

Section 5

Compound Fate and Transport

This section provides a general overview of the processes that affect the fate and transport of COCs in groundwater in the SFB. A detailed description of these processes, including relevant equations and technical references, was provided in the 1992 RI Report (JMM 1992). Because the physical constraints of the SFB on fate and transport are generally static, this section summarizes and updates the 1992 RI discussion with site-specific data collected since that time, which includes geotechnical data on soil properties presented in Table 2-4 (e.g., F_{oc} and effective porosity) and an updated list of COCs.

Fate and transport of contaminants in a basin such as the SFB is highly complex and related to a number of physical and chemical characteristics that are mostly approximated. This discussion is meant to provide a general overview of these processes, but a better approximation of these processes and the effect of the contaminants on future pumping is provided through the updated SFB groundwater model introduced in Section 6 of this report and used as part of remedial alternative selection in the Draft FS. This section is meant to forward a basic understanding of the contaminant dynamics in the SFB and the basis for the modeling of groundwater flow and contaminant transport in Section 6.

5.1 Chemical Properties

The properties of a chemical have significant impacts on the fate and transport of that chemical in groundwater. Chemicals that have high solubility generally have low adsorption and low ability to volatilize, and the opposite is true for low-solubility chemicals. These chemical properties are important for understanding how a chemical may behave and will form the basis for the chemical component of the modeling described further in Section 6. A summary of the chemical properties of the COCs, as taken from the USEPA RSLs (USEPA 2014b), are presented below:

- **Molecular weight:** The molecular weight of the compound is used for conversions such as concentration to molar units.
- **Density:** Density is a measure of the mass of a compound per unit volume. Compounds of higher density will tend to migrate vertically through the saturated zone, with lighter compounds staying near the water table.
- **Henry's Law Constant:** A measure of the ability of a chemical in aqueous solution to volatilize with low values indicating a chemical that is more likely to partition into air.
- **Water solubility:** The ability for a chemical to dissolve into water. High-solubility chemicals tend to remain in solution and have greater potential for mobility in the environment.
- **Soil organic carbon-water partition coefficient (K_{oc}):** The ratio of the mass of an organic chemical adsorbed to organic matter in soil versus mass of a chemical in solution. This value is based on several factors and taken directly from the USEPA RSL table.
- **Distribution coefficient (K_D):** The degree to which a chemical will preferentially dissolve in water or adsorb to particle surface or organic materials in the saturated zone. For organic chemicals, this is a product of the soil organic carbon-water partition coefficient (K_{oc}) and the F_{oc} in soil. In Table 5-1 a minimum and maximum K_D value was calculated for the organic compounds based on the variability in F_{oc} data collected during the well installation as described in Section 2.6.2.

Table 5-1. Chemical Properties of COCs in SFB Groundwater									
Chemical	Molecular Weight	Henry's Law Constants	Density	Water Solubility	Soil Organic Carbon-Water Partition (Koc) Coefficient (L/kg)	Distribution Coefficient (Kd) (L/kg)		Retardation Factor	
		(unitless)	(g/cm ³)	(mg/L)		MIN	MAX	MIN	MAX
TCE	131	0.4026983	1.5	1280	60.7	6.07E-03	6.98E-02	1.0	2.5
PCE	166	0.7236304	1.6	206	94.94	9.49E-03	1.09E-01	1.0	3.3
1,1-DCE	97	1.0670482	1.2	2420	31.82	3.18E-03	3.66E-02	1.0	1.8
CR VI	52	--	5.2	1.7E+06	--	--	--	--	--
CTET	154	1.1283729	1.6	793	43.89	4.39E-03	5.05E-02	1.0	2.1
1,2-DCA	99	0.048242	1.2	8600	39.6	3.96E-03	4.55E-02	1.0	2.0
PERCHLORATE	117	--	2.5	2.5E+05	--	--	--	--	--
1,4-DIOXANE	88	0.0001962	1.0	1.0E+06	2.633	2.63E-04	3.03E-03	1.0	1.1
1,2,3-TCP	147	0.0140229	1.4	1750	115.8	1.16E-02	1.33E-01	1.1	3.8
cis-1,2-DCE	97	0.1668029	1.3	6410	39.6	3.96E-03	4.55E-02	1.0	2.0
NDMA	74	0.0000744	1.0	1.0E+06	22.79	2.28E-03	2.62E-02	1.0	1.6
Nitrate (as NO3)	62	--	1.7	1.1E+06	--	--	--	--	--
ARSENIC	75	--	5.8	--	--	29		1.32E+02	6.17E+02
URANIUM, TOTAL	238	--	19.1	--	--	450		2.04E+03	9.56E+03
MANGANESE	55	--	7.3	--	--	65		2.96E+02	1.38E+03
MERCURY	201	0.467	13.5	0.06	--	52		2.37E+02	1.11E+03
1,1-DICHLOROETHANE	99	0.2297629	1.2	5040	31.82	0.003182	3.66E-02	1.0	1.8
TRICHLOROFUOROMETHANE	137	3.9656582	1.5	1100	43.89	0.004389	5.05E-02	1.0	2.1
SULFATE (AS SO4)	96	--	2.7	7.50E+05	--	--	--	--	--
IRON	56	--	7.9	--	--	25		1.14E+02	5.32E+02
1,1,1-TRICHLOROETHANE	133	0.7031889	1.3	1290	43.89	0.004389	5.05E-02	1.0	2.1
CHLORIDE (AS CL)	35	--	2.2	--	--	--	--	--	--
BORON	14	--	2.3	--	--	3		1.46E+01	6.47E+01
NITROGEN, NITRITE	47	--	1.7	1.1E+06	--	--	--	--	--
FLUORIDE	38	--	2.6	1.69	--	150		6.81E+02	3.19E+03
ASBESTOS	--	--	2.0	--	--	--	--	--	--
CHLORATE	--	--	2.5	--	--	--	--	--	--
CHROMIUM, TOTAL	52	--	7.2	--	--	1.80E+06		8.16E+06	3.8.E+07
ALUMINUM	27	--	2.7	--	--	1.5E+03		6798	31855
NICKEL	75	--	8.9	--	--	65		296	1381
THALLIUM		--	11.8	--	--	71		323	1509
ANTIMONY	122	--	6.7	--	--	45		205	957
LEAD	207	--	11.3	--	--	900		4079	19113
CADMIUM	112	--	8.7	--	--	75		341	1594
VANADIUM	51	--	6.0	--	--	1000		4532	21237

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Chemical	Molecular Weight	Henry's Law Constants	Density	Water Solubility	Soil Organic Carbon-Water Partition (Koc) Coefficient (L/kg)	Distribution Coefficient (Kd) (L/kg)		Retardation Factor	
		(unitless)	(g/cm ³)	(mg/L)		MIN	MAX	MIN	MAX
CYANIDE	26	0.0054374	0.7	1.0E+06	--	9.9		46	211
BERYLLIUM	9	--	1.9		--	790		3581	16777
COPPER	64	--	9.0		--	35		160	744
SELENIUM	79	--	4.8		--	5		24	107
ZINC	65	--	7.1		--	62		282	1318
BARIUM	137	--	3.6		--	41		187	872
SILVER	108	--	10.5		--	8.3		39	177
PCB-1248 (AROCLOR 1248)	292	0.0179886	--	0.1	76,530	7.653	8.8E+01	35.7	1870
PCB-1254 (AROCLOR 1254)	326	0.0115699	--	0.043	130,500	13.05	1.5E+02	60.1	3188
PCB-1016 (AROCLOR 1016)	258	0.0081766	--	0.42	47,700	4.77	5.5E+01	22.6	1166
PCB-1242 (AROCLOR 1242)	292	0.0077678	--	0.277	78,100	7.81	9.0E+01	36.4	1908
PCB-1260 (AROCLOR 1260)	395	0.0137367	--	0.0144	349,700	34.97	4.0E+02	159.5	8541
PCB-1221 (AROCLOR 1221)	189	0.0300899	--	15	8,397	0.8397	9.7	4.8	206
PCB-1232 (AROCLOR 1232)	189	0.0300899	--	1.45	8,397	0.8397	9.7	4.8	206
BIS(2-ETHYLHEXYL) PHTHALATE	391	0.000011	1.0	0.27	119,600	11.96	1.4E+02	55.2	2922
METHYLENE CHLORIDE	85	1.30E-01	1.3	1.30E+04	1	0.00013	1.50E-03	1.0	1.0
VINYL CHLORIDE	63	1.1365495	0.9	8800	22	0.002173	2.50E-02	1.0	1.5
TERT-BUTYL ALCOHOL	74	0.0003704	0.8	181000	3	0.0002919	3.36E-03	1.0	1.1
BENZENE	78	0.2269011	0.9	1790	146	0.01458	1.68E-01	1.1	4.6
1,1,2-TRICHLOROETHANE	133	0.0336877	1.4	4590	61	0.00607	6.98E-02	1.0	2.5
1,2-DIBROMO-3-CHLOROPROPANE	236	0.0060098	2.1	1230	116	0.01158	1.33E-01	1.1	3.8
TRANS-1,2-DICHLOROETHENE	96.94	1.70E-01	1.3	4.50E+03	40	0.00396	4.55E-02	1.0	2.0
NAPHTHALENE	128.18	0.0179886	1	31	1,544	0.1544	1.78E+00	1.7	38.7
METHYL TERT BUTYL ETHER (MTBE)	88	0.0239984	0.7	51000	12	0.001156	1.33E-02	1.0	1.3
N-NITROSODI-N-PROPYLAMINE	130	0.00022	0.9	13000	275	0.02754	3.17E-01	1.1	7.7
BENZO(A)PYRENE	252	1.90E-05	--	1.60E-03	587,400	58.74	6.76E+02	267	14346
1,1,1,2-TETRACHLOROETHANE	167.85	0.1022077	1.5406	1070	86	0.008603	9.89E-02	1.0	3.1
TOLUENE	92.14	0.2714636	0.8623	526	234	0.02339	2.69E-01	1.1	6.7
PENTACHLOROPHENOL	266	1.0016E-06	1.978	14	4,959	0.4959	5.70E+00	3.2	122
HEXACHLOROBENZENE	285	0.0695012	2	0.0062	6,195	0.6195	7.12E+00	3.8	152
1,4-DICHLOROBENZENE	147	0.0985282	1.2475	81.3	375	0.03753	4.32E-01	1.2	10
ETHYLBENZENE	106.17	0.3221586	0.8626	169	446	0.04461	5.13E-01	1.2	12
1,2,4-TRIMETHYLBENZENE	120.2	0.2518397	0.875	57	4	0.000363	4.17E-03	1.0	1.1
1,2-DICHLOROPROPANE	112.99	0.1152903	1.159	2800	61	0.00607	6.98E-02	1.0	2.5
1,2-DIBROMOETHANE	163.83	0.0866721	1.98	3030	32	0.003182	3.66E-02	1.0	1.8

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Chemical	Molecular Weight	Henry's Law Constants	Density	Water Solubility	Soil Organic Carbon-Water Partition (Koc) Coefficient (L/kg)	Distribution Coefficient (Kd) (L/kg)		Retardation Factor	
		(unitless)	(g/cm ³)	(mg/L)		MIN	MAX	MIN	MAX
4-METHYL-2-PENTANONE	100.16	0.0056419	0.7965	19000	13	0.00126	1.45E-02	1.0	1.3
1,3,5-TRIMETHYLBENZENE	120	0.3585446	0.8615	48	3	0.00034	3.91E-03	1.0	1.1
CHLOROBENZENE	113	0.1271464	1.1	498	234	0.0234	2.69E-01	1.1	6.7
N-PROPYLBENZENE	120.2	0.4292723	0.8593	52.2	4	0.000369	4.24E-03	1.0	1.1
CARBON DISULFIDE	76.13	0.5887163	1.2632	2160	22	0.002173	2.50E-02	1.0	1.5
TOTAL, 1,3-DICHLOROPROPENE	111	0.1451349	1.2	2800	2	0.000204	2.35E-03	1.0	1.0
1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE	187	21.504497	1.6	170	197	0.0197	2.27E-01	1.1	5.8
ATRAZINE	215.69	9.6484E-08	--	34.7	225	0.02245	2.58E-01	1.1	6.5

Fraction of Organic Carbon (Minimum): 1.00E-04

Fraction of Organic Carbon (Maximum): 1.15E-03

Bulk Density (g/cm³) (Minimum): 1.45

Bulk Density (g/cm³) (Maximum): 1.89

Effective Porosity (Minimum): 0.089

Effective Porosity (Maximum): 0.32

g/cm³ = grams per cubic centimeter

mg/L = milligrams per liter

L/kg = liters per kilogram

Koc = organic carbon partitioning coefficient

Kd = distribution coefficient

Table 5-1 includes the chemical properties including molecular weight, Henry's Law Constant, density, solubility, K_{oc} , and K_D values for several of the chemicals identified as COCs in Section 4.2.

5.2 Transport Processes

The movement of VOCs and inorganic chemicals in the subsurface is highly dependent on their mobility in groundwater. Several processes, such as advection, dispersion, diffusion, and sorption/desorption, affect the site-specific mobility of these compounds in the soil-water matrix in the SFB and are defined below. As stated in the 1992 RI, these parameters can vary significantly even within a small area both horizontally and vertically, so the descriptions below are averages or in some cases a range of values based on field data.

5.2.1 Advection and Dispersion

Advection and dispersion processes are primary controls on migration of compounds in groundwater systems, especially systems with relatively high groundwater velocities, groundwater pumping, and several productive groundwater zones. Under natural flow conditions in basins such as the SFB, these processes control the speed and relative spread of the plume as it moves downgradient, with the plume migrating with the flow of groundwater and spreading as it moves downgradient. In areas where pumping is occurring, advection becomes even more of a dominant process as the production wells capture contaminant plumes and pull the plumes toward the production wells.

Advective transport is the movement of the dissolved compound at an average solute velocity that is directly proportional to the average groundwater flow velocity and inversely proportional to chemical retardation (sorption). In areas with high hydraulic conductivities and resulting high groundwater flow velocities, advection is the dominant transport mechanism. As presented in the 1992 RI, natural groundwater velocities (outside of the influence of pumping) range from 290 up to 1,330 feet per year (JMM 1992). Velocities near the production wells increase during pumping with a rapid increase in velocity as water travels closer to the screen interval.

Macroscopic hydrodynamic dispersion, which is a measure of how far a plume deviates from the direction of groundwater flow, includes the effects of two processes:

- *Molecular diffusion* is the movement of the dissolved compound through the aqueous phase as a result of a concentration gradient of that compound, but is generally not significant relative to advection and mechanical dispersion in an aquifer. However, this process can be a long-term source of VOCs through diffusion from secondary sources such as lower-permeability materials to higher-permeability materials in an aquifer.
- *Mechanical dispersion*, which causes the 3D spreading of compounds in the aquifer, is a linear function of the groundwater flow velocity and the aquifer dispersivity and will increase with increasing aquifer heterogeneity. Longitudinal dispersion, which occurs in the direction of flow, is usually much greater than transverse dispersion in directions perpendicular to the flow.

Although numerical modeling is required to adequately simulate the effects of both advection and dispersion on solute transport, the effects of dispersion will increase the speed at which a plume migrates, particularly at its leading edge. For fate and transport modeling, values of dispersivity are typically 100 feet longitudinal, 10 feet transverse horizontal, and 1 foot transverse vertical for alluvial aquifers such as the SFB.

In the SFB, advection and dispersion have had a significant effect on contaminant transport, and will continue to have an impact on the distribution of impacts in the SFB and the primary reasons that releases of COCs such as TCE have developed into very large and diffuse plumes in groundwater. It can be anticipated that these processes will continue to affect the overall plume migration in the SFB, with process such as diffusion from secondary sources in finer-grained materials continuing to provide contaminants to groundwater.

5.2.2 Retardation

Sorption/desorption is an important processes influencing the advective transport of a compound in the soil-water matrix. The retardation factor is a measure of the effect of the sorption/desorption process on the rate at which some compounds move in groundwater.

Sorption is a partitioning between the stationary sorbed (e.g., soil or sediments) phase and the mobile aqueous phase (groundwater), caused by hydrophobic and weak electrostatic interactions (Fetter 1999). Compounds that are partitioned such that they are predominantly in the aqueous phase will clearly move more readily with the groundwater flow velocity, whereas compounds that are preferentially sorbed to the stationary soil matrix will be retarded in their movement with respect to the average groundwater flow. Hydrophobic interactions with the soil organic matter will typically dominate the sorption of hydrophobic organic compounds, such as TCE and PCE. Electrostatic interactions within the soil surfaces will dominate the sorption of ionic species, such as nitrate. Therefore, the effect of sorption/desorption on compound migration will be different for organic and inorganic compounds.

The distribution coefficient (K_D) defines the relative partitioning of compounds in the soil- water matrix; hence, this parameter determines the relative retardation of different compounds in the same soil-water matrix. K_D assumes that local equilibrium is achieved between the sorbed and aqueous phases; however, this may not be the case in highly transmissive aquifers. Several site-specific properties of the soil, such as organic content and surface area, can affect the value of K_D . Soils with a high surface area typically have higher sorption capacity for both hydrophobic organic and ionic species. Increasing amounts of naturally occurring organic carbon (e.g., humic and fulvic acids) can increase the capacity of the soil for sorbing nonpolar compounds. The calculation of K_D for organic compounds is presented below:

$$K_D = F_{oc} * K_{oc}$$

The minimum and maximum K_D values for the COCs identified in Section 4.2 are presented in Table 5-1. These values were calculated using the K_{oc} provided in USEPA's RSL table (USEPA 2014b) and the minimum and maximum F_{oc} values collected during recent installation of wells by LADWP. Values of K_D for inorganic compounds and K_{oc} for organic compounds are included in the table and taken from the USEPA RSLs.

The retardation factor can be used to quantify the effect of sorption/desorption processes on retarding compound migration in the subsurface. For nonpolar, organic compounds, such as TCE and PCE, the retardation factor can be calculated using the following equation:

$$\text{Retardation factor} = 1 + \text{bulk density} (K_D/\text{effective porosity})$$

Bulk density: The weight of a unit of soil divided by its volume. Values ranged from 1.45 to 1.89 grams per cubic centimeter based on samples from well installation (Table 2-4).

Effective porosity: Porosity of the soil that can transmit water. Values ranged from 0.09 to 0.32 based on samples from well installation (Section Table 2-4).

Using the minimum and maximum values of bulk density and effective porosity from the recent well installation project by LADWP included in Table 2-4, the following ranges in retardation factors were calculated for the nine high-priority organic compounds presented in Section 4.2.

Chemical	K_D		Retardation Factor Range	
	Min	Max	Min	Max
1,4-Dioxane	2.63E-04	3.03E-03	1.0	1.1
TCE	6.07E-03	6.98E-02	1.0	2.5
PCE	9.49E-03	1.09E-01	1.0	3.3
CTET	4.39E-03	5.05E-02	1.0	2.1
1,2,3-TCP	1.16E-02	1.33E-01	1.1	3.8
1,1-DCE	3.18E-03	3.66E-02	1.0	1.8
Cis-1,2-DCE	3.96E-03	4.55E-02	1.0	2.0
NDMA	2.28E-03	2.62E-02	1.0	1.6
1,2-DCA	3.96E-03	4.55E-02	1.0	2.0

For the three high-priority inorganic compounds (nitrate, perchlorate, and Cr(VI)), a retardation factor is not included in this report. These chemicals have very high solubility values with perchlorate and nitrate being generally miscible in water. Retardation of these compounds is negligible and a retardation value of 1 is generally given.

It should be noted that retardation is a complex process based on the properties of the aquifer soil and chemicals present in groundwater (e.g., multiple chemicals can compete for organic carbon and surface areas), and does not permanently sequester compounds. Compounds adsorb to the soils or organic matter based on equilibrium established between groundwater and soil as represented by the K_D value. As concentrations decrease in groundwater, the amount of mass in aquifer sediments will decrease to re-establish the equilibrium (Fetter 1999).

5.3 Degradation

Chemical and biological degradation processes can be important in determining the fate of some compounds in the subsurface. Degradation is the only natural mechanism whereby the mass of a contaminant is removed with all other processes, such as adsorption providing only temporary sequestration of the chemical. The following discussion focuses on the organic compounds that were identified as high-priority COCs in Section 4.2. Though Cr(VI) can be reduced to trivalent chromium under reducing aquifer conditions, because of the stability of the inorganic compounds (nitrate, perchlorate, and Cr(VI)) under the generally aerobic and neutral conditions of SFB, degradation of these compounds in groundwater is not a significant factor in the fate of these chemicals.

5.3.1 Chemical Processes

Hydrolysis, oxidation (loss of electrons), and reduction (gain of electrons) reactions can be important for transforming compounds in the soil-water matrix, and of these reactions. Hydrolysis is the direct reaction of dissolved compounds with the water molecules (or its components, hydrogen ion, H^+ , or hydroxide ion, OH^-), and can be an important abiotic transformation process for some compounds in

groundwater systems. In general though, hydrolysis and abiotic oxidation and reduction reactions are not expected to transform, at a significant rate, any of the high-priority COCs found in the groundwater in the SFB.

Though not currently a COC, it is apparent that 1,1,1-trichloroethane (1,1,1-TCA) in the basin, likely through dehydrohalogenation (elimination reaction whereby chlorine is lost) and/or hydrolysis (USEPA 1991), has resulted in some of the 1,1-DCE that is a current high-priority COC.

5.3.2 Microbial Processes

Biodegradation of compounds in groundwater occurs through the oxidation or reduction of a compound to produce energy by microorganisms or a consortium of microorganisms present in the saturated zone. Under aerobic conditions (environment with oxygen present) this includes an oxidation reaction by which organic matter is oxidized through reduction of oxygen in the air. Under anaerobic conditions (environment devoid of significant oxygen), this is performed using electron donors such as organic carbon combined with an electronic acceptor such as nutrients or chlorinated compounds.

For chlorinated compounds, the primary process of biodegradation is reductive dehalogenation under anaerobic conditions, whereby higher chlorinated compounds are reduced to lower chlorinated compounds through the replacement of chlorine atoms with hydrogen atoms (USEPA 1991). Though reductive dehalogenation is very efficient for higher chlorinated compounds (e.g., TCE and 1,1,1-TCA) it becomes more energetically difficult in the sequence from PCE to TCE to 1,2-DCE to vinyl chloride. For example, the formation of vinyl chloride typically requires very strongly reducing conditions where high organic substrate concentrations are present and low permeabilities in the soil matrix limit the oxygen resupply to the soils.

Reductive dechlorination of chlorinated compounds does not generally occur in an aerobic environment, though for the less chlorinated compounds such as vinyl chloride, it can be an important factor in the final conversion step carbon dioxide and water. Table 5-3 shows the general process of reductive dehalogenation, and the conditions under which the process occurs.

Table 5-3. Parent-Product Relationships of Microbial Reduction of Selected Chlorinated VOCs

Parent Compound	Aquifer Conditions	Product
PCE (or TCE as parent)	Anaerobic/reduction	TCE
		1,2-DCE (trans and cis)
		Vinyl chloride
		Ethene
	Aerobic/oxidation	Carbon dioxide
		Water
1,1,1-TCA	Anaerobic/reduction	1,1-DCA
		Ethyl chloride
		Ethane
	Aerobic/oxidation	Carbon dioxide
		Water

Table 5-3. Parent-Product Relationships of Microbial Reduction of Selected Chlorinated VOCs

Parent Compound	Aquifer Conditions	Product
Carbon tetrachloride	Anaerobic/reduction	Chloroform
		Methylene chloride
		Methyl chloride
		Methane
	Aerobic/oxidation	Carbon dioxide
		Water

5.3.3 Degradation in SFB

Though the chlorinated solvent plumes in the SFB are areally extensive for compounds such as PCE and TCE, there is little evidence of significant biotic or abiotic degradation of compounds in the SFB. For the chlorinated solvents, concentrations of daughter products such as cis-1,2-DCE and trans-1,2-DCE are fairly low outside of the source areas, and vinyl chloride is present in a very low percentage (less than 2 percent) of samples collected from the SFB. For Cr(VI), total chromium values in groundwater are almost entirely Cr(VI) indicating that it is the dominant valence state of chromium in the SFB. Some of the likely reasons for the lack of significant degradation include the following:

- Based on the relatively high DO content of the groundwater, neutral pH, and generally positive oxidation reduction potential (ORP), the aquifer is generally aerobic and oxidizing. This is not a preferable condition for reductive dehalogenation or, in the case of hexavalent chromium, reduction to trivalent chromium.
- Though the TCE plume and PCE plumes are large, they are also diffuse with a very large area of impacts near the MCL and areas with concentrations greater than 1,000 µg/L being generally confined to the source areas. The low mass of solvents is non-conducive to significant microorganism populations developing that are able to degrade the compounds.