490				3300	1050	40	3100	750	40
18. Offutt AFB/FPTA3	170				450	140	20	480	85	20
Plattsburgh AFB/FT-002	550	19.			4300	1250		4670	1500	
20. Sterling/OW-31/OW-41										
21. Sterling/Unit K								850	250	28
22. USCG Site	75	280	210		280	210		270	200	
23. Westover ARB/FT-03	120				380	150	38	450	310	38
Westover ARB/FT-08	200	100 24.	90	35	660	380	79	560	250	35
max	1300	13700	10100	50	11900	9100	79	9400	8300	56
75th percen.	777	1335	1138	35	2600	1400	50	3100	1025	37
median	**555**	**970**	**750**	**33**	**1215**	**610**	**35**	**1205**	**668**	**30**
25th percen.	313	228	205	23	450	350	20	540	258	20
min	75	100	90	20	250	140	10	200	85	10
Average	585	1933	1493	32	2137	1208	36	2046	1172	30
n	20	11	11	6	21	21	13	20	20	15

Note:
1. The widest chlorinated solvent plume in the source area was used to determine the source width. It was delineated to the lowest concentration reported .

TABLE B-1
STATISTICAL ANALYSIS OF CHLORINATED SITE DATA

BIOCHLOR: Chlorinated Solvent Plume Database
Air Force Center for Environmental Excellence (AFCEE)

AFFECTED GROUNDWATER PLUME CHARACTERISTICS CONT'D

	trans-DCE Plume Characteristics			VC Plume Characteristics			Ethene Plume Characteristics			Chloride Plume Characteristics		
Facility/Site Name	**Length (ft)**	**Width (ft)**	**Thickness (ft)**	**Length (ft)**	**Width (ft)**	**Thickness (ft)**	**Length (ft)**	**Width (ft)**	**Thickness (ft)**	**Length (ft)**	**Width (ft)**	**Thickness (ft)**
1. Aerojet Superfund Site				1400	1100	25	990	730	25	2000	2000	
2. Altus AFB/LF-04	2750	875								3750	1500	
3. Cape Canaveral AS/CCFTA-2	1190	140	20	1225	875	20	1155	490	20	1435	840	20
4. Cape Canaveral AS/Facility 1381	1890	1320		3000	1800	10	1500	570		3200	600	
5. Chemical Distribution Facility				1395	540	20						
6. Chemical Manufacturer										1520	400	
7. Chlorinated Site #1												
8. Chlorinated Site #2												
9. Chlorinated Site #3												
10. Eielson AFB/Site 45/57	1200	300					410	170				
11. Hill AFB/OU-5										4520	2950	
12. Industrial Facility/Plume 1				325	280	10	120	200	10			
13. Industrial Facility/Plume 2				270	450	10	210	130	10			
14. Kelly AFB				860	1370	25						
15. Landfill #1				1080	960	50	600	600	50	1400	650	
16. Landfill #2				1100	730					420	340	
17. Offutt AFB/Bldg. 301												
18. Offutt AFB/FPTA3				470	200	20	320	115	20	600	435	20
19. Plattsburgh AFB/FT-002				3300	1250					3600		
20. Sterling/OW-31/OW-41				700	200	24	1100	700	24			
21. Sterling/Unit K				690	280	28	700	400	28	1400	480	28
22. USCG Site				265	90					270	270	
23. Westover ARB/FT-03										900	400	38
24. Westover ARB/FT-08	440	110	35	180	120	35	320	100		850	240	35
max	2750	1320	35	3300	1800	50	1500	730	50	4520	2950	38
75th percen.	1890	875	31	1310	1030	26	1045	585	26	2900	840	35
median	**1200**	**300**	**28**	**860**	**540**	**22**	**600**	**400**	**22**	**1418**	**480**	**28**
25th percen.	1190	140	24	398	240	18	320	150	18	863	400	20
min	440	110	20	180	90	10	120	100	10	270	240	20
Average	1494	549	28	1084	683	23	675	382	23	1848	854	28
n	5	5	2	15	15	12	11	11	8	14	13	5

TABLE B-1
STATISTICAL ANALYSIS OF CHLORINATED SITE DATA

BIOCHLOR: Chlorinated Solvent Plume Database
Air Force Center for Environmental Excellence (AFCEE)

AFFECTED GROUNDWATER PLUME CHARACTERISTICS CONT'D

	BTEX Plume Characteristics			TCA Plume Characteristics			1,1-DCA Plume Characteristics			1,1-DCE Plume Characteristics		
Facility/Site Name	**Length (ft)**	**Width (ft)**	**Thickness (ft)**	**Length (ft)**	**Width (ft)**	**Thickness (ft)**	**Length (ft)**	**Width (ft)**	**Thickness (ft)**	**Length (ft)**	**Width (ft)**	**Thickness (ft)**
1. Aerojet Superfund Site							2500	2000	25			
2. Altus AFB/LF-04	2875	500								1560	625	
3. Cape Canaveral AS/CCFTA-2	1540	438	20	300	200	20	1250	440	20	1200	340	20
4. Cape Canaveral AS/Facility 1381	240	480		130	170		1670	800		1670	800	
5. Chemical Distribution Facility				1170	345	20	1410	525	20	1380	420	20
6. Chemical Manufacturer/Waste Site	3200	1400		2700	1200		1900	320				
7. Chlorinated Site #1/Hanger	560	560	30	560	750	30	2000	750	30			
8. Chlorinated Site #2/Tank Farm												
9. Chlorinated Site #3/Junkyard												
10. Eielson AFB/Site 45/57	640	340										
11. Hill AFB/OU-5				2520	385	36	1629	301	11	1820	350	36
12. Industrial Facility/Plume 1	60	40										
13. Industrial Facility/Plume 2	170	60										
14. Kelly AFB/MP Site												
15. Landfill #1	1000	500	50									
16. Landfill #2/VC Site												
17. Offutt AFB/Bldg. 301												
18. Offutt AFB/FPTA3	650	440	30									
19. Plattsburgh AFB/FT-002	3600	900										
20. Sterling/OW-31/OW-41	960	540	24				1040	340	24			
21. Sterling/Unit K	870	300	28							1000	200	28
22. USCG Site												
23. Westover ARB/FT-03	630	580	38									
24. Westover ARB/FT-08	750	350	50									
max	3600	1400	50	2700	1200	36	2500	2000	30	1820	800	36
75th percen.	1270	550	41	2183	659	32	1925	763	25	1643	574	30
median	**750**	**480**	**30**	**865**	**365**	**25**	**1650**	**483**	**22**	**1470**	**385**	**24**
25th percen.	595	345	27	365	236	20	1370	335	20	1245	343	20
min	60	40	20	130	170	20	1040	301	11	1000	200	20
Average	1183	495	34	1230	508	27	1675	685	22	1438	456	26
n	15	15	8	6	6	4	8	8	6	6	6	4

TABLE B-1
STATISTICAL ANALYSIS OF CHLORINATED SITE DATA

BIOCHLOR: Chlorinated Solvent Plume Database
Air Force Center for Environmental Excellence (AFCEE)

MAXIMUM CONCENTRATIONS FOR SITE-SPECIFIC GROUNDWATER PARAMETERS

	Chlorinated Solvent Plume Maximum Concentrations (mg/L)								Max. Total	Maximum TPH
Facility/Site Name	**PCE**	**TCE**	**cis-DCE**	**trans-DCE**	**VC**	**TCA**	**DCA**	**1,1-DCE**	**BTEX (mg/L)**	**(mg/L)**
1. Aerojet Superfund Site		3.900	2.800	0.084	2.600		1.400	0.039	0.025	
2. Altus AFB/LF-04		8.910	1.340	0.033				0.004	0.024	0.883
3. Cape Canaveral AS/CCFTA-2	0.056	15.800	98.500	0.389	6.520	0.258	0.443	0.039	0.331	
4. Cape Canaveral AS/Facility 1381	0.003	39.400	4.120	0.025	1.350	0.130	0.026	0.238	0.006	
5. Chemical Distribution Facility	60.000	64.000	0.400		<0.025	30.000	0.150	3.800		
6. Chemical Manufacturer/Waste Site	9.500	17.000	7.300	0.010	0.010	3.700	0.033		37.027	
7. Chlorinated Site #1/Hanger	0.041	0.075	0.476			0.242	0.084		1.696	
8. Chlorinated Site #2/Tank Farm	1.420	0.547	0.146				0.004		0.057	
9. Chlorinated Site #3/Junkyard	0.062	0.720				0.002				
10. Eielson AFB/Site 45/57		2.610	0.029	0.049					0.213	2.311
11. Hill AFB/OU-5		0.259	0.016			0.064	0.006	0.002		
12. Industrial Facility/Plume 1	0.002	5.000	21.000	0.009	3.700			0.004	1.830	
13. Industrial Facility/Plume 2		570.000	300.000	0.210	3.000	0.180		0.260	75.800	
14. Kelly AFB/MP Site	49.000	4.300	12.000		1.300					
15. Landfill #1	1.800	0.450	29.000		1.300	0.120	0.440		9.700	
16. Landfill #2/VC Site	0.001	0.002	0.004		0.083		0.003		0.031	
17. Offutt AFB/Bldg. 301	0.002	17.500	1.230	0.009	0.001		0.001	0.029		
18. Offutt AFB/FPTA3		0.009	0.273	0.002	0.792				3.233	
19. Plattsburgh AFB/FT-002	0.002	0.562	12.600	0.009	1.520				6.596	
20. Sterling/OW-31/OW-41					0.712		11.150	0.032	0.501	
21. Sterling/Unit K			1.250	0.138	6.520			0.823	28.960	
22. USCG Site	2.860	0.332	0.164		0.034					
23. Westover ARB/FT-03		0.008	0.032						1.657	
24. Westover ARB/FT-08	0.001	12.800	0.732	0.003	0.002				32.557	
max	60.000	570.000	300.000	0.389	6.520	30.000	11.150	3.800	75.800	2.311
75th percen.	2.330	15.050	10.825	0.084	2.700	0.258	0.441	0.249	8.924	1.954
median	**0.056**	**3.255**	**1.240**	**0.025**	**1.300**	**0.180**	**0.059**	**0.039**	**1.676**	**1.597**
25th percen.	0.002	0.362	0.191	0.009	0.071	0.120	0.005	0.016	0.096	1.240
min	0.001	0.002	0.004	0.002	0.001	0.002	0.001	0.002	0.006	0.883
Average	8.317	34.736	22.428	0.075	1.840	3.855	1.145	0.479	11.125	1.597
n	15	22	22	13	16	9	12	11	18	2

TABLE B-1
STATISTICAL ANALYSIS OF CHLORINATED SITE DATA

BIOCHLOR: Chlorinated Solvent Plume Database
Air Force Center for Environmental Excellence (AFCEE)

ELECTRON ACCEPTOR/METABOLIC BY-PRODUCT DATA

Facility/Site Name	Δ Dissolved Oxygen (DO, mg/L)	Δ Sulfate (SO_4^{2-}, mg/L)	Δ Nitrate (NO_3^-, mg/L)	Δ Ferrous Iron (Fe II, mg/L)	Δ Methane (mg/L)	Max. Ethene (mg/L)	Max. Ethane (mg/L)	Max Dissolved H_2 (mg/L)	Max. Acetone (mg/L)	Max. Methanol (mg/L)
1. Aerojet Superfund Site	0.450	11.100	0.325		1.463	0.289	0.290			
2. Altus AFB/LF-04	3.500	-710.000	0.080					4.33E-06		
3. Cape Canaveral AS/CCFTA-2	0.363	33.600	0.150	3.100	1.374	0.225	0.055	3.63E-06		
4. Cape Canaveral AS/Facility 1381	0.100	70.540		3.250	3.644	0.018		4.49E-06		
5. Chemical Distribution Facility										
6. Chemical Manufacturer/Waste Site	2.58	201	1.87	19.937		0.114				
7. Chlorinated Site #1/Hanger	2.47									
8. Chlorinated Site #2/Tank Farm										
9. Chlorinated Site #3/Junkyard		0.001	0.081							
10. Eielson AFB/Site 45/57		1.550	0.170	-14.065	-0.010	0.001				
11. Hill AFB/OU-5	4.695	9.700	5.645	-0.300				6.05E-07		
12. Industrial Facility/Plume 1	1.420	44.000	0.050	6.000	4.581	7.572				8.170
13. Industrial Facility/Plume 2	1.370	33.400	-0.070	6.620	0.515	0.437				2.840
14. Kelly AFB/MP Site									0.120	
15. Landfill #1	8.500		0.150	309.980	8.269	0.906			0.590	
16. Landfill #2/VC Site	7.34	-6.13	0.41	149.980	9.490	0.001	0.017		0.064	
17. Offutt AFB/Bldg. 301	6.175	14.000	4.580	5.300	0.184			1.57E-06		
18. Offutt AFB/FPTA3	0.050	26.470	-1.180	23.300	22.399	0.895				
19. Plattsburgh AFB/FT-002	0.400	5.590	-0.040	15.800	-9.510					
20. Sterling/OW-31/OW-41	-1.067	140.333	0.637	4.750	4.591	7.750	3.850			
21. Sterling/Unit K	-1.867	132.333	0.215	31.600	1.491	2.400	3.800			
22. USCG Site		61.4	-0.17	-15.950	-0.730	0.004	0.004	1.23E-05		
23. Westover ARB/FT-03	3.530	18.850	2.395	600.000	0.180					
24. Westover ARB/FT-08	7.297	9.100	3.947	279.700	4.286	0.005				
max	8.500	201.000	5.645	600.000	22.399	7.750	3.850	1.23E-05	0.590	8.170
75th percen.	4.404	52.700	1.254	31.600	4.584	0.903	2.923	4.45E-06	0.355	6.838
median	**1.945**	**18.850**	**0.170**	**6.620**	**1.477**	**0.257**	**0.173**	**3.98E-06**	**0.120**	**5.505**
25th percen.	0.372	7.345	0.065	3.250	0.183	0.008	0.027	2.09E-06	0.092	4.173
min	-1.867	-710.000	-1.180	-15.950	-9.510	0.001	0.004	6.05E-07	0.064	2.840
Average	2.628	5.097	1.013	84.059	3.264	1.473	1.336	4.49E-06	0.258	5.505
n	18	19	19	17	16	14	6	6	3	2

Note:
1. Values for ΔDO, ΔSO4, and ΔNO3 calculated as average background concentration minus minimum plume concentration. Values for ΔFe and Δmethane calculated as maximum plume concentration minus average background concentration.

TABLE B-1
STATISTICAL ANALYSIS OF CHLORINATED SITE DATA

BIOCHLOR: Chlorinated Solvent Plume Database
Air Force Center for Environmental Excellence (AFCEE)

WATER QUALITY PARAMETERS

Facility/Site Name	Δ Chloride (mg/L)	Min. Redox Potential (mV)	Total Organic Carbon: Background Average TOC (mg/L)	Total Organic Carbon: Δ Total TOC (mg/L)	Avg. pH	Alkalinity: Minimum (mg/L)	Alkalinity: Maximum (mg/L)	Avg. Temperature (°C)
1. Aerojet Superfund Site	49.9	-125			7.0	66	310	21.8
2. Altus AFB/LF-04	378.0	-179	15.7	-7.4	6.9	320	422	14.8
3. Cape Canaveral AS/CCFTA-2	96.9	-250	21.1	19.5	7.0	319	500	22.4
4. Cape Canaveral AS/Facility 1381	97.1	-340	8.6	0.4	7.2	239	354	26.1
5. Chemical Distribution Facility								
6. Chemical Manufacturer/Waste Site	589.0	-336	6.6	17.5	6.9	82	460	17.5
7. Chlorinated Site #1/Hanger			11.2	3.7	6.7	175	500	7.5
8. Chlorinated Site #2/Tank Farm					5.6			23.7
9. Chlorinated Site #3/Junkyard								
10. Eielson AFB/Site 45/57		-118			6.9	112	321	8.3
11. Hill AFB/OU-5	77.0	83	3.5	1.1	7.3	208	512	18.2
12. Industrial Facility/Plume 1	-235.9	-60			7.3	259	339	5.9
13. Industrial Facility/Plume 2	-101.2	-60			7.0	223	450	5.7
14. Kelly AFB/MP Site	40.9				6.7	315	315	26.2
15. Landfill #1	155.3	-116	0.5	299.5	6.5	42	424	10.4
16. Landfill #2/VC Site	124.0	-137		17.0	5.7	25	317	14.5
17. Offutt AFB/Bldg. 301	19.6	-70	34.9	-27.1	7.4	207	346	16.0
18. Offutt AFB/FPTA3	208.4	-170			7.2	520	760	13.4
19. Plattsburgh AFB/FT-002	21.4	158			7.2	86	330	10.8
20. Sterling/OW-31/OW-41	1871.7				7.0	515	940	20.8
21. Sterling/Unit K	5097.7				6.6	410	780	20.6
22. USCG Site	-74.0	102	21.7	-8.7	5.9	70	260	18.3
23. Westover ARB/FT-03	3.5	-40	6.2	19.9	6.4	90	320	12.3
24. Westover ARB/FT-08	0.0	-105	3.2	91.2	7.5	10	260	10.8
max	5097.7	158	34.9	299.5	7.5	520	940	26.2
75th percen.	181.9	-60	18.4	19.6	7.2	315	500	20.8
median	**77.0**	**-116**	**8.6**	**10.3**	**7.0**	**207**	**354**	**15.4**
25th percen.	11.5	-170	4.8	-1.5	6.6	82	320	10.8
min	-235.9	-340	0.5	-27.1	5.6	10	260	5.7
Average	443.1	-104	12.1	35.5	6.8	204	439	15.7
n	19.0	17	11	12	22	21	21	22

Note:

1. Values for Δchloride and Δtotal TOC calculated as maximum plume concentration minus average background concentration.

TABLE B-1
STATISTICAL ANALYSIS OF CHLORINATED SITE DATA

BIOCHLOR: Chlorinated Solvent Plume Database
Air Force Center for Environmental Excellence (AFCEE)

REDUCTIVE DECHLORINATION PARAMETERS

Facility/Site Name	AFCEE Score	AFCEE Score (Sufficient Info Only)	PCE Rate Constant (1/yr)	TCE Rate Constant (1/yr)	DCE Rate Constant (1/yr)	VC Rate Constant (1/yr)	TCA Rate Constant (1/yr)	DCA Rate Constant (1/yr)
1. Aerojet Superfund Site	23	23		2.1	1.2	1.7		1.2
2. Altus AFB/LF-04	5			1.5	20.9			
3. Cape Canaveral AS/CCFTA-2	28	28		0.9	0.7	0.6		0.3
4. Cape Canaveral AS/Facility 1381	19	19						0.2
5. Chemical Distribution Facility	4			0.4	0.4	12.2	1.6	
6. Chemical Manufacturer/Waste Site	17	17	2.4	3.1	2.2		3.2	
7. Chlorinated Site #1/Hanger	3							
8. Chlorinated Site #2/Tank Farm	5							
9. Chlorinated Site #3/Junkyard	2							
10. Eielson AFB/Site 45/57	14	14						
11. Hill AFB/OU-5	9	9						
12. Industrial Facility/Plume 1	16	16		0.3	0.8	2.3		
13. Industrial Facility/Plume 2	7	7						
14. Kelly AFB/MP Site	5		1.1	3.2	1.6			
15. Landfill #1	12	12						
16. Landfill #2/VC Site	3	3				0.7		
17. Offutt AFB/Bldg. 301	1	1						
18. Offutt AFB/FPTA3	22	20						
19. Plattsburgh AFB/FT-002	12	12		0.5	0.1	0.4		
20. Sterling/OW-31/OW-41	12	14						
21. Sterling/Unit K	17	19						
22. USCG Site	13	13	0.8	2.5	3.6	7.6		
23. Westover ARB/FT-03	16	18						
24. Westover ARB/FT-08	18	18		0.7				
max	28.0	28	2.4	3.2	20.9	12.2	3.2	1.2
75th percen.	17.0	19	1.7	2.4	2.2	4.9	2.8	0.7
median	**12.0**	**15**	**1.1**	**1.2**	**1.2**	**1.7**	**2.4**	**0.3**
25th percen.	5.0	12	0.9	0.5	0.7	0.6	2.0	0.2
min	1.0	1	0.8	0.3	0.1	0.4	1.6	0.2
Average	11.8	15	1.4	1.5	3.5	3.6	2.4	0.5
n	24.0	18	3	10	9	7.0	2.0	3

1. Low AFCEE scores may be due to conditions that are not conducive to natural attenuation or to insufficient information. These scores were determined from data collected at the most contaminated well at each site.
2. Bracketed values indicate the standard error of the rate constant estimate.

APPENDIX C - REDOX REACTIONS AND THE ROLE OF HYDROGEN IN THE SUBSURFACE

The role of hydrogen in anaerobic biodegradation reactions is shown in the conceptual model shown in Figure C-1 (Wiedemeier *et al*., 1999). The figure is arranged thermodynamically, with reactions releasing larger amounts of energy (i.e., aerobic biodegradation and nitrate reduction) shown on the left side of the figure and reactions that releasing smaller amounts of energy (such as methanogenesis) shown on the right side of the figure. The figure focuses on the thermodynamic flow of electron acceptors and electron donors in a moderately to highly reduced anaerobic system after oxygen and nitrate are consumed.

As discussed in Wiedemeier *et al*. 1999:

A general indication of the *potential* mass flux is shown by the thickness of the pipes connecting each vessel. For each reaction, the flux is inferred based on typical concentrations observed under field conditions. Typical concentrations of the various constituents are shown as the level in the various reservoirs in the process diagram. For example, fermentation produces dissolved hydrogen which flows through a small pipe into each of the dissolved hydrogen reservoirs. Because the reactions that use hydrogen are much faster than the reactions that generate hydrogen, the pipes leading out from each hydrogen reservoir are much larger than the pipes leading in. Since the inlet pipe smaller (low capacity) than the outlet pipe (high capacity) at each hydrogen reservoir, the amount in the reservoir (representing dissolved hydrogen concentrations in groundwater) are typically very low (< 0.001 mg/L) at all times.

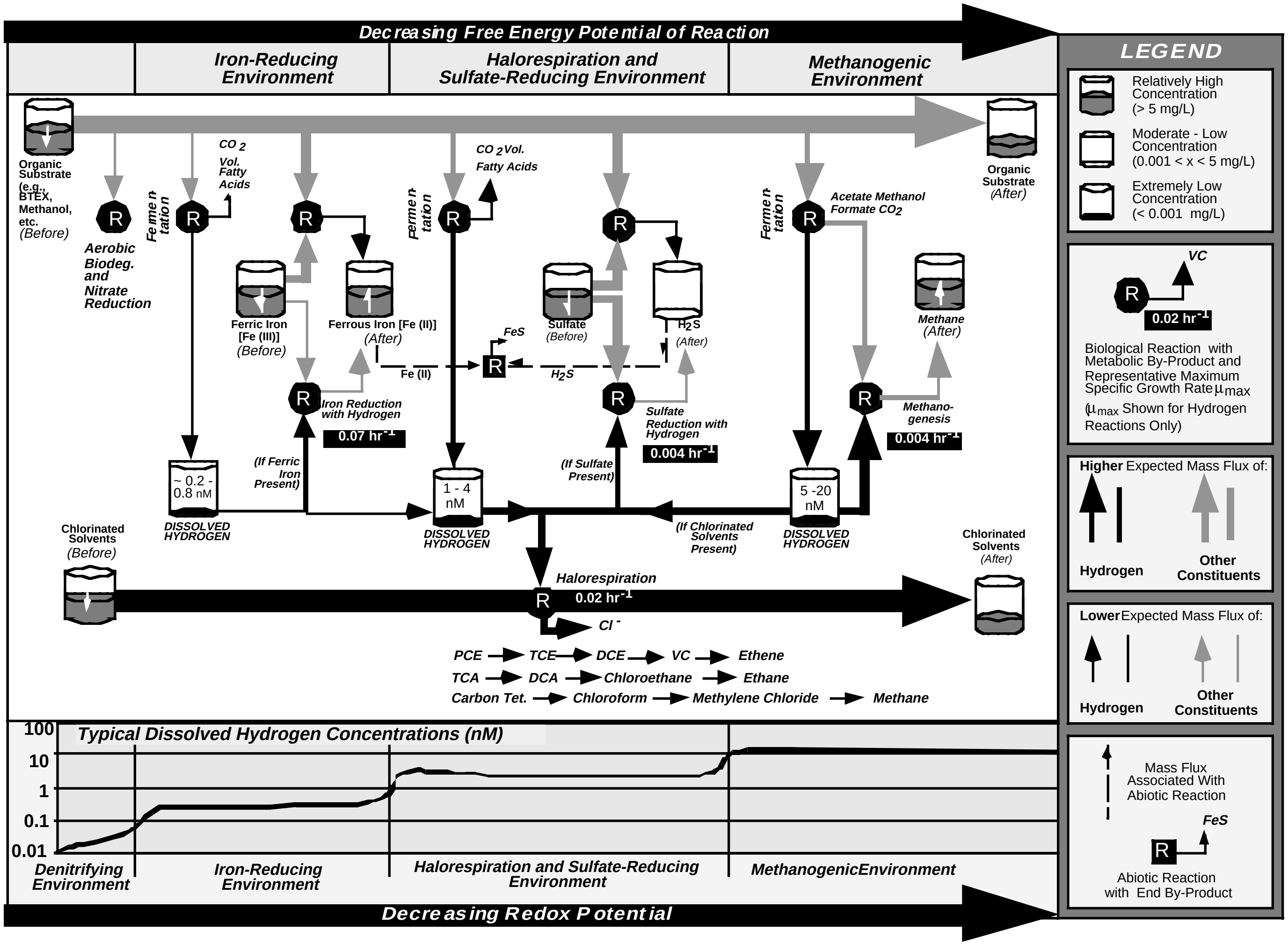


Figure C-1. Thermodynamic flow of electron donors and electron acceptors pathways at chlorinated solvent sites undergoing halorespiration (Wiedemeier et al., 1999).

APPENDIX D – BIOCHLOR MODEL DESCRIPTION

Governing Equations

The BIOCHLOR software solves a set of coupled partial differential equations to describe the reactive transport of chlorinated solvent species, such as PCE, TCE, DCE, VC and ETH, in saturated ground-water systems. The equations describe one-dimensional advection, three-dimensional dispersion, linear sorption, and sequential, first-order biotransformation. All equations, except the first, are coupled to a parent species equation through the reaction term as shown below:

$$R_1 \frac{\partial c_1}{\partial t} = D_x \frac{\partial^2 c_1}{\partial x^2} + D_y \frac{\partial^2 c_1}{\partial y^2} + D_z \frac{\partial^2 c_1}{\partial z^2} - v_s \frac{\partial c_1}{\partial x} - k_1 c_1 \quad (1)$$

$$R_2 \frac{\partial c_2}{\partial t} = D_x \frac{\partial^2 c_2}{\partial x^2} + D_y \frac{\partial^2 c_2}{\partial y^2} + D_z \frac{\partial^2 c_2}{\partial z^2} - v_s \frac{\partial c_2}{\partial x} + y_1 k_1 c_1 - k_2 c_2 \quad (2)$$

$$R_3 \frac{\partial c_3}{\partial t} = D_x \frac{\partial^2 c_3}{\partial x^2} + D_y \frac{\partial^2 c_3}{\partial y^2} + D_z \frac{\partial^2 c_3}{\partial z^2} - v_s \frac{\partial c_3}{\partial x} + y_2 k_2 c_2 - k_3 c_3 \quad (3)$$

$$R_4 \frac{\partial c_4}{\partial t} = D_x \frac{\partial^2 c_4}{\partial x^2} + D_y \frac{\partial^2 c_4}{\partial y^2} + D_z \frac{\partial^2 c_4}{\partial z^2} - v_s \frac{\partial c_4}{\partial x} + y_3 k_3 c_3 - k_4 c_4 \quad (4)$$

$$R_5 \frac{\partial c_5}{\partial t} = D_x \frac{\partial^2 c_5}{\partial x^2} + D_y \frac{\partial^2 c_5}{\partial y^2} + D_z \frac{\partial^2 c_5}{\partial z^2} - v_s \frac{\partial c_5}{\partial x} + y_4 k_4 c_4 - k_5 c_5 \quad (5)$$

where c_1, c_2, c_3, c_4, and c_5 are concentrations of PCE, TCE, DCE, VC, and ETH, respectively [mg/L]; D_x, D_Y, and D_Z are the hydrodynamic dispersion coefficients [ft^2/yr]; v_s is the seepage velocity [ft/yr]; k is the first-order degradation coefficient [1/yr]; y is the yield coefficient [a dimensionless value; for example, y_1 would represent the mg of TCE produced per unit mg of PCE destroyed]; and R_1, R_2, R_3, R_4, and R_5 are respective retardation factors. In BIOCHLOR, the retardation factor values of different species are averaged to compute an "effective retardation factor, R", which is in turn used to compute the effective transport velocity and dispersion coefficients. Also, biotransformation is assumed to occur only in the aqueous phase (which is a conservative assumption) and hence all the degradation reaction terms are divided by R.

Analytical Solution Strategy

The Domenico (1987) solution with some minor improvements suggested by Martin-Hayden and Robbins (1997) was used as the base solution to solve the three dimensional problem. The solution was directly used to solve the independent equation 1. However, since equations 2 to 5 are coupled equations, the Domenico solution cannot be used to solve them. Therefore, in BIOCHLOR a new transformation procedure is used to first uncouple equations 2 to 5 and recast them in the form of equation 1 (Sun and Clement, 1999; Sun et al. 1999a, Sun et al. 1999b). The transformation equations used are:

$$a_2 = c_2 + \frac{y_1 k_1}{k_1 - k_2} c_1 \quad (6)$$

$$a_3 = c_3 + \frac{y_2 k_2}{k_2 - k_3} c_2 + \frac{y_1 y_2 k_1 k_2}{(k_1 - k_3)(k_2 - k_3)} c_1 \quad (7)$$

$$a_4 = c_4 + \frac{y_3 k_3}{k_3 - k_4} c_3 + \frac{y_2 y_3 k_2 k_3}{(k_2 - k_4)(k_3 - k_4)} c_2 + \frac{y_1 y_2 y_3 k_1 k_2 k_3}{(k_1 - k_4)(k_2 - k_4)(k_3 - k_4)} c_1 \quad (8)$$

$$a_5 = c_5 + \frac{y_4 k_4}{k_4 - k_5} c_4 + \frac{y_3 y_4 k_3 k_4}{(k_3 - k_5)(k_4 - k_5)} c_3 + \frac{y_2 y_3 y_4 k_2 k_3 k_4}{(k_2 - k_5)(k_3 - k_5)(k_4 - k_5)} c_2 + \frac{y_1 y_2 y_3 y_4 k_1 k_2 k_3 k_4}{(k_1 - k_5)(k_2 - k_5)(k_3 - k_5)(k_4 - k_5)} c_1 \quad (9)$$

It can be shown that using transformation equations 6 to 10, the reactive transport equations 2 to 5 can be written in a transformed "a" domain where the coupled transport equations reduce to a form similar to equation 1. For illustration purposes, the steps involved in proving the strategy for a one-dimensional, 2-species transport problem is given below.

Consider the following set of one-dimensional fate and transport equations that describe two reacting species that are coupled by first-order decay reactions:

$$\frac{\partial c_1}{\partial t} = D_x \frac{\partial^2 c_1}{\partial x^2} - v \frac{\partial c_1}{\partial x} - k_1 c_1 \quad (10)$$

$$\frac{\partial c_2}{\partial t} = D_x \frac{\partial^2 c_2}{\partial x^2} - v \frac{\partial c_2}{\partial x} + y_1 k_1 c_1 - k_2 c_2. \quad (11)$$

Since equation 10 is already in the standard form, it can be solved using a standard analytical solution. Based on Sun et al. (1999a) work, a transformation for the second equation can be written as:

$$a_2 = c_2 + \frac{y_1 k_1}{k_1 - k_2} c_1. \quad (12)$$

Differentiating equation 12 partially with respect to time we get,

$$\frac{\partial a_2}{\partial t} = \frac{\partial c_2}{\partial t} + \frac{y_1 k_1}{k_1 - k_2} \frac{\partial c_1}{\partial t} \quad (13)$$

Substituting (10) and (11) into (12) we get,

$$\frac{\partial a_2}{\partial t} = D_x \frac{\partial^2 c_2}{\partial x^2} - v \frac{\partial c_2}{\partial x} + y_1 k_1 c_1 - k_2 c_2 + \frac{y_1 k_1}{k_1 - k_2} \left[D_x \frac{\partial^2 c_1}{\partial x^2} - v \frac{\partial c_1}{\partial x} - k_1 c_1 \right] \quad (14)$$

Equation 14 can be rearranged as,

$$\frac{\partial a_2}{\partial t} = D_x \frac{\partial^2}{\partial x^2} \left[c_2 + \frac{y_1 k_1}{k_1 - k_2} c_1 \right] - v \frac{\partial}{\partial x} \left[c_2 + \frac{y_1 k_1}{k_1 - k_2} c_1 \right] + y_1 k_1 c_1 - k_2 c_2 + \frac{y_1 k_1^2 c_1}{k_1 - k_2}. \quad (15)$$

Using (12), equation 15 can be written as:

$$\frac{\partial a_2}{\partial t} = D_x \frac{\partial^2 a_2}{\partial x^2} - v \frac{\partial a_2}{\partial x} - k_2 c_2 + y_1 k_1 c_1 - \frac{y_1 k_1^2 c_1}{k_1 - k_2}. \quad (16)$$

Combining the last three terms, equation 16 can be simplified to:

$$\frac{\partial a_2}{\partial t} = D_x \frac{\partial^2 a_2}{\partial x^2} - v \frac{\partial a_2}{\partial x} - k_2 a_2 \quad (17)$$

To solve (11), first a standard, one-dimensional solution should be used to solve (17) for computing a_2 values and to solve (10) for computing c_1 values (note that c_1 is always same as a_1). Then, c_2 values can be computed using equation 12 in an inverse mode. This procedure can be repeated for solving any number of coupled reactive species. A more general analysis of this solution strategy, and a detailed comparison of the analytical results against the numerical results of the RT3D code are discussed in Sun and Clement (1998).

If retarding species are assumed then an effective retardation factor is used to divide the transport velocity, dispersion coefficients and degradation rates (since degradation is assumed to occur only in the aqueous phase). It should be noted that the proposed analytical solution strategy would work only when the constant effective retardation factor is used to represent the retardation characteristics of all the transported species.

DOMENICO SINGLE SPECIES ANALYTICAL MODEL

Domenico (1987) developed a semi-analytical solution for reactive transport with first order decay and a two-dimensional (i.e., planar) source geometry. BIOCHLOR uses the Domenico solution with Martin-Hayden and Robbins (1997) improvements and assumes that degradation reactions occur only in the aqueous phase. BIOCHLOR evaluates centerline concentrations at y=0, z=0 and the 2-D array at z=0. The model equation, boundary conditions, assumptions, and limitations are discussed below.

Domenico Model with First Order Decay

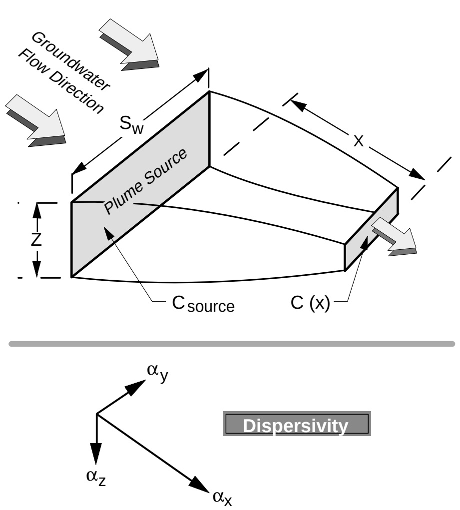
$$C(x,y,z,t) = \frac{C_o}{8} f_x f_y f_z$$

$$f_x = \exp\left(\frac{x\left[1-\left(1+4\lambda\alpha_x/v_s\right)^{0.5}\right]}{2\alpha_x}\right) * erfc\left(\frac{x - vt\left(1+4\lambda\alpha_x/v_s\right)^{0.5}}{2\left(\alpha_x vt\right)^{0.5}}\right) +$$

$$\exp\left(\frac{x\left[1+\left(1+4\lambda\alpha_x/v_s\right)^{0.5}\right]}{2\alpha_x}\right) * erfc\left(\frac{x + vt\left(1+4\lambda\alpha_x/v_s\right)^{0.5}}{2\left(\alpha_x vt\right)^{0.5}}\right)$$

$$f_y = \mathrm{erf}\left(\frac{(y+Y/2)}{2(\alpha_y x)^{0.5}}\right) - \mathrm{erf}\left(\frac{(y-Y/2)}{2(\alpha_y x)^{0.5}}\right) \qquad f_z = \mathrm{erf}\left(\frac{(z+Z)}{2(\alpha_z x)^{0.5}}\right) - \mathrm{erf}\left(\frac{(z-Z)}{2(\alpha_z x)^{0.5}}\right)$$

Definitions



C(x, y, z, t)	Concentration at distance x downstream of source and distance y off centerline of plume at time t (mg/L)
Co	Concentration in Source Area at t=0 (mg/L)
x	Distance downgradient of source (ft)
y	Distance from plume centerline of source (ft)
z	Distance from top of saturated zone to measurement point (assumed to be 0; concentration is always given at top of saturated zone).
α_x	Longitudinal ground-water dispersivity (ft)
α_y	Transverse ground-water dispersivity (ft)
α_z	Vertical ground-water dispersivity (ft)
θ_e	Effective Soil Porosity
λ	First-Order Degradation Rate Coefficient(day^{-1})
v_s	Seepage Velocity (ft/yr)=Ki/(θ_e)
v	Chemical Velocity (ft/yr)=v_s/R
K	Hydraulic Conductivity (ft/yr)
R	Constituent retardation factor
i	Hydraulic Gradient (cm/cm)
Y	Source Width (ft)
Z	Source Depth (ft)

Note that because biotransformation is assumed to occur only in the aqueous phase, the first order rate constant, λ, has been divided by R. However, R can be canceled out by replacing v (the compound velocity (i.e., v_s/R)) in the original Domenico solution with v_s, (the seepage velocity).

The Domenico solution was modified for chloroethane (CA) reactive transport to take into consideration both biotic and abiotic reactions. The first order rate constant for abiotic decay, λ_A, is added to the biological rate constant for reductive dechlorination, λ, as shown below. All other terms in the Domenico equation remain the same.

$$f_x = \exp\left(\frac{x\left[1-\left(1+4(\lambda+\lambda_A)\alpha_x/v_s\right)^{0.5}\right]}{2\alpha_x}\right) * \operatorname{erfc}\left(\frac{x - vt\left(1+4(\lambda+\lambda_A)\alpha_x/v_s\right)^{0.5}}{2\left(\alpha_x vt\right)^{0.5}}\right) +$$

$$\exp\left(\frac{x\left[1+\left(1+4(\lambda+\lambda_A)\alpha_x/v_s\right)^{0.5}\right]}{2\alpha_x}\right) * \operatorname{erfc}\left(\frac{x + vt\left(1+4(\lambda+\lambda_A)\alpha_x/v_s\right)^{0.5}}{2\left(\alpha_x vt\right)^{0.5}}\right)$$

The initial conditions of the Domenico model are:

1. $c(x, y, z, 0) = 0$ (Initial concentration = 0 for x, y, z, > 0)
2. $c(0, Y, Z, 0) = C_0$ (Source concentration for each vertical plane source = C_0 at time 0)

The key assumptions in the model are:

1. The aquifer and flow field are homogenenous and isotropic.
2. The ground-water velocity is fast enough that molecular diffusion in the dispersion terms can be ignored (may not be appropriate for simulation of transport through clays).
3. Adsorption is a reversible process represented by a linear isotherm.