

5.0 CONTAMINANT FATE AND TRANSPORT

This section discusses the physical and chemical processes that affect contaminant migration in matrices at the Site. The properties of the chemicals detected beneath the Site are reviewed, and the interactions of these chemicals within groundwater and surface water are summarized. Difficulties and concerns associated with their presence in the subsurface also are presented.

5.1 POTENTIAL ROUTES OF MIGRATION

Contaminant presence at the Site is apparently a result of operational activities at the former location of the Untz Dry Cleaners during the years 1960 to 1975. During this period, typical dry cleaning solvents were released to the environment. Results of sampling of several matrices, including soil, sediment, surface water, and groundwater, by NCDEHNR in 1992 and EPA in 1996 have indicated that contaminants associated with dry cleaning solvents (i.e., PCE) and their potential degradation products (i.e., TCE, cis 1,2-DCE) are present in groundwater beneath the site and have been detected in a local, unnamed stream northeast of the former dry cleaner location. These constituents have not been detected in soil and sediment samples. The reader is referred to Section 4 for a discussion of sample analytical results.

As indicated by previous sampling results, potential routes of migration for PCE and associated degradation products within the area of the Site are principally through flow of water within the groundwater. Continued use of groundwater by local residents as a water source and natural hydraulic flow of groundwater will result in the continued migration and spreading of contaminants. In addition, if groundwater is discharging to nearby streams, the possibility exists that contaminants may be detected in the surface water bodies. The following paragraphs will discuss the persistence of chlorinated hydrocarbons in the environment and factors affecting the length of persistence.

5.2 CONTAMINANT PERSISTENCE

Although semi-volatile organic compounds, pesticides, and metals were detected in groundwater samples from the Site, only volatile organic compounds were observed in significant quantities above MCLs. Therefore, this discussion will focus on VOC properties.

5.2.1 Chemical Properties of Contaminants

From the perspective of groundwater and surface water contamination, the most significant contaminant characteristic is solubility (Gorelick et. al., 1993). The solubility of a solute is defined as the mass of the solute that will dissolve in a unit volume of solution under specified conditions. The solubility defines the maximum possible concentration that commonly occurs in groundwater or surface water, for any given contaminant.

The most simple organic compounds are hydrocarbons, which consist solely of carbon and hydrogen. Hydrocarbons can be divided into two classes, aromatic hydrocarbons, which contain a benzene ring, and aliphatic hydrocarbons, that don't contain a benzene ring (Fetter, 1993). Hydrocarbons such as benzene, toluene, ethylbenzene, and xylene (BTEX) consist of hydrocarbon molecules combined with aromatic compounds.

Halogenated organic compounds are characterized by a variable number of single, double, and triple bonds and the presence of chlorine, bromine, fluorine, or iodine. These compounds are widely used and have been frequently found as contaminants in groundwater. Tetrachloroethene (PCE), trichloroethene (TCE), and 1,1,1-trichloroethane are examples of these compounds. Each of these chemicals has a low flammability and a high vapor density, which makes them very useful as solvents for the degreasing of metal parts. PCE and TCE are denser than water, and if spilled on the ground in quantities great enough to overcome the residual saturation, may migrate vertically downward through an aquifer (Fetter, 1993). They are also soluble in water and can migrate in a dissolved phase in the direction of groundwater flow.

Regardless of whether a liquid is composed of a single type of molecule, such as TCE, or a mixture, it is the nature of the intermolecular bonding in the liquid that contributes to its generally low solubility in water. Liquids with infinite solubilities (e.g., acetone) are referred to as being miscible with water. Liquids with finite solubilities (e.g., trichloroethene) are generally referred to as immiscible with water, even if the solubility is high.

Low density immiscible liquids, or light non-aqueous phase liquids (LNAPLs), will float on the surface of the higher density groundwater and surface water. High density liquids, or dense non-aqueous phase liquids (DNAPLs), sink through water until they reach the aquifer or surface water bottom. Gasoline is an example of an LNAPL, and PCE and TCE are examples of DNAPLs. While these liquids do not go completely into solution in groundwater, they do contain compounds with limited solubilities in water (Gorelick et. al., 1993).

5.2.2 Site-Specific Chemical Properties

The various VOCs detected in soils and groundwater at the Site are classified as halogenated aliphatic compounds (HACs); i.e., PCE, TCE, and 1,2-DCE. **Table 5-1** lists physical properties for the various organic contaminants detected in soils (ranked by their aqueous solubility). **Table 5-2** lists physical properties that can affect fate and transport of contaminants in the surface and subsurface, as discussed in the previous sections.

HACs are characterized by open-chain structures; a variable number of single, double, and triple bonds; and the presence of chlorine, bromine, fluorine, or iodine. HACs have many applications, such as solvents, degreasers, dry cleaning agents, refrigerants, and organics synthesis agents (Moore et al, 1984). PCE was the most frequently detected HAC in North Belmont groundwater samples.

In general, HACs have low to moderate solubilities, high volatilities, low to moderate partition coefficients, high mobilities, and densities greater than water (Table 5-1). As a result, they are relatively easily leached from the soil into the groundwater (if conditions are suitable). Once in the subsurface, the HACs typically undergo progressive dehalogenation. Generally, the time required for each step may be widely variable and degradation may or may not occur, depending on subsurface conditions (the presence of nutrients, microorganisms, etc.).

5.2.3 Contaminant Transport — Groundwater

Surface and subsurface soils sampled within the immediate vicinity of the former Untz Dry Cleaner facility have not revealed contamination by PCE and associated degradation products. Leaching of chemicals from soil is a process of migration involving the movement of a chemical downward through soil by percolation of water. Typically, the more precipitation, the greater the chance for chemicals to leach (Ney, 1990). Leaching is a concern because of the potential for a chemical to move through the soil and contaminate the groundwater. Many factors affect whether or not a chemical leaches in soil, including solubility of the chemical, biodegradation, hydrolysis, dissociation, sorption, volatility, rainfall, and evaporation. A chemical that is water-soluble can leach in soil and is likely to be biodegraded by soil microbes. If biodegradation is rapid, then leaching may be minimal. A chemical that is insoluble in water can be adsorbed in soil, moved with soil particles, and perhaps very slowly biodegrade, if at all.

The presence of chlorinated hydrocarbons in the unsaturated soils serves as a renewable source of groundwater contamination. As the water table fluctuates over time, the saturated portion of the flow system repeatedly comes in contact with contaminated soil (Gorelick, et. al., 1993). Each rise of the water table serves to recharge the contaminants in the groundwater. Infiltration from above also contributes to the contaminant distribution in groundwater. Once a chemical enters the groundwater regime, several transport mechanisms are present that may aid in the spreading of the contamination. These mechanisms include diffusion, advection, mechanical dispersion, and hydrodynamic dispersion.

Diffusion is the process by which a contaminant in water will move from an area of greater concentration toward an area where it is less concentrated. Diffusion will occur as long as a concentration gradient exists, even if the fluid is not moving, and as a result, a contaminant may spread away from the place where it is introduced into a porous medium. Diffusion may also occur when the concentration of a contaminant is higher in one stratum than in an adjacent stratum (Fetter, 1993) provided that the adjacent stratum has the requisite porosity.

Advection is the movement of dissolved solute with flowing groundwater (Gorelick et. al., 1993). The amount of contaminant being transported is a function of its concentration in the groundwater and the quantity of groundwater flowing, and advection will transport contaminants at different rates in each stratum.

Table 5-1. Physical Properties of Organic Contaminants at the North Belmont PCE Site

Chemical	Specific Gravity (g/cc)	Aqueous Solubility (mg/L)	Vapor Pressure (mm Hg)	Henry's Law (atm-m ³ mol)	Log K _{oc} (mL/g)	Log K _{ow}	Vapor Density (g/L)	Water Diffusion Coefficient (sq.cm/sec)	Est. Half-Life (days)	
									Soil	GW
Acetone	^a 0.79	—	^a 266	^a 3.9E-05	^a 0.43	^a 0.24	^a 2.37	—	^b 1-7	^b 2-14
Chloroform	^a 1.48	^a 8200	^a 160	^a 3.2E-03	^a 1.64	^a 1.95	^a 4.88	^a 9.1E-06	^b 28-180	^b 56-1800
1,1-DCA	^a 1.18	^a 5060	^a 182.1	^a 4.3E-03	^a 1.48	^a 1.78	^a 4.04	—	^b 32-154	^b 64-154
1,1-DCE	^a 1.22	^a 400	^a 495	^a 2.1E-02	^a 1.81	^a 2.13	^a 3.96	^h 9.5E-06	28-180	56-132
cis-1,2-DCE	^a 1.28	^a 3500	^{oc} 200@25°C	—	—	—	^{oc} 3.34	—	—	—
trans-1,2-DCE	^a 1.21	^a 6300	^a 265	0.384	^a 1.77	^a 2.09	^a 3.96	^c 9.5E-06	—	—
Methylene chloride	^a 1.33	^a 2000	^a 349	^a 2.0E-03	^a 0.94	^a 1.30	1.89	^c 1.1E-06	^b 7-28	^b 14-56
PCE	^a 1.62	^a 150	^a 14	121	^a 2.42	^a 2.60	^a 6.78	^c 7.5E-06	180-360	360-720
Toluene	^a 0.87	^a 490	^a 22	^a 6.7E-03	^a 2.06	^a 2.65	^a 3.77	—	^b 4-22	^b 7-28
1,1,1-TCA	^a 1.34	^a 300	^a 100	^a 1.8E-02	^a 2.18	^a 2.48	^a 5.45	ⁱ 8E-06	^h 140-273	^h 140-546
1,1,2-TCA	^a 1.44	^a 4500	^a 19	^a 9.9E-04	^a 1.75	^a 2.18	^a 5.45	^h 8E-06	^h 136-360	^h 136-720
TCE	^a 1.46	^a 1100	^a 57.8	87	^a 2.10	^a 2.53	^a 5.37	^c 8.3E-06	^c 180-360	^c 321-1653
TCFM	^a 1.49	^a 110	^a 687	^a 0.11	^a 2.20	^a 2.53	^a 5.85	4.415	180-360	360-720

Notes: — = Value not provided

a = Montgomery, J.H., and Welkom, L.M., 1990, Groundwater Chemicals Desk Reference, Lewis Publ., Chelsea, MI, 650p.

b = Howard, P.H., et. al., 1991, Handbook of Environmental Degradation Rates, Lewis Publ., Chelsea, MI, 725p.

c = Lucius, J.E., et. al., 1990, Properties and Hazards of 108 Selected Substances, USGS Open File Report, 90-408, 559p.

h = Tetra Tech, Inc., 1988, Chemical Data for Predicting the Fate of Organic Chemicals in Water, Vol.2, Database EPRI EA-5818, Vol.2, Elec. Power Res. Inst., Palo Alto, CA, 411p.

i = Mendoza, C.A., and Frind, E.O., 1990b, Advective-Dispersive Transport of Dense Organic Vapors in the Unsaturated Zone, 2. Sensitivity Analysis, Water Res., Vol.26, p.388-398.

oc = Verschuren, K., 1983, Handbook of Environmental Data on Organic Chemicals, 2nd Ed., Van Nostrand, Reinhold, NY, 131p.

Table 5-2. Physical Properties of Organic Contaminants

Property	Range	Qualitative Description	Source
Sorption- Soil Adsorption Coefficient (K_{cc})	< 10	Very weakly sorbed	Little, A.D. Inc., 1989
	10 - 100	Weakly sorbed	
	100 - 1000	Moderately sorbed	
	1000 - 10,000	Moderately to strongly sorbed	
	10,000 - 100,000	Strongly sorbed	
	> 100,000	Very strongly sorbed	
Mobility- Based on a combination of solubility(s) (mg/L) and soil adsorption (K_{cc})	$x > 3500$ and $K_{cc} < 50$	Very high mobility	Cohen and Mercer, 1993; Ney, 1990
	$3500 > s > 850$ and $50 < K_{cc} < 500$	High mobility	
	$800 > s > 150$ and $150 < K_{cc} < 2000$	Moderate mobility	
	$150 > s > 15$ and $500 < K_{cc} < 20,000$	Low mobility	
	$15 > s > 0.2$ and $2000 < K_{cc} < 20,000$	Slight mobility	
	$s < 0.2$ and $K_{cc} > 20,000$	Immobile	
Volatility- Henry's Law Constant - (H) (atm m ³ /mol)	$H < 3 \times 10^{-7}$	Non-volatile	Fetter, C.W., 1988
	$3 \times 10^{-7} < H < 10^{-5}$	Low volatility	
	$10^{-6} < H < 10^{-3}$	Moderate volatility	
	$H > 10^{-3}$	High volatility	

Groundwater flow through different porous media occurs at variable rates due to the arrangement of particles in the subsurface. As contaminated groundwater travels through the stratum, the fluid does not all travel at the same velocity, and as a result, mixing occurs along the flow path. This mixing is termed mechanical dispersion, and it results in a dilution of the contaminant at the advancing edge of flow (Fetter, 1993).

Mechanical dispersion is composed of two contaminant front mixing methods - longitudinal and transverse dispersion. Longitudinal dispersion occurs along the direction of the flow path, while transverse dispersion occurs normal to the flow path and causes lateral spreading of the contaminant. Mechanical dispersion and diffusion combine in groundwater flow to create hydrodynamic dispersion. This process begins when a contaminant enters the aquifer. Once introduced, the advecting groundwater carries the mass of contaminant with it, and in the process, the contaminant spreads, thereby decreasing the maximum concentration with time. However, the contamination is now spread over a much wider area.

The adsorption of a solute onto an aquifer material (e.g., clay) results in a reduction of concentration in the aqueous phase and a retardation of the velocity of contaminant migration. The degree of retardation experienced by a particular organic contaminant will depend on the fraction of organic carbon (f_{oc}) of the aquifer materials. The higher the f_{oc} , the more sites there are available for adsorption.

5.2.4 Contaminant Transport — Surface Water

During the NCDEHNR Site Investigation of June 1992, a surface water sample was collected "from near the bridge on Acme Road, approximately 1,200 feet downstream of the site drainage to the intermittent creek" (NCDEHNR, 1993). This sample was analyzed for VOC content and revealed two compounds at or above detection limits. The two compounds and the concentrations of the compounds were, respectively: 1,1,1-trichloroethane at 11 $\mu\text{g/L}$ and PCE at 5 $\mu\text{g/L}$. The PCE detection was an estimated value. During the October 1996 sampling effort by SESD, two compounds were detected in one surface water sample. However, the compounds, cis-1,2-dichloroethene and chloroform, were detected at estimated concentrations.

Once the contaminant has entered the regime of the stream, various processes, including volatilization, chemical reaction, air-water exchange, and biologic interaction, will act to reduce the concentration or degrade the chemical form. Depending upon water temperature in the stream and dissolved oxygen content of the water, the contaminant will diminish downstream due to mass transfer to the air (volatilization). In addition, a contaminant in a stream that is flowing and has turbulent activity will partition substantially into air from water if the aqueous solubilities of these substances are commensurately low.

The reactivity and solubility of an organic chemical in water will also affect the concentration of the substance. In certain situations, a chemical of interest may be involved in a rapid, reversible transformation in the water phase. Such a reaction results in the alteration of the overall rate of diffusive transport. Depending upon the presence or absence of polar and nonpolar compounds in the water, the organic chemical may bind to another compound transforming the chemical into another compound, become bound to another compound without changing form, or not bind to another compound but undergo other reactions or transformations (Schwarzenbach et. al., 1993).

Organic chemicals may also be transformed by biologic interaction in surface waters. Microorganisms, plants, and animals may uptake or act to bind the chemical, transforming the chemical structure or removing the chemical from the possibility of further interaction. Depending upon the biologic health and interaction of the surface water body, an organic chemical may be rapidly transformed or affixed to plant tissues or other compounds via the biologic agent. Schwarzenbach et. al., (1993) thoroughly discusses biological transformation reactions.

5.2.5 Degradation Mechanisms in the Natural Environment

There are several mechanisms active within the natural environment that affect the transport and persistence of chemicals once they are released to the environment. These mechanisms include:

1. Phototransformation
2. Biodegradation
3. Metabolic reactions/Bioaccumulation
4. Hydrolysis
5. Dissociation/Redox reactions
6. Sorption

Each of these mechanisms, except for sorption which was discussed above, are introduced in this section.

Phototransformation, the degradation of a chemical through absorption of sunlight, will occur as long as the chemical can absorb sunlight, and can occur in air, soil, or water, and on surfaces of water, soil, plants, and animals. Environmental influences such as depth of the chemical in soil and water, sorption to soil, sensitizers, and pH, can have an effect on the rate of phototransformation. The rate of phototransformation is the time that it takes for a parent chemical to be transformed to one-half ($t_{1/2}$) of its original amount. This rate could differ in soil, in water, and on surfaces. The faster the rate, the less likelihood of continued exposure in the environment. If the phototransformation half-life is less than 30 days, then accumulation, bioaccumulation, or food-chain contamination is unlikely; if it is 30 to 90 days, some food-chain contamination is possible; and if it is greater than 90 days, food-chain contamination is likely (Ney, 1990).

Biodegradation is the biological process by which aerobic microbes or anaerobic microbes break down organic chemicals to either a higher- or a lower-molecular-weight chemical(s). This is a very important process by which soil microbes or aquatic microbes can detoxify chemicals (Ney, 1981); however, the process may also result in the formation of a more toxic chemical. Chemicals that are highly water-soluble can biodegrade, but those with low water solubility usually will not.

Reduction of the concentration of a particular organic contaminant due to biological transformation does not ensure a reduction in toxicity. Many of the daughter products of transformation processes are as toxic, or more toxic, than their parents. Biotransformation of TCE, for example, can result in the formation of vinyl chloride, which is more toxic (and stable) than its parent (Gorelick et. al., 1993).

Hydrolysis is one of the most important mechanisms in the environment for the breakdown of a parent chemical (Ney, 1981). It occurs in soils, water, plants, animals, and possibly air. The hydrolysis of pesticides has even occurred on plant surfaces. Hydrolysis is the chemical interaction of water with the contaminant which alters the chemical's structure and, in turn, alters its transport within the environment. Many environmental factors influence the rate of hydrolytic degradation such as temperature, pH, solubility, sunlight, ad- or absorption, and volatility. The rate of hydrolyzation of a chemical is the time that it takes for one-half of the original concentration ($t_{1/2}$) of the chemical to become structurally altered (Ney, 1990).

Bioaccumulation is the uptake of chemicals by a plant or animal, and the storage of the chemicals or its degradation product within the tissues of that organism. Metabolic reactions involve uptake by plants into their root systems and uptake by animals through normal feeding habits. These reactions produce metabolites. These metabolites are usually translocated throughout the plant. Also, animals producing metabolites translocate these throughout their bodies.

Dissociation or ionization of a chemical takes place in the solid, aqueous, or volatilized state. The ionization takes place when the chemical becomes electrically charged through the loss or gain of electrons. When an atom, molecule, or ion loses electrons, it is oxidized; when electrons are gained, it is reduced. These reactions are referred to as oxidation-reduction, or redox, reactions.

Oxidation typically involves the loss of electrons during a chemical reaction. In general, substituted aromatic compounds such as ethylbenzene, naphthalene, and phenol can be oxidized. Oxidation rates for aromatic compounds are typically an order of magnitude faster than for chlorinated aliphatic compounds. Overall, abiotic (without biological life) oxidation of organic compounds in groundwater systems is extremely limited (Olson and Davis, 1990).

Reduction reactions transfer electrons to a compound. For a chlorinated aliphatic compound, this results in a less chlorinated compound (e.g., the formation of vinyl chloride from 1,1-DCE). Dehydrohalogenation involves the loss of both a hydrogen ion and a halogen, and the resultant formation of a double carbon bond (e.g., the formation of dichloroethene from trichloroethane).

Aromatic hydrocarbons are typically flammable liquids that have lower densities and boiling points than the chlorinated hydrocarbons. They are moderately soluble in water, have high volatilities, high mobilities, and have moderate partition coefficients.

Chlorinated ethanes and chlorinated ethenes have been found to undergo degradation. Degradation is defined as the process of an organic molecule becoming smaller by chemical or biological means (Fetter, 1993). Figure 5-1 illustrates the degradation of PCE and TCE, due to substitution, dehydrohalogenation, oxidation, or reduction reactions.

Environmental conditions influencing the type and rate of these reactions include pH, temperature, state of oxidation or reduction, microorganisms present, and types of other chemicals present.

5.3 SITE-SPECIFIC FATE AND TRANSPORT

5.3.1 Introduction and Objective

Roy F. Weston, Inc., (WESTON®) completed an analytical fate and transport model for the tetrachloroethene (PCE) plume observed in groundwater in the saprolite and bedrock at the Site. The objective of this modeling effort was to estimate the distance that the PCE plume will travel downgradient of the presumed source area before degrading below applicable regulatory levels (the Federal Maximum Contaminant Level (MCL) and North Carolina Drinking Water Standards (NCDWS) of 5.0 micrograms per liter ($\mu\text{g/L}$) and the North Carolina Groundwater Quality Standard (NCGWQS) of 0.7 $\mu\text{g/L}$).

The following text outlines the field activities completed, summarizes the methodologies employed for the modeling effort, and discusses the results obtained.

5.3.2 Background

The results of the environmental investigation at the Site indicate that elevated levels of PCE exist in weathered bedrock (saprolite) and competent bedrock groundwater. The highest PCE concentration detected in the groundwater within the saprolite was 2,500 $\mu\text{g/L}$ in MW-6 and the highest PCE concentration noted in groundwater in the bedrock was 3,500 $\mu\text{g/L}$ in CW-6. Consequently, this modeling effort has focused on groundwater in both the saprolite and the bedrock. Furthermore, groundwater-quality data for the Site indicates that concentrations of trichloroethene (TCE) and cis-1,2-Dichloroethene (cis-1,2 DCE) were detected in excess of NCGWQSs. However, these compounds were detected at lower concentrations and therefore were not evaluated in this modeling effort.

5.3.3 Field Activities and Results

Groundwater level measurements, slug testing, and groundwater sampling performed by WESTON were utilized in developing the site conceptual model. The results of these activities are summarized below.

5.3.3.1 Groundwater-Level Measurements/Hydraulic Gradient

In October 1996, groundwater levels were measured in monitor wells MW-1 through MW-22 and CW-1 through CW-9 and referenced to surveyed top-of-casing elevations. Using these data, a hydraulic gradient of 0.0298 foot per foot (ft/ft) and 0.0275 ft/ft were calculated for the saprolite and bedrock, respectively.

5.3.3.2 Slug Testing

Rising head slug tests were performed in monitor wells MW-6 through MW-22 in January 1997. Using the Bouwer-Rice (Bouwer and Rice, 1976) and the Hvorslev (Hvorslev, 1951) methods, hydraulic conductivities were calculated for wells screened in the saprolite and in the bedrock. **Tables 5-3** and **5-4** display the hydraulic conductivities calculated from slug test data for the saprolite and bedrock, respectively. Appendix A contains data and graph sheets for each slug test method solution for each monitor well.

Table 5-3. Hydraulic Conductivities in the Saprolite at the North Belmont PCE Site in January 1997

Well	Hydraulic Conductivity (ft/day)	
	Bouwer-Rice	Hvorslev
MW-6	0.56	0.50
MW-7	0.78	0.71
MW-8	0.24	0.27
MW-9	1.22	1.23
MW-10	1.34	1.57
MW-11	1.25	1.31
MW-12	1.93	1.91
MW-13	1.94	1.99

Table 5-4. Hydraulic Conductivities in the Bedrock at the North Belmont PCE Site in January 1997.

Well	Hydraulic Conductivity (ft/day)	
	Bouwer-Rice	Hvorslev
MW-14	0.066	0.057
MW-15	0.55	0.48
MW-16	0.46	0.44
MW-17	0.52	0.52
MW-18	2.87	2.56
MW-19 ¹	0.019	0.016
MW-20	2.06	1.83
MW-21	3.41	3.18
MW-22	2.38	2.16

NOTE: ft/day: feet per day

¹ not used to calculate geometric mean

The geometric mean of the saprolite hydraulic conductivity values is 0.98 ft/day and the geometric mean of the bedrock hydraulic conductivity values is 0.90 ft/day. The data from well MW-19 was not used in the calculation due to its anomalously low hydraulic conductivity and location (south of the modeled area).

5.3.3.3 Groundwater Sampling

Groundwater samples were collected from wells MW-4, MW-6 through MW-22, CW-1, and CW-5 through CW-8 in October 1996. Samples were analyzed for VOCs, SVOCs, pesticides, PCBs, and total metals content. However, for the purposes of the modeling effort, only the VOC data will be utilized (see Section 4.0 for the analytical results).

5.3.4 Transport Modeling Calculations

The analytical transport model BIOSCREEN was used to estimate the downgradient attenuation of PCE. The BIOSCREEN model was developed by the US Air Force Center for Environmental Excellence (AFCEE) and EPA, and is based on the Domenico analytical solute transport model. This model was developed to determine natural attenuation of fuel compounds, but can also be used for chlorinated compounds if the first-order decay coefficient is used to predict biodegradation. BIOSCREEN is a very flexible model in that it allows the use of separate decay coefficients for the solute (groundwater) phase and the source. It can also estimate dispersion parameters from plume length. The model parameters input into the BIOSCREEN model are presented in **Table 5-5**. Input screen and centerline screen printout for the modeling effort are found in Appendix C.

Table 5-5. BIOSCREEN Model Input Parameters for the North Belmont PCE Site

Model	Saprolite	Bedrock	Source
Hydrogeology			
Hydraulic Conductivity (ft/day)	0.98	0.90	Measured
Hydraulic Gradient (ft/ft)	0.0298	0.0275	Measured
Porosity	0.10	0.103	Estimated from model
Dispersion			
Longitudinal Dispersivity (ft)	22.2	32.1	Estimated from plume length
Transverse Dispersivity (ft)	2.2	3.2	Estimated from plume length
Adsorption			
Bulk Density (g/cm ³)	1.7	2.2	Davis & DeWiest, 1966
Partition Coefficient (K _{oc})	318	318	Montgomery, 1991
Fraction Organic Carbon	0.001	0.0001	Measured/Model Estimate
Biodegradation			
Solute Half-Life (years)	4	3.4	Howard et al, 1991/Model Estimate
Source Half-Life (years)	6	8-9	(Howard et al, 1991/Model Estimate)
Initial Source Concentration (µg/L)	25,000	17,000	Model Estimate

Average groundwater velocity was calculated according to the following equation:

$$\text{Velocity} = \frac{\text{hydraulic gradient} \times \text{hydraulic conductivity}}{\text{effective porosity}}$$

Using the hydraulic gradient of 0.0298 ft/ft, the geometric mean hydraulic conductivity of 0.98 ft/day and an effective porosity of 0.1, a groundwater velocity of 106 ft/year was calculated for the saprolite. Using the hydraulic gradient of 0.0275 ft/ft, the geometric mean hydraulic conductivity of 0.90 ft/day and an effective porosity of 0.1, a groundwater velocity of 87.6 ft/year was calculated for the bedrock.

The retardation factor of PCE in the soil present at the Site was calculated using the following equation:

$$R_d = \frac{P_b \times (K_{oc} \times f_{oc})}{n_e} + 1$$

Where:

R_d	=	Retardation Factor
P_b	=	Bulk Density
n_e	=	Effective Porosity
K_{oc}	=	Organic Carbon Distribution Coefficient for PCE
f_{oc}	=	Organic Carbon Content of Soil

Using a bulk density of 1.7 g/cm³, an effective porosity of 0.1, an organic carbon distribution coefficient of 318 ml/g (Montgomery, 1991), and an average organic carbon content in the soil of 0.001, the resulting retardation factor is 6.4 for the saprolite. This retardation factor was used to adjust the average groundwater velocity to reflect an average contaminant velocity in the saprolite using the following relationship:

$$R_d = v/v_c$$

Where:

R_d	=	Retardation Factor
v	=	Average Groundwater Velocity
v_c	=	Contaminant Velocity

Using the saprolite retardation factor of 6.4 and the saprolite average groundwater velocity of 106 ft/year, the resulting contaminant velocity for the saprolite is estimated as 16.6 ft/year. Using the same equation and the values listed in **Table 5-5**, the contaminant velocity for the bedrock is estimated as 51.5 ft/year. These values were entered into BIOSCREEN to represent contaminant flow conditions at the Site. The modeling involved two stages: simulating the current (October 1996) observed conditions at the Site following a hypothetical release, then using the information derived to simulate future contaminant transport. To simulate the current plume, a source of PCE was introduced into the model domain at the location of well MW-14. The duration of the initial simulation was estimated based upon the minimum elapsed time (21 years) since closure of the Site (1975). The strength of the source, the seepage velocity, and the

biodegradation values were adjusted during the initial time step until the predicted concentrations approximated the current measured values (analyses from MW-6, CW-5, MW-12, and MW-8 were used for the saprolite model and analyses from CW-6, MW-16, CW-7, and MW-22 were used for the bedrock model).

The bedrock groundwater was modeled in two ways. First, the bedrock was modeled with the source area located in the vicinity of well CW-6, due to the high PCE concentration at this location. Secondly, the bedrock was modeled with the source area in the vicinity of well MW-14 with the groundwater at CW-6 treated as a migrating high concentration slug. However, this model ultimately had two problems. First, the model could not predict the PCE contamination in well MW-22 (i.e., contamination could not be modeled as traveling this far) and the model required a much greater source concentration with a lower half-life than the solute phase. Therefore, modeling CW-6 as the source location of the bedrock groundwater contamination has been determined to be a more accurate representation of the chemical and physical characteristics of the Site.

Once the models had been calibrated, the predictions were repeated at five-year intervals until all predicted concentrations were below 5 µg/L and 0.7 µg/L, respectively. The approximate migration distances from the source area for the 5.0 µg/L and 0.7 µg/L iso-concentration contours in the saprolite are presented in **Table 5-6** and the approximate migration distances from the source area for the 5.0 µg/L and 0.7 µg/L iso-concentration contours in the bedrock are presented in **Table 5-7**.

Table 5-6. Estimated Contaminant Migration Distances for the Saprolite at North Belmont PCE Site.

Time (from years present)	Distance from Source Area to Downgradient Iso-concentration Contour Line (feet)	
	5.0 µg/L	0.7 µg/L
0 (current)	500-600	600-700
5	600-700	700-800
10	700	800-900
15	700-800	800-900
20	720-800	900-1,000
25	700-800	900-1,000
30	600-700	900-1,000
35	400-500	900-1,000
40	200-300	900-1,000
50	100	700-800

Note: µg/L = Micrograms per liter

Table 5-7. Estimated Contaminant Migration Distances for the Bedrock at the North Belmont PCE Site

Time (from years present)	Distance from Source Area to Downgradient Iso-concentration Contour Line (feet)	
	5.0 µg/L	0.7 µg/L
0 (current)	1,400	1,600
5	1,600-1,800	1,800-2,000
10	1,600-1,800	2,000
15	1,600	2,100
20	1,400	2,250
25	1,200-1,400	2,200
30	1,000-1,200	2,100
35	1,000	1,800
40	800	1,600
50	400-600	1,200-1,400

Note: µg/L = Micrograms per liter

Based on the input data and modeling results, the PCE plume in the saprolite is predicted to completely attenuate below the MCL of 5.0 µg/L within approximately 60 years, and below the NCGWQS of 0.7 µg/L within approximately 80 years. The PCE plume in the bedrock is predicted to completely attenuate below the MCL of 5.0 µg/L within approximately 80 years, and below the NCGWQS of 0.7 µg/L within approximately 100 years.

Certain assumptions were made in the above calculations and apply to the results described:

1. Concentrations in the wells were assumed to be indicative of the center of plume at the appropriate distance from the source.
2. The PCE concentration in MW-6 and CW-6 are currently the highest concentrations in the saprolite and bedrock groundwater, respectively and also represent the source locations.
3. The contaminant attenuation observed between the modeled wells is approximately representative of conditions across the Site.
4. The direction of groundwater flow is horizontal and vertical flow between the saprolite and bedrock is negligible.
5. The saprolite and bedrock are homogeneous, isotropic, and of uniform thickness.
6. Recharge rates are insignificant relative to regional flow.
7. Groundwater flow directions and velocities are constant over time.

5.3.5 Sensitivity Analysis

A sensitivity analysis was performed on the following variables utilized in the model calibrations: effective porosity, fraction of organic carbon, and half-lives. These are the only variables used in the model calculations which were not empirically-determined.

Four successive model iterations were completed in which the value of one variable was increased or decreased by 25%. Following each alteration, the time required for the plume to dissipate below 5.0 µg/L was determined, as well as the maximum distance the plume traveled above 5.0 µg/L.

The concentration of 5.0 µg/L was used because this is the MCL for PCE. The results of the sensitivity analysis for the saprolite are presented in **Table 5-8**.

Table 5-8. Sensitivity Analysis Results for the North Belmont PCE Site Modeling Effort.

Iteration No.	Scenario	Time after which plume will be below 5.0 µg/L (years)	Maximum Distance from source area after which plume will be below 5.0 µg/L (feet)/years
1	Calibrated Values	60	700-800/20
2	Increase f_{oc} 25%	60	600-700/20
3	Decrease f_{oc} 25%	60	900-1,000/20
4	Increase n_e 25%	60	700-800/20
5	Decrease n_e 25%	60	800/20
6	Increase sol-half 25%	60	900-1,000/30
7	Decrease sol-half 25%	60	600-700/10
8	Increase source-half 25%	40	700-800/20
9	Decrease source-half 25%	80	700-800/20
10	Increase source conc. 25%	60	700-800/20
11	Decrease source conc. 25%	60	700-800/25

Note: µg/L = Micrograms per liter

The sensitivity analysis for these variables shows that, under conservative assumptions, for each of these variables except source half-life (a 25% change in source half-life induced an approximate 35% change), the plume attenuated to below 5.0 µg/L in approximately 60 years.

The maximum distance the plume traveled above MCLs was most affected by the solute (groundwater) half-life (which also affected the timing of this event) and the fraction of organic carbon.