

## Complexity of Groundwater Contaminants at DOE Sites

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### Introduction

The U.S. Department of Energy (DOE) is responsible for the remediation and long-term stewardship of one of the world's largest groundwater contamination portfolios, with a significant number of plumes containing various contaminants, and considerable total mass and activity (1; 2). As of 1999, the DOE's Office of Environmental Management was responsible for remediation, waste management, or nuclear materials and facility stabilization at 144 sites in 31 states and one U.S. territory, out of which 109 sites were expected to require long-term stewardship (3, p.25). Currently, 19 DOE sites are on the National Priority List (6). The total number of contaminated plumes on DOE lands is estimated to be 10,000 (7). However, a significant number of DOE sites have not yet been fully characterized (6). The most prevalent contaminated media are groundwater and soil, although contaminated sediment, sludge, and surface water also are present. Groundwater, soil, and sediment contamination are present at 72% of all DOE sites (6, Page 1-14).

A proper characterization of the contaminant inventory at DOE sites is critical for accomplishing one of the primary DOE missions—planning basic research to understand the complex physical, chemical, and biological properties of contaminated sites (the 20-year Strategic Plan of DOE's Office Science Office, February 2004 (8)). (Note that the definitions of the terms "site" and "facility" may differ from one publication to another. In this report, the terms "site," "facility" or "installation" are used to identify a contiguous land area within the borders of a property, which may contain more than one plume. The term "plume" is used here to indicate an individual area of contamination, which can be small or large.)

Even though several publications and databases contain information on groundwater contamination and remediation technologies (e.g., 6, 9-17), no statistical analyses of the contaminant inventory at DOE sites has been prepared since the 1992 report by Riley and Zachara (18). The DOE Groundwater Data Base (GWD) (16) presents data as of 2003 for 221 groundwater plumes at 60 DOE sites and facilities (listed in Table S1 in Supporting Information). Note that Riley and Zachara (18) analyzed the data from only 18 sites/facilities including 91 plumes.

In this paper, we present the results of statistical analyses of the data in the GWD (16) as guidance for planning future basic and applied research of groundwater contaminants within the DOE complex. Our analyses include the evaluation of a frequency and ranking of specific

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contaminants and contaminant groups, contaminant concentrations/activities and total contaminant masses and activities. We also compared the results from analyses of the GWD with those from the 1992 report by Riley and Zachara (18). The difference between our results and those summarized in the 1992 report by Riley and Zachara (18) could be caused by not only additional releases, but also by the use of modern site characterization methods, which more accurately reveal the extent of groundwater contamination.

Contaminated sites within the DOE complex are located in all major geographic regions of the United States, with highly variable geologic, hydrogeologic, soil, and climatic conditions. We assume that the information from the 60 DOE sites included in the GWD (16) are representative for the whole DOE complex. These 60 sites include the major DOE sites and facilities, such Rocky Flats Environmental Technology Site, Colorado; Idaho National Laboratory, Idaho; Savannah River Site, South Carolina; Oak Ridge Reservation, Tennessee; and Hanford Reservation, Washington. These five sites alone account for 71% of the value of the remediation work (6, pp. 1-9). For assumptions and uncertainties used in this paper see Section S1 in Supporting Information. For the results of testing the integrity of the GWD see Section S2 in Supporting Information.

## Frequency of Occurrence of Contaminants

**Contaminant Groups.** The GWD contaminants detected in groundwater at 60 DOE sites and facilities can be grouped into the following eight contaminant groups:

- Chlorinated hydrocarbons
- Fuels and fuel components (i.e., petroleum/fuel hydrocarbons)
- Explosives
- Metals
- Radioactive isotopes (excluding tritium)
- Tritium
- Sulfates
- Nitrates

We identified tritium as an individual contaminant group (apart from other radioisotopes, which are combined in a separate group), because tritium is present in groundwater only in a dissolved state. Tritium in groundwater is subject to the processes of radioactive decay, dispersion, or dilution, with no transformation between the dissolved and solid states. Contrary to tritium, other radioactive isotopes are affected by radionuclide transformation between the dissolved and solid states.

Table S1 in Supporting Information lists the types of contaminant groups for each groundwater plume. In their 1992 report, Riley and Zachara (18) also identified the presence of radionuclides, metals, organic solvents, and fuel hydrocarbons. In addition, they identified polychlorinated biphenyls (PCBs) and organic ligands. Five contaminant groups (chlorinated hydrocarbons, fuel and fuel components, explosives, metals, and radioactive isotopes) contain more than one contaminant, and three groups include only a single component (tritium, sulfates, or nitrates). The most frequent contaminant groups (as percentage of the number of plumes surveyed for this contaminant group) are: chlorinated hydrocarbons (84%), tritium (51%), other radioactive isotopes (47%), nitrates (46%), metals (43%), sulfates (32%), fuel (11%), and explosives (10%) (Table S2).

Statistical analysis shows that single contaminants are contained in 23.5% of all plumes, binary combinations of contaminant groups are found in 29.4%, ternary—in 29%, quaternary—in 11.8%, and quinary—in 5% (Figure S1). The most frequent binary combinations of contaminant groups are those of mixed waste, including chlorinated hydrocarbons and tritium—35% of all plumes, metals and isotopes—28%, chlorinated hydrocarbons and isotopes—24%, isotopes and nitrate—23% (Figure 2. See also Table S3). Chlorinated hydrocarbons are also found in association with nitrate (30% of plumes), sulfate (26%), and metals (24%). A binary combination of radioactive contaminants, including tritium and other radioactive isotopes, is present at 31% of plumes. Calculations of binary combinations of contaminant groups (as a percentage of plumes coded for the presence or absence of a contaminant group that is present with at least one other contaminant group) show that the most frequently occurring group is chlorinated hydrocarbons (2/3 of all plumes), followed by tritium (51%), isotopes and nitrates (both 45%), metals (43%), sulfate (31%), explosives (10%), and fuel (8%).

In ternary combinations, the most frequent contaminant groups are mixed wastes—chlorinated hydrocarbons (20.8%), radionuclides (19.3%), and metals (15.6%) (See Table S4a). This combination was also the most frequent in 1992 (I8, Table 4) along with a combination of metals, anions, and radionuclides. A quaternary combination of contaminant groups most frequently includes mixed wastes—nitrates (21.2%), metals (18.3%), chlorinated hydrocarbons (17.3%), and tritium (16.3%) (See Table S4b). This combination is different from that identified in 1992—metals, anions, radionuclides, and chlorinated hydrocarbons. The most frequent quinary combination of contaminant groups also contains mixed waste—metals, tritium, other radioactive isotopes, nitrates, and chlorinated hydrocarbons (See Table S4c).

**Specific Contaminants.** We calculated the frequency of occurrence of specific contaminants in multiple-contaminant groups as a percentage of: (a) all individual compounds in a given contaminant group, (b) a number of plumes containing the given contaminant group, and (c) a number of all plumes in the GWD.

*Chlorinated hydrocarbons.* The most common chlorinated hydrocarbons in the GWD were (in descending order, given as a percent of occurrence in all plumes): TCE—57.5%, PCE—31.7%, DCE—16.3%, carbon tetrachloride (CT)—15.8%, and VC—8.1% (Table S5a). These chlorinated hydrocarbons were also common in 1992 (I8, Figure 7a).

*Fuels and fuel components.* No fuel component occurred in more than 5% of all plumes in the GWD, which seems low as discussed above. The most common fuel contaminants were benzene, diesel, jet fuel, MTBE, and toluene (Table S5b). In 1992, the most frequent fuel hydrocarbons were toluene, xylenes, benzene, ethylbenzene (I8, Figure 8a).

*Explosives.* No explosive occurred in more than 5% of all plumes in the GWD. The most frequent explosives were perchlorate, DNT (dinitrotoluene), HMX (high melting explosive, octahydro-1,3,5,7-tetranitro-1,3,5,7-tetraazazine), RDX (royal demolition explosive/cyclonite/hexogen/cyclotrimethylene-trinitramine), trinitrobenzene (TNB), trinitrotoluene (TNT), and teryl (Table S5c). In 1992, the following explosives (at a very few sites) were found—HMX, RDX, and trinitrotoluene (I8, Table 5).

*Metals.* The metals occurred in more than 5% of all plumes in the GWD, with the highest content of chromium, molybdenum, and selenium, followed by arsenic, and lead at lower

percentages (Table S5d). In 1992, the most common metals in groundwater (in descending order of occurrence) were lead, chromium, arsenic, zinc, and copper (18, Figure 5a);

*Tritium and other radionuclides.* The most common radionuclide in the GWD was tritium, occurring in 38% of all plume in the GWD. Three other radionuclides occurred in more than 5% of all the plumes are: uranium—19.5%, strontium—10.9%, and technetium—7.2% (Table S5e). In 1992, the most common radionuclides were tritium, uranium, and strontium (18, Figure 6a), whereas technetium was ranked as the 7<sup>th</sup> radionuclide.

Based on our analysis, out of 69 contaminants occurring in at least one of the plumes listed in the GWD, nine contaminants occur in more than 15% of the plumes in the GWD. These contaminants are (in descending order of occurrence): TCE, tritium, nitrates, PCE, sulfates, U, Cr, DCE and CT.

A comparison of the present data with those reported by Riley and Zachara (18) shows that the frequency of occurrence of individual contaminants has changed over the past decade. For example, technetium, CT, and MTBE were not significant contaminants in 1992, but they have recently become contaminants of concern at DOE facilities.

The frequency of occurrence of individual contaminants in binary combinations of contaminant groups is as follows (Table S6) is as follows:

- (a) chlorinated hydrocarbons (including TCE, PCE, DCE, and CT) with nitrate and sulfates,
- (b) chlorinated hydrocarbons (TCE and PCE) with tritium,
- (c) chlorinated hydrocarbons (TCE and PCE) with metals (chromium),
- (d) radioisotopes (tritium and uranium) with nitrate, (e) metals (chromium) with sulfate, and
- (f) sulfate with nitrate.

**Plume Volumes and Maximum Contaminant Concentrations.** The GWD lists the volumes of 134 plumes, or 61% of the total 221 plumes. The plume volumes vary over approximately 6 orders of magnitude—from  $5 \times 10^4$  to  $3.5 \times 10^{10}$  gallons, with a mean value of  $1.15 \times 10^9$  gallons (Table S7). The statistical distribution of plume volumes is close to lognormal (Figure S2). The total volume of 134 plumes is  $1.54 \times 10^{11}$  gal ( $5.85 \times 10^{11}$  L). Assuming that the remaining 87 plumes (with no volumes given in the GWD) are characterized by the same statistical distribution, the estimated total volume of contaminated groundwater would be  $2.55 \times 10^{11}$  gal ( $9.65 \times 10^{11}$  L), i.e. approximately 1 trillion liters. This estimated volume of 221 plumes in the GWD exceeds the value of  $1 \times 10^{10}$  gal ( $3.79 \times 10^{10}$  L) given in the 1997 Federal Register, but it is about one half of that reported in (20, Pages 15 and 21)— $4.75 \times 10^{11}$  gal ( $1.8 \times 10^{12}$  L). The estimated volume of 221 plumes in the GWD is 6.7 times less than the estimate of  $1.7 \times 10^{12}$  gal ( $6.44 \times 10^{12}$  L) for 5,000 DOE plumes identified by the Subsurface Contaminants Focus Area (20). These comparisons are commensurate with our belief that the GWD is a significant sample of groundwater contamination in the DOE complex.

The distribution of the maximum contaminant concentrations for individual compounds detected in at least 10 groundwater plumes are given in Figures S3-S8. Because some concentration populations extend to the detection limit, the concentration distributions appear to

be left-truncated. For the past decade, the ranges of PCE and TCE concentrations remained practically the same (Figure S3a). A normal quantile score (calculated as a probability corresponding to the normal distribution of quantile values) versus maximum concentrations of chlorinated hydrocarbons indicates that the DCE and, to a lesser extent, TCE distributions consist of two superimposed, lognormal distributions (Figure S4). This may be a result of the contribution from both primary contamination and degradation of PCE, and the DCE distribution could result from degradation of both PCE and TCE.

The Cr concentration distribution is lognormal and left truncated (Figures S3b and S6). The Cr concentration has essentially remained in the same range as that in 1992 (18). The lognormal and left truncated patterns are also typical for <sup>3</sup>H, Sr and Tc activities (Figure S3b, Figure S7 and Table S8). The present maximum tritium concentration is approximately one order of magnitude higher than that a decade ago from (18). The present maximum Sr concentration in groundwater (Figure S3c) is more than two orders of magnitude greater than that reported 1992 (18). Figure S3b also shows the box-and-whiskers plot for technetium, which was not included in the 1992 report (18), and uranium, which had a one order higher minimum and maximum concentration than that reported in 1992.

The sulfate and, to a greater degree, nitrate concentration distributions (Figure S8) are relatively peaked and strongly positive kurtosis. The quartile plots of the maximum concentrations of sulfates and nitrates indicate that both distributions comprise of two parts: (a) low-concentration segments exhibiting a log-normal distribution, and (b) high-concentration segments departing from a log-normal distribution. For sulfates, the log-normal distribution segment likely represents background concentrations, whereas the high concentrations might be caused by groundwater contamination. The presence of low and high concentration segments of the nitrate distribution is likely to reflect different anthropogenic causes of groundwater contamination. For example, low concentrations could be caused by leakage of nitrates from sewage lines and agricultural releases, and higher concentrations could indicate discharges from fuel processing, uranium recovery, or fuel fabrication (19). Figure S3c shows that the present maximum concentration of nitrates in groundwater is lower by a factor of 2 than that in 1992 (18).

To assess a relative (apparent) risk of the groundwater plumes, we calculated a normalized concentration as a ratio given by

$$C_{ci} = (C - C_{st}) / (C_{max} - C_{st}) \quad (1)$$

where  $C$  is the maximum contaminant concentration in a plume,  $C_{max}$  is the maximum contaminant concentration within a contaminant group, and  $C_{st}$  is the drinking water standard for this contaminant.  $C_{st}$  is determined from various drinking water standards as shown in Table S11. The  $C_{ci}$  values vary from negative values, when the contaminant concentration is below  $C_{st}$ , to 1, which corresponds to the highest contaminant hazard of a particular contaminant. As an example, the plumes with the five largest estimates of  $C_{ci}$  for the five most prevalent chlorinated hydrocarbons are shown in Figure S9. For PCE, TCE, CT, and DCE only positive  $C_{ci}$  values are shown, because the scale of the vertical axis (apparent risk) is logarithmic.

**Maximum Contaminant Masses/Activities.** The maximum contaminant masses/activities were calculated for plumes with known maximum concentrations and volumes from

$$M_{\max} = C_{\max} * V \quad (2)$$

where  $C_{\max}$  is the maximum concentration/activity of a compound, and  $V$  is the total plume volume. The total mass/activity for a contaminant and contaminant group is calculated as a sum of the masses/activities of calculated for each plume. For the plumes with either no reported concentration or volume, we estimated the maximum contaminant mass by assuming the same statistical distribution of concentrations (for a given contaminant) or volumes as for the plumes with the known information. The results are summarized in Tables S9 and S10.

The contaminant masses above the regulatory limits were calculated from the formula

$$M_{\max, \text{reg}} = (C_{\max} - C_{\text{reg}}) * V \quad (3)$$

where  $M_{\max, \text{reg}}$  is the maximum estimate of the mass/activity of each compound, and  $C_{\text{reg}}$  is the regulatory limit (Table S11). The regulatory limits were chosen for calculations according to the following precedence: Maximum Contaminant Limit (MCL), California Maximum Contaminant Limit (CA MCL), Treatment Technology (TT), California Response Limit (CA RL), Secondary Drinking Water Standard (SDWS), California Secondary Drinking Water Standard (CA SDWS). For contaminants without a regulatory limit (designated in Table S11 with an asterisk, \*) no limit-corrected mass/activity was calculated. For contaminants with no concentration and volume data in the database (designated with a double asterisk, \*\*) no mass/activity was calculated. Note from Tables S9 and S10 that the contaminant masses and activities above the regulatory limits are not significantly different from the total masses and activities.

The ranking of contaminant masses (as a percentage of the total contaminant mass) at all DOE sites is as follows: nitrates—55%, chlorinated hydrocarbons—23% (including TCE—17% and PCE-6%), sulfates—15%, PCE—6%, diesel—5%. According to the statistics of radioactive activities, virtually 100% of the total activity is attributed to tritium. Note the ranking according to occurrence is different than the ranking according to mass. For instance nitrates are the fourth ranked contaminant group by occurrence, but the first ranked group by contaminant mass. Isotopes are the second ranked group by occurrence, but virtually 100% of the total activity is due to tritium. The five largest sites by estimated maximum contaminant group mass (kg) or activity (pCi) are given in Figure 3.

**Multiple Factor Analysis and  $k$ -means Clustering of the Groundwater Plumes.** To assess the complexity and to integrate the different groundwater plume characteristics (Tables S1 and S12) we used a multiple factor analysis, MFA (22) followed by a  $k$ -means cluster analysis of main factors characterizing groundwater plumes. The approach and the results of this analysis are given in Section S3 in Supporting Information. Based on the basic plume characteristics, the plumes are classified into 5 clusters as given in Tables S13h,i. Using the basic plume characteristics together with the CT concentrations, the plumes are classified into 5 clusters as given in Tables S14g,h.

We suggest using the quantitative information about the individual contaminants and contaminant mixtures in decision making to establish priorities to advance the basic research on

environmental problems and developing remediation technologies for groundwater plumes throughout the DOE complex. The data analysis presented in this report could be of value to environmental managers, stakeholders, funding sources, site operators, the R&D community, as well as other interested parties.

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**Supporting Information is available free of charge via the internet at <http://pubs.acs.org>.**

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## Supporting Information

### Complexity of Groundwater Contaminants at DOE Sites

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**The file “Supporting Information” includes:**

- S1. Assumptions and uncertainties—1 page.
- S2. Corroboration of the GWD (2003) data using the LBNL Records—1 page.
- S3. Multiple factor analysis and *k*-means clustering of the groundwater plumes—2 pages, 14 Tables and 11 Figures.

## **S1. Assumptions and uncertainties**

We assume that the GWD records are representative of the concentrations of contaminants present in multi-contaminant plumes, for which several types of chemical reactions could typically occur. The sources of uncertainty in the results of the DOE GWD data analysis, as compared to the actual situation, is inconsistency in the data collection from different sites located in various climatic conditions, a partial representation of all DOE sites, and the difference in site characterization technologies.

Maximum concentration/activity and plume volume are available for many plumes in the GWD. For a given plume, the GWD does not include concentration/activity data other than the maximum concentration. In this paper, the total mass/activity of a contaminant in a plume was calculated by multiplying the plume volume by the maximum concentration/activity. This approach overestimates the contaminant mass/activity as a result of many simplifying assumptions. The approach does not take into account the actual concentrations/activities throughout the plume, which are almost always lower than the maximum concentration/activity. The approach does not take into the portion of the plume volume occupied by single contaminants in multi-contaminant plumes. Despite these significant limitations, the simplified approach provides a “first cut” comparison of contaminant predominance in the DOE complex on a mass/activity basis using the data available in the GWD. These total masses/activities should not be taken as representative of the actual masses/activities, though, and were calculated purely to provide relative comparisons between contaminants on a mass/activity basis. The uncertainty in calculations of contaminant masses/activities could be caused by the lack of information on the spatial distribution of contaminant concentrations within a plume. For example, using the entire plume volumes (rather than the volume occupied by a particular contaminant) and maximum contaminant concentrations (the maximum concentration exceeds real values at the plume edges), which are listed in the database, we are likely to overestimate the contaminant mass/activity.

## **S2. Corroboration of the GWD (2003) data using the LBNL Records**

To assess the reliability of the GWD, we compared the LBNL records entered in the GWD (2003) with those from LBNL's Environmental Restoration Program (ERP) database, including the number of plumes, contaminant groups, contaminants in each plume, and maximum concentrations (LBNL, 2000, 2002, 2003). We found that the records in the GWD generally match the ERP records from the time period from the 4<sup>th</sup> Quarter of Federal Fiscal Year 2001 (July 1<sup>st</sup>, 2001) through the 4<sup>th</sup> Quarter of Federal Fiscal Year 2002 (September 30<sup>th</sup>, 2002). This comparison also indicates an accurate data entry (for this period) to the GWD. We found that the plume areas in the GWD generally match the actual areas determined at the LBNL sites. However, the plume volumes in the GWD and calculated using the actual LBNL aquifer thickness and porosity data are different by a factor from 1/8 to 3.

To assess the degree of overestimating the calculated contaminant masses/activities, using the assumption of an evenly contaminant distribution over the entire plume volume, we used the results of observations of the chlorinated hydrocarbons at the Old Town plume of LBNL (LBNL, 2000). We estimated that individual chlorinated hydrocarbons occurred in 1% to 89% of the total plume area, with a median value of approximately 20%. We determined that the higher the contaminant concentration relative to other contaminants, the higher the proportion of the plume occupied by the contaminant. The analysis of the Old Town plume at LBNL indicates that the assumption of the evenly distributed contaminant concentrations over the entire plume may be applicable for the high contaminant concentrations, but is likely to lead to the overestimation of the mass of lower concentration contaminants by a factor from 100 to 200-400.

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### **S3. Multiple Factor Analysis and *k*-means Clustering of the Groundwater Plumes**

The groups of plume characteristics were classified as main or supplementary for the MFA. The basic analysis included the following 5 groups of groundwater plume characteristics (see Table S1):

Group 1. Identification of the presence (identified as 1) or absence (identified as 0) of contaminant groups.

Group 2. Two categories of data are included in this group:

- (a) Number of contaminant groups (Ngr) that are present at the site, and
- (b) Contamination severity index (Sv), which we defined depending on the severity of contamination and complexity of remediation:

1–sulfates (SO<sub>4</sub>) and/or nitrates (NO<sub>3</sub>), 2–CVOCs and/or fuels (F1), 4–explosives (Expl), 8–tritium (H3), and 16–metals (M) and/or radioisotopes (RI).

Group 3. Plume volumes (Vol), which are expressed as log<sub>10</sub> of the plume volume (given in gallons),

Group 4. Plume depths (Dp) and velocities (Vel), which are expressed as log<sub>10</sub> of the plume depth (ft) and velocity (ft/yr), and

Group 5. Climatic conditions, which were identified as dry or moist, using the identifiers 1 and 2, respectively (according to the map of DOE's climate zones—

[http://www.energycodes.gov/implement/pdfs/color\\_map\\_climate\\_zones\\_Mar03.pdf](http://www.energycodes.gov/implement/pdfs/color_map_climate_zones_Mar03.pdf)

Groups 1, 2, and 3 are considered the main plume characteristics, and the Groups 4 and 5 are supplementary ones. Table S12 summarizes data groups used in the MFA calculations. In addition to the aforementioned analysis of 5 basic groups of plume characteristics, we also analyzed the carbon tetrachloride (CT) concentrations.

The CT data were presented as a ratio of its concentration in groundwater to the MCL. The results of the MFA and cluster analysis are summarized in Table S13 and Figure S9 for basic plume characteristics. The correlation matrix of the quantitative variables shows the overall low correlation between the various plume characteristics (Tables S13c). The correlation coefficient between the number of contaminant groups and the severity index is 0.583 for 124 plumes used for the analysis of the basic plume characteristics. From the results of the MFA, the variability of the basic plume characteristics can mostly be described by the first four factors (their cumulative variability is about 70%) (Figure S10a).

Table S13g and Figure S10b provide the contributions of different groups of data to the multiple factors. The contaminant severity and the number of contaminant groups provide a major contribution to the 1<sup>st</sup> factor. The types of contaminant groups and CT concentrations provide the major contribution to the 2<sup>nd</sup> factor. The contribution of the supplementary data (climate and plume depth and velocity) is insignificant. The 1<sup>st</sup> factor is mostly related to the presence of radioactive contaminants, and the 2<sup>nd</sup> factor is mostly related to the presence of sulfates, and to a lesser degree the presence of nitrates and metals.

The relationships between the groups of variables can be performed using the  $L_g$  and RV coefficients. The  $L_g$  coefficient is defined as the scalar product between the matrices associated with each group; the  $L_g$  of 0 corresponds to no relationship between the groups, and it increases when the relationship between the groups becomes stronger. The RV coefficient is defined as the quotient of the  $L_g$  coefficient and is determined as the product of the norms of the matrices associated with each group; the RV coefficients vary from 0 (no relationship between the groups) to 1 (a strong relationship between the groups) (Greenacre and Blasius. 2006). The strongest relationship is, as expected, between the types of contaminant groups and the contamination severity. The relationships between contaminant groups and the plume depth/velocity, and contaminant groups and climate are weak, and there is no a significant relationship with the plume volume. The *k*-means analysis was conducted using the first four factors of the MFA for the basic plume characteristics. The plumes classified into 5 clusters as given in Tables S13h,i.

As an example of the MFA and the cluster analysis using the concentration data, we analyzed the CT concentrations combined with the aforementioned 5 groups of basic plume characteristics. The CT data were presented as a ratio of CT concentration in groundwater to the MCL of CT. The CT group was identified as a main and quantitative group of data. The results of the MFA and *k*-means analysis including the CT concentration data are shown in Table S14 and Figure S11. The variability of basic plume characteristics and CT concentrations can be mostly described by the first three factors—cumulative variability exceeds 70% (Table S14d and Figure S11a). The correlation coefficient between the number of contaminant groups and the severity index 0.563 for 26 plumes used in the analysis of CT concentrations. The best correlation is between the plume depths and groundwater velocity. The correlation between the CT concentration and basic plume characteristics is low. Based on the *k*-means analysis of the first three factors of the MFA for the basic plume characteristics combined with CT concentration data, the plumes are classified into 5 clusters as given in Tables S14g,h.

### **Literature cited in Section S3**

Greenacre and Blasius. 2006. Multiple Correspondence Analysis and Related Methods, Chapman & Hall/CRC Statistics in the Social and Behavioral Science. Volume 1.

**Table S1. Data used in the MFA and cluster analysis of groundwater plume characteristics (see abbreviations at the bottom of the table)**

Plume name	Plume code	VOCs	FI	Expl	Mt	H3	RI	SO4	NO3	Ngr	Sv	Vol	Dp	Vel	Cl	CCI4
Albuquerque Inhalation Toxicology Laboratory - Lagoon	11	0	0	0	0	0	0	1	0	1	1	7.59	2.19	1.94	1	
Albuquerque Inhalation Toxicology Laboratory - Diesel	12	0	1	0	0	0	0	0	0	1	2	5.88	2.19	1.94	1	
Ambrosia Lake	133	0	0	0	1	0	1	0	1	3	16		2.00	1.18	1	
Amchitka - Long Shot	8	0	0	0	1	1	1	0	0	3	16		3.36	1.00	2	
Amchitka - Milrow	9	0	0	0	1	1	1	0	0	3	16		3.60	1.00	2	
Amchitka - Cannikin	10	0	0	0	1	1	1	0	0	3	16		3.77	1.00	2	
Argonne Lab - 317	6	1	0	0	0	0	0	0	0	1	2	6.95	1.54	1.57	1	
Argonne Lab - 319	7	1	0	0	0	1	0	0	0	2	8	6.60	1.30	1.57	1	
Ashtabula	134	1	0	0	1	0	1	1	1	5	16	6.18	1.48	0.60	2	
BNL - OU V VOC	13	1	0	0	1	1	0	0	0	3	16	7.58	2.18	2.48	2	
BNL -Sr90 - Chemical Holes	14	0	0	0	0	0	1	0	0	1	16	7.22	1.48	1.40	2	
BNL -HFBR Tritium	15	1	0	0	0	1	0	0	0	2	8	6.95	1.70	2.48	2	
BNL -OU I VOC	178	1	0	0	0	1	1	0	0	3	16	8.77	1.30	2.48	2	
BNL -OU I/IV VOC	179	1	0	0	0	1	0	0	0	2	8	7.47	1.85	2.48	2	
BNL -Sr-90 - BGGR	180	1	0	0	0	0	1	0	0	2	16	8.65	1.78	1.40	2	
BNL -Sr-90 Former HWMF	181	1	0	0	0	1	1	0	0	3	16	8.86	1.30	1.40	2	
BNL -OU VI VOC	189	1	0	0	0	0	0	0	0	1	2	8.30	1.95	2.48	2	
BNL -Sr-90 Waste Concentration Facility	190	1	0	0	0	1	1	0	0	3	16	8.53	1.48	1.40	2	
BNL -OU III VOC	191	1	0	0	0	1	0	0	0	2	8	9.73	1.70	2.48	2	
Canonsburg	135	0	0	0	1	0	1	0	0	2	16	7.77	1.30		2	
Central Nevada Test Area	16	0	0	0	1	1	1	0	0	3	16	8.30	3.51	2.00	1	
Durango	136	0	0	0	1	0	1	0	0	2	16	7.73	2.00		1	
ETEC-1, FSDF	17	1	1	0	1	1	1	0	0	5	16	7.48	2.48	1.70	1	
ETEC-2, Bldg. 56 Landfill	18	1	0	0	1	0	1	0	0	3	16	10.54	2.48	1.70	1	
ETEC-3, RMHF	19	1	0	0	1	1	1	0	0	4	16	10.41	2.36	1.70	1	
Falls City	137	0	0	0	1	0	1	0	1	3	16		2.30	2.30	2	
Fernald-Great Miami Aquifer	138	1	0	0	1	0	1	0	1	4	16	9.30		3.00	2	
Gasbuggy	20	0	0	0	1	1	1	0	0	3	16	10.30	3.63	0.00	1	
Gnome-Coach	21	0	0	0	1	1	1	0	0	3	16	8.60	3.08	2.00	1	
Grand Junction Project Office	141	0	0	0	1	0	1	0	0	2	16	9.00			1	
Grand Junction (UMTRA)	142	0	0	0	1	0	1	0	0	2	16	7.64	1.70		1	
Green River	143	0	0	0	1	0	1	0	1	3	16	7.40	1.48	2.48	1	
Gunnison	144	0	0	0	1	0	1	0	0	2	16	6.00	2.00	2.30	1	
Hanford - 100-HR-3 (H)	22	0	0	0	1	1	1	0	1	4	16	6.18	2.00	3.70	1	
Hanford - 100-HR-3 (D/DR Area)	23	0	0	0	1	1	0	1	0	3	16	6.00	2.00	3.70	1	
Hanford - 100-KR-4	24	0	0	0	1	1	1	0	1	4	16	7.00	2.00	3.70	1	
Hanford - 100-NR-2	25	0	1	0	1	1	1	1	1	6	16	6.60	2.00	3.70	1	
Hanford - 200-UP-1	26	1	0	0	0	1	1	0	1	4	16	5.95	2.40	3.00	1	130
Hanford - 200-ZP-1	27	1	0	0	0	1	1	0	1	4	16	5.70	2.40	3.00	1	6900
Hanford - 100-BC-5	28	0	0	0	1	1	1	0	1	4	16	5.13	2.00	2.30	1	
Hanford - 200-BP-5	29	0	0	0	0	1	1	0	1	3	16	5.13	2.40	3.07	1	
Hanford - 300-FF-5	30	1	0	0	0	1	1	0	1	4	16	5.88	2.00	3.70	1	
Hanford - 100-FR-3	31	1	0	0	1	1	1	0	1	5	16	7.94	2.00	3.22	1	
Hanford - 200-PO-1	32	0	0	0	1	1	1	0	1	4	16	7.85	2.40	3.00	1	
INL - WAG-1	33	1	0	0	0	1	1	0	0	3	16	7.47	2.32	3.30	1	
INL - WAG-2	34	0	0	0	1	1	0	0	0	2	16	7.55	1.90	3.30	1	
INL - WAG-3	35	0	0	0	0	1	1	0	0	2	16	8.39	2.65	3.30	1	
INL - WAG-4	36	0	0	0	0	1	0	1	1	3	8	7.21	2.81	3.30	1	
INL - WAG-7	37	1	0	0	0	1	1	0	0	3	16	7.10	2.78	3.30	1	6

Kansas Plant - Blue River	38	1	1	0	0	0	0	0	0	0	2	2	7.77	1.48	3.48	2	
Kansas Plant - Indian Creek	39	1	0	0	0	0	0	0	0	0	1	2	5.83	1.60	3.06	2	
Lakeview	145	0	0	0	1	0	0	1	0	2	16	6.88	1.60	2.30	1		
LBNL - B-51/64	41	1	1	0	1	0	0	0	0	3	16	6.84	1.00	1.00	1	12	
LBNL - B-71	42	1	0	0	0	0	0	0	0	1	2	8.31	1.30	1.00	1		
LBNL - B-7E	43	0	1	0	0	0	0	0	0	1	2	6.53	1.40	1.00	1		
LBNL - Old Town	44	1	1	0	0	0	0	0	0	2	2	8.08	1.48	1.00	1	3422	
LBNL - B-75	45	1	0	1	0	1	0	0	0	3	8	8.05	1.48	1.70	1		
LBNL - B-74	46	0	1	0	0	0	0	0	0	1	2	7.80	1.08	1.70	1		
LBNL - B-37	47	1	0	0	0	0	0	0	0	1	2	8.29	1.48	1.00	1		
LBNL - Test Lab/Central Lab Area	226	1	0	0	0	0	0	0	0	1	2	7.52	1.08	1.70	1		
LBNL - B-51L	227	1	1	0	0	0	0	0	0	2	2	6.67	1.08	1.70	1		
LBNL - B-76 Area	228	1	1	0	0	1	0	0	0	3	8	7.84	1.30	1.00	1		
LLNL - TFA-1B	48	1	0	0	1	0	0	1	0	3	16	7.14	2.10	1.85	1		
LLNL - TFB-1B	49	1	0	0	1	0	0	0	0	2	16	7.62	1.90	1.85	1	2	
LLNL - TFC-SE-1B	50	1	0	0	1	0	0	0	0	2	16	7.62	1.95	1.85	1		
LLNL - TFD-W-1B	51	1	0	0	1	0	0	1	0	3	16	7.03	1.78	1.78	1		
LLNL - TFE-E-2	52	1	0	0	0	1	0	1	1	4	8	7.47	2.00	1.85	1		
LLNL - TF5475N-3A	53	1	0	0	0	1	0	0	0	2	8	7.21	1.98	1.60	1	27	
LLNL - TF5475-S-3A	54	1	0	0	0	1	0	0	0	2	8	7.24	2.02	1.60	1	14	
LLNL - TFG-1B	55	1	0	0	1	1	0	0	0	3	16	6.87	2.00	1.85	1		
LLNL - B292-1B	56	0	0	0	0	1	0	0	0	1	8	6.86	1.70	1.60	1		
LLNL - T5475-2	57	1	0	0	1	1	0	1	0	4	16	7.63	2.00	1.85	1	3	
LLNL - TF518-5	58	1	0	0	1	1	0	1	1	5	16	7.65	2.02	1.85	1	150	
LLNL - TFA-2	192	1	0	0	1	0	0	1	0	3	16	7.32	2.18	1.85	1		
LLNL - TFA-3A	193	1	0	0	1	0	0	1	1	4	16	6.05	2.26	1.65	1	3	
LLNL - TFB-2	194	1	0	0	1	0	0	1	1	4	16	6.92	2.18	1.85	1	2	
LLNL - TFC-1B-TCE	195	1	0	0	1	0	0	1	1	4	16	7.97	1.95	1.85	1		
LLNL - TFD-NE-2	196	1	0	0	0	0	0	1	0	2	2	7.43	2.13	1.78	1		
LLNL - TFD-ETC-N-2	197	1	0	0	0	0	0	1	1	3	2	6.61	1.98	1.85	1	10	
LLNL - TFD-SE-2	198	1	0	0	0	0	0	1	1	3	2	7.65	2.02	1.85	1		
LLNL - TFD-NE-3A	199	1	0	0	0	0	0	1	0	2	2	7.17	2.15	1.78	1		
LLNL - TFD-ETC-S-3A	200	1	0	0	0	0	0	1	1	3	2	6.63	2.06	1.70	1	1	
LLNL - TFD-S-3A	201	1	0	0	1	0	0	1	1	4	16	6.97	2.19	1.70	1		
LLNL - TFD-ETC-N-3A/3B	202	1	0	0	0	0	0	1	0	2	2	9.87	2.08	1.70	1	89	
LLNL - TFD-3B	203	1	0	0	0	1	0	1	1	4	8	7.80	2.18	1.70	1	8	
LLNL - TFD-HEL-3B	204	1	0	0	0	0	0	1	1	3	2	8.93	2.08	1.48	1	22	
LLNL - TFD-HEL-4	205	1	0	0	1	0	0	1	1	4	16	7.65	2.10	1.85	1	7	
LLNL - TFD-SE-4	206	1	0	0	0	0	0	1	1	3	2	7.07	2.15	1.85	1	1	
LLNL - TFD-5	207	1	0	0	0	0	0	1	1	3	2	5.43	2.32	1.78	1	1	
LLNL - TFD-SE-5	208	1	0	0	0	0	0	1	1	3	2	9.59	2.24	1.85	1		
LLNL - TFD-S-5	209	1	0	0	0	0	0	1	1	3	2	6.65	2.33	1.85	1		
LLNL - TFE-2	210	1	0	0	0	0	0	0	0	1	2	7.83	2.00	1.78	1		
LLNL - B419-3A	211	1	0	0	0	1	0	1	1	4	8	5.27	2.02	1.60	1	61	
LLNL - TFE-SW-3B	212	1	0	0	1	1	0	1	1	5	16	6.61	2.18	1.78	1	4	
LLNL - B419-3B	213	1	0	0	0	0	0	1	0	2	2	6.97	2.06	1.78	1		
LLNL - TFE-E-4	214	1	0	0	1	1	0	1	1	5	16	7.37	2.15	1.85	1	13	
LLNL - TF518-Perched	215	1	0	0	0	0	0	1	1	3	2	6.70	1.52		1		
LLNL - TF5475-5	216	1	0	0	1	1	0	1	1	5	16	6.85	2.10	1.40	1	10	
LLNL - TFC-N-1B	217	1	0	0	1	0	0	1	0	3	16	6.00	1.95	1.85	1		
LLNL - TFG-S-1B	218	1	0	0	1	1	0	1	0	4	16	6.30	2.02	1.78	1		
LLNL - TFD-ETC-S-2	219	1	0	0	0	0	0	1	1	3	2	7.00	2.00	1.85	1	3	

LLNL Site 300 - CGSA Building 875	59	1	0	0	0	0	0	0	0	0	1	2	7.30	1.30	3.00	1
LLNL Site 300 - B834 Core Area	60	1	0	0	0	0	0	0	0	1	2	2	7.00	1.30	2.57	1
LLNL Site 300 - Pit 6 Landfill	61	1	0	1	0	1	0	0	0	1	4	8	7.18	1.40	3.00	1
LLNL Site 300 - HEPA B815	62	1	0	0	0	0	0	0	0	1	2	2	6.83	1.40	2.00	1
LLNL Site 300 - Pits 3&5	63	1	0	1	0	1	1	0	0	1	5	16	6.60	1.00	2.27	1
LLNL Site 300 - B850	64	0	0	0	0	1	1	0	0	1	3	16	10.00	1.18	2.57	1
LLNL Site 300 - B854	65	1	0	1	0	0	0	0	0	1	3	4	10.00	1.30	2.57	1
LLNL Site 300 - B832	66	1	0	1	0	0	0	0	0	1	3	4	10.00	0.78	2.57	1
LLNL Site 300 - B801/Pit 8	67	1	0	0	0	0	0	0	0	0	1	2	7.77	1.70	2.57	1
LLNL Site 300 - B833	68	1	0	0	0	0	0	0	0	0	1	2		1.34	2.57	1
LLNL Site 300 - B851	69	0	0	0	0	0	1	0	0	0	1	16		2.00	2.57	1
LLNL Site 300 - HEPA HE Lagoons	70	0	0	1	0	0	0	0	0	1	2	4	9.41	1.40	2.00	1
LLNL Site 300 - CGSA Northern Plume	220	1	0	0	0	0	0	0	0	0	1	2	8.76	1.30	3.00	1
LLNL Site 300 - EGSA Debris Burial Trenches	221	1	0	0	0	0	0	0	0	0	1	2	6.70	1.18	3.08	1
LLNL Site 300 - HEPA Burn Pit	222	1	0	1	0	0	0	0	0	1	3	4	7.70	1.95	2.00	1
LLNL Site 300 - Pit 1 Landfill	223	0	0	1	0	0	0	0	0	1	2	4	7.78	1.70	2.57	1
LLNL Site 300 - Pit 2 Landfill	224	0	0	0	0	0	0	0	0	1	1	1	6.70	1.70	2.57	1
LLNL Site 300 - B830	225	1	0	1	0	0	0	0	0	1	3	4	8.28	0.78	2.57	1
Los Alamos National Laboratory (TA-16 - Deep Groundwater Only)	40	0	0	1	1	1	1	0	0	1	5	16		2.88	2.39	1
Maybell	146	0	0	0	1	0	1	0	0	1	3	16		2.00		1
Mexican Hat	147	0	0	0	1	0	1	1	1	1	4	16				1
Miamisburg Project - OU 1	71	1	0	0	0	1	0	0	0	0	2	8	9.81	1.40	2.18	2
Miamisburg Project - Well 411 Area	139	1	0	0	0	1	0	0	0	0	2	8		1.40		2
Miamisburg Project - Tritium	150	1	0	0	0	1	1	0	0	0	3	16		1.40		2
Miamisburg Project - Tributary Valley VOCs	151	1	0	0	0	1	0	0	0	0	2	8		1.40	2.18	2
Monticello Remedial Action Project	148	0	0	0	1	0	1	0	0	0	2	16		1.70		1
Monument Valley	149	0	0	0	0	0	0	0	1	1	2	1		1.90	2.08	1
Naturita	152	0	0	0	1	0	1	0	0	0	2	16		2.00	1.30	1
New Rifle	72	0	0	0	1	0	1	0	0	1	3	16		2.90		1
NTS - Frenchman Flat	73	0	0	0	0	1	1	0	0	0	2	16		3.30		1
NTS - West Pahute Mesa	74	0	0	0	0	1	1	0	0	0	2	16		3.20		1
NTS - Yucca Flat	75	0	0	0	0	1	1	0	0	0	2	16		3.30		1
NTS - Central Pahute Mesa	76	0	0	0	0	1	1	0	0	0	2	16		3.20		1
NTS - Climax Mine	77	0	0	0	0	1	1	0	0	0	2	16		3.20		1
NTS - Rainer																
Mesa/Shoshone Mesa	153	0	0	0	0	1	1	0	0	0	2	16		1.48	1.48	1
ORNL - Central	78	1	0	0	1	1	1	0	0	0	4	16	7.85	2.00	3.00	2
ORNL East	79	1	1	0	0	0	0	0	0	0	2	2	7.84			2
ORNL West	80	0	0	0	0	1	1	0	0	0	2	16	8.90	2.00		2
ORNL - Melton Valley	81	1	0	0	0	1	1	0	0	0	3	16	7.35	2.00	3.00	2
ORNL - Y-12	82	1	1	0	1	0	1	0	0	1	5	16	9.00	2.70	3.00	2
ORNL - Bear Creek Valley	83	1	0	0	0	0	1	0	0	1	3	16	9.00	2.00	3.00	2
ORNL - ETTP Main Plant	84	1	1	0	0	0	1	0	0	0	3	16	7.80	1.30	2.00	2
ORNL - ETTP K-27	85	1	0	0	0	1	1	0	0	0	3	16	4.70	1.48	0.00	2
ORNL - ETTP 1070-A	86	1	0	0	0	0	0	0	0	0	1	2	7.15	1.48	2.00	2
Old Rifle	154	0	0	0	1	0	1	0	0	1	3	16		1.48	1.48	1
Paducah Plant - GW OU (NW Plume)	155	1	0	0	0	0	1	0	0	0	2	16	5.86	2.00	2.56	2
Paducah Plant - GW OU (NE Plume)	156	1	0	0	0	0	1	0	0	0	2	16	8.46	2.00	2.56	2
Paducah Plant - GW OU (SW Plume)	157	1	0	0	0	0	1	0	0	0	2	16	8.41	2.00	2.56	2
Pantex Plant - Northeast On-site Perched Aquifer	87	1	0	1	1	0	0	0	0	0	3	16	8.70	2.43	2.00	1
Pantex Plant - Southeast On-site Perched Aquifer	88	1	0	1	1	0	0	0	0	0	3	16	7.66	2.42	2.00	1
Pantex Plant - On-site Ogallala Aquifer	89	1	0	0	0	0	0	0	0	0	1	2		2.60	2.40	1

Pinellas Plant (1)	158	1	0	0	0	0	0	0	0	1	2				2
Pinellas Plant (2)	159	0	0	0	0	0	0	0	1	0					2
Pinellas Plant (3)	160	1	0	0	0	0	0	0	0	1	2				2
Portsmouth Plant - 5 Unit Plume	91	1	0	0	0	0	0	0	0	1	2	1.00	1.56		2
Portsmouth Plant - X-749	92	1	0	0	0	0	1	0	0	2	16	1.00	1.86		2
Portsmouth Plant - X-740	93	1	0	0	0	0	0	0	0	1	2	1.00			2
Portsmouth Plant - X701B	94	1	0	0	0	0	1	0	0	2	16	1.00	1.86		2
Portsmouth Plant - 7 Unit Plume	95	1	0	0	0	0	1	0	0	2	16	1.00	2.82		2
Portsmouth Plant - X-120	96	1	0	0	0	0	0	0	0	1	2	1.00	1.56		2
Project Shoal	97	0	0	0	1	1	1	0	0	3	16	3.08	2.00		1
Rio Blanco	102	0	0	0	1	1	1	0	0	3	16	3.77	1.00		1
Riverton	164	0	0	0	1	0	1	1	0	3	16	2.00	2.48		1
Rocky Flats - Mound Plume	98	1	0	0	0	0	1	0	0	2	16	9.08	1.00	1.48	1
Rocky Flats - East Trenches	99	1	0	0	0	0	0	0	0	1	2	8.46	1.00	1.48	1
Rocky Flats - Solar Ponds	100	0	0	0	0	0	1	0	1	2	16	7.55		1.48	1
Rocky Flats - 903 Pad	101	1	0	0	0	0	0	0	0	1	2	7.60		1.48	1
Rocky Flats - 881 Hillside Drum Storage Area	161	1	0	0	0	0	0	0	0	1	2				1
Rocky Flats - Carbon Tetrachloride Spill	162	1	0	0	0	0	0	0	0	1	2				1
Rocky Flats - Industrial Area	163	1	0	0	0	0	0	0	0	1	2				1
Rocky Flats - Rulison	103	0	0	0	1	1	1	0	0	3	16	3.93	1.00		1
Rocky Flats - Alluvial	104	0	0	0	1	1	0	0	0	2	16	1.60	0.48		1
Rocky Flats - Salt Lake City	165	0	0	0	1	0	1	0	0	2	16	1.70	2.23		1
Rocky Flats - Fuel Oil Spill	169	0	1	0	0	0	0	0	0	1	2	2.70			1
Rocky Flats - Navy Landfill	188	1	0	0	0	0	0	0	0	1	2	3.70	0.00		1
Rocky Flats - Chemical Waste Landfill (ChWLF)	105	1	0	0	0	0	0	0	0	1	2	2.70			1
Rocky Flats - Tijeras Arroyo	106	1	0	0	0	0	0	0	0	1	2	2.51			1
Rocky Flats - TA5	107	1	0	0	0	0	0	0	0	1	2	2.70			1
Rocky Flats - Canyons	187	0	1	0	0	0	0	0	1	2	2	2.51	0.00		1
SRS - A-Area Burning/Rubble Pits	109	1	0	0	0	0	0	0	0	1	2	6.90	2.11	2.48	2
SRS - A/M Area Groundwater	110	1	0	0	1	0	0	0	0	2	16	7.59	2.60	2.79	2
SRS - C Area Burning/Rubble Pits	111	1	0	0	0	0	0	0	0	1	2	1.78	3.78		2
SRS - C-Area Groundwater Operable Unit	112	1	0	0	0	1	0	0	0	2	8	1.85	3.78		2
SRS - CMP Pits	113	1	0	0	0	0	0	0	0	1	2	1.85	2.00		810
SRS - D-Area Groundwater	114	1	0	0	1	1	1	1	1	6	16	0.70	2.70		2
SRS - D-Area Oil Seepage Basins	115	1	1	0	0	0	0	0	0	2	2	1.60	1.78		2
SRS - F Area Seepage Basins	116	0	0	0	1	1	1	0	1	4	16	0.00	3.56		2
SRS - H Area Seepage Basins	117	1	0	0	1	1	1	0	1	5	16	0.00	3.56		2
SRS - Central Shops GW OU	118	1	0	0	0	0	0	0	0	1	2	1.78			2
SRS - K Area Burning/Rubble Pit	119	1	0	0	0	0	0	0	0	1	2	1.70	1.70		2
SRS - K Area Groundwater Operable Unit	120	1	0	0	0	1	0	0	0	2	8	1.70	1.70		2
SRS - L Area Burning/Rubble Pit	121	1	0	0	0	0	0	0	0	1	2	1.54	1.70		13
SRS - L Area Southern Groundwater	122	1	0	0	0	1	0	0	0	2	8	1.78	2.18		14
SRS - Miscellaneous Chemical Basin	123	1	0	0	0	0	0	0	0	1	2	2.35	2.79		2
SRS - Mixed Waste Management Facility Northeast Plume	124	1	0	0	0	1	0	0	0	2	8	1.78	3.56		2
SRS - Mixed Waste Management Facility Northwest Plume	125	1	0	0	0	1	0	0	0	2	8	1.78	3.56		2
SRS - Mixed Waste Management Facility Southeast Plume	126	1	0	0	0	1	1	0	0	3	16	1.78	3.56		2

South Valley Plume	108	1	0	0	0	0	0	0	0	0	1	2		2.38	3.74	1	
Spook	170	0	0	0	1	0	1	0	1	3	16			2.60		2	
Tuba City	171	0	0	0	0	0	1	1	1	3	16				0.00	1	
Weldon Project - Quarry	172	0	0	1	0	0	1	0	0	2	16				0.00	2	
Weldon Project - Chemical Plant (exposives)	173	0	0	1	0	0	0	0	1	2	4				0.00	2	
Weldon Project - Chemical Plant (VOC)	174	1	0	0	0	0	0	0	0	1	2				0.00	2	
Weldon Project - Chemical Plant (Uranium East)	175	0	0	0	0	0	1	0	0	1	16			2.85	1.78	2	
Weldon Project - Chemical Plant (Uranium West)	176	0	0	0	0	0	1	0	0	1	16			1.30		2	
Weldon-North Plateau Plume	172	0	0	0	0	1	1	0	0	2	16					2	
Stanford Center - Former Hazardous Waste Storage Area	183	1	0	0	0	0	0	0	0	1	2					1	
Stanford Center - Former Solvent Underground Storage Tank Area	184	1	0	0	0	0	0	0	0	1	2					1	
Stanford Center - Plating Shop Area	185	1	0	0	0	0	0	0	0	1	2					1	
Stanford Center - Test Lab/Central Lab Area	186	1	0	0	0	0	0	0	0	1	2				1.90	1	
<b>Notes:</b>																	
<b>Ngr</b>	Number of contaminant groups						<b>FI</b>	Fuels									
<b>Sv</b>	Severity index						<b>Exp</b>	Explosives									
<b>Vol</b>	log10 of plume volume in gallons						<b>Mt</b>	Metals									
<b>Dp</b>	Log10 of plume depth (in feet)						<b>H3</b>	Tritium									
<b>Vel</b>	log10 of groundwater velocity (in ft/yr)						<b>RI</b>	radioisotopes									
<b>CI</b>	Climate index						<b>SO4</b>	Sulfate									
<b>CCl4</b>	Ration of Carbon Tet concentration to th						<b>NO3</b>	Nitrates									

**Table S2. Frequency of occurrence of contaminant groups in groundwater plumes (total number of plumes in the GWD is 221). The contaminant groups are sorted according to the frequency of their occurrence.**

<b>Contaminant Groups</b>	<b>Plumes surveyed for specific contaminant groups</b>	<b>Number and % of plumes with specific contaminant groups</b>
CVOCs	175	147 (84%)
Tritium	164	84 (51%)
Isotopes	196	92 (47%)
Nitrates	155	71 (46%)
Metals	177	76 (43%)
Sulfate	139	44 (32%)
Fuel	146	16 (11%)
Explosives	146	15 (10%)

**Table S3. Ranking of plumes with binary association of contaminant groups (given as a percent of plumes identified for both groups). Mixed wastes are in bold.**

Percent	Contaminant groups	
35%	<b>CVOCs</b>	<b>Tritium</b>
31%	<b>Tritium</b>	<b>Isotopes</b>
30%	CVOCs	Nitrate
28%	<b>Metals</b>	<b>Isotopes</b>
26%	VOCs	Sulfate
24%	<b>CVOCs</b>	<b>Isotopes</b>
24%	Metals	Nitrate
24%	CVOCs	Metals
23%	<b>Isotopes</b>	<b>Nitrate</b>
23%	<b>Metals</b>	<b>Tritium</b>
22%	Sulfate	Nitrate
19%	<b>Tritium</b>	<b>Nitrate</b>
17%	Metals	Sulfate
10%	<b>Tritium</b>	<b>Sulfate</b>
7%	Explosives	Nitrate
7%	CVOCs	Fuel
6%	CVOCs	Explosives
5%	<b>Isotopes</b>	sulfate
3%	<b>Fuel</b>	<b>Isotopes</b>
3%	Explosives	Metals
3%	Fuel	Metals
3%	<b>Explosives</b>	<b>tritium</b>
2%	Fuel	Nitrate
2%	<b>Fuel</b>	<b>Tritium</b>
2%	<b>Explosives</b>	<b>Isotopes</b>
1%	Fuel	Sulfate
0%	Fuel	Explosives
0%	Explosives	Sulfate

**Table S4. Ternary, quaternary, and quinary combinations of contaminant groups in groundwater plumes. The most frequent contaminant groups are shown in bold.**

	<b>CVOCs</b>	<b>Fuels</b>	<b>Explosives</b>	<b>Metals</b>	<b>Tritium</b>	<b>Isotopes</b>	<b>Sulfates</b>	<b>Nitrates</b>	<b>Number of contaminant groups</b>
(a) Ternary									
<b>Number of plumes</b>	40 3		7	30	29	37	18	28	192
<b>Frequency (%)</b>	<b>20.8</b>	1.6 3.	6	<b>15.6</b>	15.1	<b>19.3</b>	9.4 14	.6	100
(b) Quaternary									
<b>Number of plumes</b>	18 0		1	19	17	15	12	22	104
<b>Frequency (%)</b>	<b>17.3</b>	0.0 1.	0	<b>18.3</b>	<b>16.3</b>	14.4 11	.5	<b>21.2</b>	100
(c) Quinary									
<b>Number of plumes</b>	10 2		2	10	9	7	5	10	55
<b>Frequency (%)</b>	<b>18.2</b>	3.6 3.	6	<b>18.2</b>	<b>16.4</b>	12.7 9.	1	<b>18.2</b>	100

**Table S5. Occurrence of individual contaminants in contaminated groups****(a) Chlorinated hydrocarbons (number of plumes is 147)**

VOCs	TCE	PCE	DCE	CT	VC	DCA	TCA	Chloro-form	CVOC (undivided)	Freon	chloride	carbon disulfide	chlor-ethane	dibromide
Number of plumes with a specific compound	127	70	36	35	18	12	10	8	7	6	2	1	1	1
Frequency of occurrence among other CVOCs compounds (%)	38.0	21.0	10.8	10.5	5.4	3.6	3.0	2.4	2.1	1.8	0.6	0.3	0.3	0.3
Frequency of occurrence in CVOCs contaminated plumes (%)	86.4	47.6	24.5	23.8	12.2	8.2	6.8	5.4	4.8	4.1%	1.4	0.7	0.7	0.7
Frequency of occurrence in all plumes (%)	57.5	31.7	16.3	15.8	8.1	5.4	4.5	3.6	3.2	2.7	0.9	0.5	0.5	0.5

**(b) Fuel or fuel components (number of plumes is 16)**

<b>Fuel</b>	benzene	diesel	jet fuel	MTBE	toluene	benzene	benzene	gas	methyl-naphthalene	other
Number of plumes with a specific fuel compound	7	7	2	2	2	1	1	1	1	1
Frequency of occurrence among other fuel compounds (%)	29.2	29.2	8.3	8.3	8.3	4.2	4.2	4.2	4.2	4.2
Frequency of occurrence in fuel contaminated plumes (%)	43.8	43.8	12.5	12.5	12.5	6.3	6.3	6.3	6.3	6.3
Frequency of occurrence in all plumes (%)	3.2	3.2	0.9	0.9	0.9	0.5	0.5	0.5	0.5	0.5

**(c) Explosives (number of plumes is 15)**

<b>Explosives</b>	Per-chlorate	DNT	HMX	RDX	TNB	TNT	Tetryl
Number of plumes with a specific explosive compound	9	5	5	4	4	3	1
Frequency of occurrence among other explosive compounds (%)	29.0	16.1	16.1	12.9	12.9	9.7	3.2
Frequency of occurrence in explosive contaminated plumes (%)	60.0	33.3	33.3	26.7	26.7	20.0	6.7
Frequency of occurrence in all plumes (%)	4.1	2.3	2.3	1.8	1.8	1.4	0.5

**(d) Metals (number of plumes is 70)**

<b>METALS</b>	<b>Cr</b>	<b>Mo</b>	<b>Se</b>	<b>As</b>	<b>Pb</b>	<b>Hg</b>	<b>Mn</b>	<b>Cd</b>	<b>Ni</b>	<b>Ba</b>	<b>V</b>
Number of plumes with specific metals	42	16	13	9	7	6	6	5	4	3	3
Occurrence with other metals	33.3	12.7	10.3	7.1	5.6	4.8	4.8	4.0	3.2	2.4	2.4
Occurrence in metal contaminated plumes	60.0	22.9	18.6	12.9	10.0	8.6	8.6	7.1	5.7	4.3	4.3
Occurrence in all plumes	19.0	7.2	5.9	4.1	3.2	2.7	2.7	2.3	1.8	1.4	1.4

<b>METALS</b>	<b>Bo</b>	<b>Co</b>	<b>Fe</b>	<b>Mg*</b>	<b>Al</b>	<b>Be</b>	<b>Cu</b>	<b>Zn</b>
Number of plumes with specific metals	2	2	2	2	1	1	1	1
Occurrence with other metals	1.6	1.6	1.6	1.6	0.8	0.8	0.8	0.8
Occurrence in metal contaminated plumes	2.9	2.9	2.9	2.9	1.4	1.4	1.4	1.4
Occurrence in all plumes	0.9	0.9	0.9	0.9	0.5	0.5	0.5	0.5

**(e) Radioactive isotopes (number of plumes is 98)**

<b>Radionuclides</b>	U	Str	Tc	I*	Ra	Th*	Cs*	Gross Alpha	Am**	Carbon 14**	Co*	PU*	Gross Beta	other*
Number of plumes	44	24	16	8	4	4	3	3	1	1	1	1	1	1
Occurrence with other radionuclides	39.3	21.4	14.3	7.1	3.6	3.6	2.7	2.7	0.9	0.9	0.9	0.9	0.9	0.9
Occurrence in plumes with radionuclides	44.9	24.5	16.3	8.2	4.1	4.1	3.1	3.1	1.0	1.0	1.0	1.0	1.0	1.0
Occurrence in all plumes	19.9	10.9	7.2	3.6	1.8	1.8	1.4	1.4	0.5	0.5	0.5	0.5	0.5	0.5

**Table S6. Types and ranking of plumes with binary combinations of individual contaminants. Mixed waste is in bold.**

<b>Co-contaminants</b>		<b>Percent of identified plumes</b>
Chlorinated Hydrocarbons – Nitrate and Sulfate		
TCE	nitrate	28%
TCE	sulfate	25%
PCE	sulfate	20%
PCE	nitrate	17%
<b>Chlorinated Hydrocarbons – Tritium</b>		
<b>TCE</b>	<b>tritium</b>	<b>29%</b>
<b>PCE</b>	<b>tritium</b>	<b>21%</b>
Chlorinated Hydrocarbons – Metals		
TCE	Cr	20%
PCE	Cr	16%
<b>Radioisotopes-Nitrate</b>		
<b>Tritium</b>	<b>Nitrate</b>	<b>19%</b>
<b>Uranium</b>	<b>Nitrate</b>	<b>17%</b>
Metals-Sulfate		
Cr	Sulfate	18%
Sulfate-Nitrate		
Sulfate	Nitrate	22%

**Table S7. Summary of statistics of plume volumes (volumes are gallons).  
Total number of plumes is 134.**

Mean	1.15E+09
Standard Error	3.81E+08
Median	3.53E+07
Mode	1.00E+06
Standard Deviation	4.41E+09
Sample Variance	1.94E+19
Kurtosis	3.53E+01
Skewness	5.63E+00
Range	3.50E+10
Minimum	5.00E+04
Maximum	3.50E+10
Confidence Level (95.0%)	7.53E+08

**Table S8. Statistics of maximum activities (pCi/L) of tritium and radioisotopes in groundwater plumes**

Statistical values	Tritium	Sr	Tc	U
Standard Error	1.61E+09	4997291	1247321	933.2892
Minimum	15	8	25	1
1 <sup>st</sup> quartile (Q1)	1820	35.75	311.5	
Median (Q2)	18400	483	3798.5	201
Mean	1.62E+09	5054433	1298130	
3 <sup>rd</sup> quartile (Q3)	219000	5393.5	48000	
Maximum	1E+11	1E+08	20000000	12400
IQR	217180	5357.75	47688.5	
Q1-3IQR	-649720	-16037.5	-142754	
Q1-1.5IQR	-215360	-5322	-47377	
Q3+1.5IQR	436180	10751.25	95688.5	
Q3+3IQR	870540	21466.75	191065.5	
Standard Deviation	1.27E+10	22348563	4989284	3365.022
Sample Variance	1.61E+20	4.99E+14	2.49E+13	11323374
Kurtosis	61.99988	19.99709	15.9669	12.69662
Skewness	7.873997	4.471674	3.994273	3.548152
Range	1E+11	99999992	19999975	12399
Number of occurrences	62	20	16	13
Confidence Level(95.0%)	3.23E+09	10459453	2658604	2033.462

Table S9. Maximum contaminant mass estimates

## (a) Chlorinated hydrocarbons

Contaminants	Number of plumes with a specific contaminant	Plumes with known concentration and volume			All plumes	
		% of plumes	Mass (kg)		Mass (kg)	
			Maximum	Above regulatory limit	Maximum	Above regulatory limit
TCE	127	74	1.67E+07	1.67E+07	2.25E+07	2.25E+07
PCE	70	81	6.07E+06	6.07E+06	7.45E+06	7.45E+06
CT	35	86	1.40E+05	1.40E+05	1.63E+05	1.63E+05
DCE	36	69	7343	7275	10574	1.05E+04
chloroform	8	88	1064	4.5	1216	5.2
VC	18	78	380.3	379.0	488.9	487.3
methylene chloride	2	100	71.5	31.9	71.5	31.9
TCA	10	50	126.9	114.3	253.8	228.5
DCA	12	75	135.6	84.1	180.8	112.1
Freon*	6	100	62.2		62.2	
carbon disulfide	1	100	13.5	0.0	13.5	0.0
VOC (undivided)**	7	0				
chloroethane**	1	0				
ethylene dibromide**	1	0				
<b>Total VOCs</b>	334		2.29E+07	2.29E+07	3.01E+07	3.01E+07

## (b) Fuel and fuel components

Contaminants	Number of plumes with a specific contaminant	Plumes with known concentration and volume			All plumes	
		% of plumes	Mass (kg)		Mass (kg)	
			Maximum	Above regulatory limit	Maximum	Above regulatory limit
Diesel*	7	71	5.15E+06		7.21E+06	
gas*	1	100	31.23		31.23	
Benzene	7	86	7.24	6.09	8.45	7.1
dichlorobenzene	1	100	1.99	0	1.99	0
MTBE	2	100	2.42	1.93	2.4	1.9
Toluene	2	50	0.38	0	0.8	0
methylnaphthalene*	1	100	0.17		0.2	
ethylbenzene	1	100	0.004	0	0.004	0
jet fuel**	2	0				
<b>Total fuel</b>	24		5147664		7206714	

## (c) Explosives

Contaminants	Number of plumes with a specific contaminant	Plumes with known concentration and volume			All plumes	
		% of plumes	Mass (kg)		Mass (kg)	
			Maximum	Above regulatory limit	Maximum	Above regulatory limit
RDX*	4	75	20000		26666.7	
TNB*	4	75	8500		11333.3	
HMX*	5	80	4300		5375	
DNT*	5	40	680		1700	
TNT*	3	67	1200		1800	
perchlorate	9	89	460	0	517.5	0
tertyl*	1	100	2.2		2.2	
<b>Total</b>	31		35142		47395	

## (d) Metals

Contaminants	Number of plumes with a specific contaminant	Plumes with known concentration and volume			All plumes	
		% of plumes	Mass (kg)		Mass (kg)	
			Maximum	Above regulatory limit	Maximum	Above regulatory limit
Mg*	2	100	647,746		647,746	
Fe <sup>†</sup>	2	100	1,941,214	1,940,295	1,941,214	1,940,295
Mn <sup>†</sup>	6	50	128,574	121,686	257,148	243,372
Cr	39	100	276,486	272,076	276,486	272,076
Bo	2	100	18,054	0	18,054	0
Cr-6*	3	1300	276,486		21,268	
Mo*	16	13	4,554		36,431	
Ba	3	100	5894	6.9	5893.9	6.94
Ni	4	100	16955	15227.4	16955.1	15227.4
Cu <sup>†</sup>	1	100	1260	0	1259.7	0
Pb	7	71	1831	1669.4	2562.8	2337.12
As	9	33	229.8	79.5	689.3	238.47
Be	1	100	1068.9	1056.8	1068.9	1056.77
Cd	5	40	150.7	116.6	376.6	291.45
Co*	2	100	131.2		131.2	
Zn <sup>†</sup>	1	100	67.5	0	67.5	0
Hg	6	83	35.2	13.7	42.2	16.38
Al**	1	0				
Se**	13	0				
V**	3	0				
<b>Total metals</b>	126		3,320,735		3,227,393	

**(e) Nitrates and sulfates**

Contaminants	Number of plumes with a specific contaminant	Plumes with known concentration and volume			All plumes	
		% of plumes	Mass (kg)		Mass (kg)	
			Maximum	Above regulatory limit	Maximum	Above regulatory limit
Nitrates	71	72	52,605,366	52,603,153	73,234,921	73,231,840
Sulfates <sup>†</sup>	44	84	17,926,614	16,248,125	21,318,136	19,322,095
<b>Total sulfates and nitrates</b>	115		70531980		94553057	

**Table S10. Maximum activity estimates for the tritium and other radionuclides**

Contaminants	Number of plumes with a specific contaminant	Plumes with known concentration and volume			All plumes	
		% of plumes	Activity (pCi/l)		Activity (pCi/l)	
			Maximum	Above regulatory limit	Maximum	Above regulatory limit
Tritium	84	60	4,784,809	4,779,627	8,038,479	8,029,774
<b>Radioisotopes</b>						
Tc	16	81	7008.5		8625.85	
Sr	24	63	2705.6	2704	180.37	4326
I*	8	88	5.19		6	
U	44	27	3.44	3	12.61	12
Cs*	3	33	1.4		4.2	
Ra	9	22	0.4	0	1.8	2
Gross Alpha	3	100	0.91	0.9	0.91	0.9
Gross Beta	1	100	0.6	0.4	0.6	0.4
other (provide names)*	1	100	0.03		0.03	
Pu*	1	100	0.04		0.04	
Th*	4	25	0.12		0.48	
Co*	1	100	0		0	
Am**	1	0				
Carbon 14**	1	0				
<b>Total radionuclides</b>	117		9,726		8,833	

**Table S11. Regulatory concentration limits used in calculations of the maximum mass/activity of contaminants in groundwater.**

Contaminants	Limits ( $\mu\text{g/L}$ or $\text{pCi/L}$ )	limit type	Notes
<b>VOCs</b>			
PCE/TCE/VC/DCE/	5	MCL	PCE and TCE CA VC MCL is 0.5 For 1,1 DCE (most conservative DCE MCL). CA MCL for 1,1-DCE & cis-1,2-DCE is 6. CA MCL for trans-1,2_DCE is 10.
CT	5	MCL	CA MCL is 0.5
DCE	7	MCL	
chloroform	80	MCL	for total trihalomethanes applied singly to chloroform
VC	2	MCL	
methylene chloride	5	MCL	Also called dichloromethane. Same as CA MCL
TCA	200	MCL	Standard for 1,1,1-TCA. Same as CA MCL. CA MCL for 1,1,2-TCA is 5.
DCA	5	MCL	Standard for 1,2-DCA. Same as CA MCL for 1,1-DCA. CA MCL for 1,2-DCA is 0.5
carbon disulfide	1600	CA RL	no MCL
<b>Fuel and Fuel Components</b>			
Benzene	5	MCL	CA MCL is 1
dichlorobenzene	75	MCL	MCL for p-dichlorobenzene (1,4)--CA MCL = 5. MCL for o-dichlorobenzene (1,2-) = 600--the same as CA MCL.
MTBE	13	CA MCL	no MCL
Toluene	1000	MCL	CA MCL is 150.
ethylbenzene	700	MCL	CA MCL is 300.
<b>Explosives</b>			
perchlorate	60	CA RL	no MCL
<b>Metals</b>			
Fe <sup>+</sup>	300	SDWS	CA SDWS is same.
Mn <sup>+</sup>	50	SDWS	CA SDWS is same.
Cr	100	MCL	CA MCL is 50
Bo	10000	CA RL	no MCL
Cr-6*	NA		Cr-VI is regulated under total Cr MCL.
Ba	2000	MCL	CA MCL is 1000

Ni	100	CA MCL	no MCL
Cu <sup>†</sup>	1000	SDWS	CA SDWS is 1000. TT is 1300.
Pb	15	TT	
As	10	MCL	As of 1/23/06. CA MCL is 50 currently
Be	4	MCL	same as CA MCL
Cd	5	MCL	same as CA MCL
Zn <sup>†</sup>	5000	SDWS	CA SDWS is same.
Hg	2	MCL	MCL for inorganic form. Same as CA MCL.
Al <sup>**</sup>	200	CA SDWS	no MCL
Se <sup>**</sup>	50	MCL	same as CA MCL
V <sup>**</sup>	500	CA RL	no MCL
<b>Tritium</b>			
Total tritium	20,000	CA MCL	no MCL
<b>Radioisotopes</b>			
Sr	8	CA MCL	For Sr-90
U	20	CA MCL	no MCL on activity basis. U MCL is on mass basis and is utilized in metals group results.
Ra	5	MCL	same as CA MCL
Gross Alpha	15	MCL	same as CA MCL except CA standard is for alpha excluding that from Ra and U.
Gross Beta	50	CA MCL	MCL is in unites of millirems/year.
<b>Sulfates and nitrates</b>			
Nitrates	10	MCL	
Sulfates <sup>†</sup>	250,000	SDWS	

**Table S12. The basic groups of plume characteristics used in the FMA.**

<b>Groups of plume characteristics</b>	<b>Qualitative or quantitative data</b>	<b>Number of data categories</b>	<b>Main (1) or supplementary (0) data</b>
Contaminant groups (Cntm)	Qualitative 8		1
Severity index (Sv)	Quantitative	2	1
Plume volume (Vol)	Quantitative 1		1
Depth and Velocity (Dp+V)	Quantitative 2		0
Climate Qualita	tive	1	0

Table S13. Results of multiple factor analysis of groundwater plumes

**(a) Descriptive statistics of data groups**

Variable	Number of sites *)	Minimum	Maximum	Mean	Std. deviation
Ngr	124	1.000	6.000	2.742	1.182
Sv	124	1.000	16.000	10.258	6.405
Vol	124	4.699	10.544	7.535	1.184
Dp	124	0.778	3.627	1.888	0.504
Vel	124	0.000	3.699	2.130	0.732

\*) 124 is the number of sites with all groups of data

**(b) Frequences of qualitative groups**

Variable	Present-1, Absent-0	Frequencies	%
VOCs	0	27	21.774
	1	97	78.226
FI	0	112	90.323
	1	12	9.677
Expl	0	112	90.323
	1	12	9.677
Mt	0	80	64.516
	1	44	35.484
H3	0	73	58.871
	1	51	41.129
RI	0	85	68.548
	1	39	31.452
SO4	0	87	70.161
	1	37	29.839
NO3	0	76	61.290
	1	48	38.710
Cl	1	98	79.032
	2	26	20.968

**(c) Correlation matrix - Pearson correlation coefficients**

Variables	Ngr	Sv	Vol	Dp	Vel
Ngr	1	0.583	-0.111	0.312	0.101
Sv	0.583	1	-0.025	0.342	0.132
Vol	-0.111	-0.025	1	-0.035	-0.101
Dp	0.312	0.342	-0.035	1	0.101
Vel	0.101	0.132	-0.101	0.101	1

**(d) Bart table of contaminant groups**

	VOCs-0	VOCs-1	F0	F-1	Exp-0	Exp-1	M-0	M-1	H-0	H-1	R-0	R-1
VOCs-0	27	0	23	4	24	3	13	14	12	15	13	14
VOCs-1	0	97	89	8	88	9	67	30	61	36	72	25
F0	23	89	112	0	100	12	72	40	64	48	77	35
F-1	4	8	0	12	12	0	8	4	9	3	8	4
Exp-0	24	88	100	12	112	0	71	41	64	48	74	38
Exp-1	3	9	12	0	0	12	9	3	9	3	11	1
M-0	13	67	72	8	71	9	80	0	51	29	58	22
M-1	14	30	40	4	41	3	0	44	22	22	27	17
H-0	12	61	64	9	64	9	51	22	73	0	60	13
H-1	15	36	48	3	48	3	29	22	0	51	25	26
R-0	13	72	77	8	74	11	58	27	60	25	85	0
R-1	14	25	35	4	38	1	22	17	13	26	0	39
SO4-0	22	65	76	11	75	12	62	25	48	39	50	37
SO4-1	5	32	36	1	37	0	18	19	25	12	35	2
NO3-0	15	61	66	10	72	4	50	26	46	30	53	23
NO3-1	12	36	46	2	40	8	30	18	27	21	32	16

**(e) Eigenvalues and percentages of factors**

	F1	F2	F3	F4	F5	F6	F7	F8	F9	F10
Eigenvalue	1.748	1.220	0.949	0.684	0.601	0.554	0.459	0.378	0.172	0.070
Variability (%)	25.573	17.853	13.883	10.009	8.793	8.104	6.710	5.535	2.512	1.081
Cumulative%	25.573	43.426	57.308	67.317	76.110	84.214	90.923	96.458	98.969	100.000

**(f) LG and RV coefficients****LG coefficients**

	Crim	Sv	Vd	Dp+V	Q	MFA
Crim	3.138	0.783	0.088	0.349	0.207	2.294
Sv	0.783	1.070	0.008	0.139	0.026	1.065
Vd	0.088	0.008	1.000	0.010	0.010	0.627
Dp+V	0.349	0.139	0.010	1.667	0.018	0.285
Q	0.207	0.026	0.010	0.018	1.000	0.139
MFA	2.294	1.065	0.627	0.285	0.139	2.281

**RV coefficients**

	Crim	Sv	Vd	Dp+V	Q	MFA
Crim	1.000	0.427	0.050	0.152	0.117	0.857
Sv	0.427	1.000	0.008	0.104	0.025	0.682
Vd	0.050	0.008	1.000	0.008	0.010	0.415
Dp+V	0.152	0.104	0.008	1.000	0.014	0.146
Q	0.117	0.025	0.010	0.014	1.000	0.092
MFA	0.857	0.682	0.415	0.146	0.092	1.000

**(g) Correlations between variables and factors**

	F1	F2	F3	F4	F5	F6	F7	F8	F9	F10
Ng	0.858	-0.147	0.373	-0.026	0.046	0.300	-0.085	0.053	-0.026	-0.080
Sv	0.842	0.343	-0.072	0.184	-0.046	-0.126	-0.183	-0.130	-0.090	0.242
Vd	-0.250	0.725	0.551	0.194	0.029	0.048	0.251	0.068	0.011	0.014
Dp	0.430	0.000	0.006	0.168	-0.006	-0.218	0.186	0.046	-0.054	-0.177
Vd	0.191	0.078	-0.094	-0.330	-0.022	-0.048	0.039	-0.044	0.146	0.026

**(h) Factors corresponding to cluster centroids (from k-means clustering)**

Cluster	F1	F2	F3	F4
1	0.213	0.135	0.098	0.068
2	0.124	0.063	0.410	0.073
3	0.701	0.070	0.064	0.034
4	0.085	0.580	0.054	0.032
5	0.100	0.070	0.085	0.409

**(i) Classification of plumes into 5 clusters (plume names corresponding to plume codes are given in Table S1)**

Cluster 1	Cluster 2	Cluster 3	Cluster 4	Cluster 5
11	12	6	178	29
13	7	134	180	41
15	14	189	181	48
179	144	22	190	49
191	43	24	16	50
17	56	25	18	51
143	195	28	19	57
23	204	31	20	192
26	205	32	21	217
27	208	42	35	61
30	65	47	193	63
33	66	226	197	70
34	225	58	198	222
36	85	210	200	223
37	155	212	206	110
38	87	214	207	
39		216	209	
145		59	211	
44		67	219	
45		220	64	
46		221	156	
227		78	157	
228		86	98	
52		99		
53		109		
54				
55				
194				
196				
199				
201				
202				
203				
213				
218				
60				
62				
224				
71				
81				
82				
83				
84				
88				
90				

Table S14. Results of multiple factor analysis of groundwater plumes with CCl4 concentrations

**(a) Descriptive statistics of data groups**

Variable	Observations*)	Minimum	Maximum	Mean	Std. deviation
Ngr	26	2.000	5.000	3.423	0.987
Sv	26	2.000	16.000	10.462	6.408
Vol	26	5.272	9.872	7.143	1.023
CCl4_r	26	0.200	1380.000	84.085	296.050
Dp	26	1.000	2.778	2.069	0.311
Vel	26	1.000	3.301	1.881	0.571

\*) 26 is the number of sites with all groups of data

**(b) Frequencies of qualitative groups**

Variable	Categories	Frequencies	%
VOCs	1	26	100.000
FI	0	24	92.308
	1	2	7.692
Expl	0	26	100.000
Mt	0	16	61.538
	1	10	38.462
H3	0	13	50.000
	1	13	50.000
RI	0	22	84.615
	1	4	15.385
SO4	0	9	34.615
	1	17	65.385
NO3	0	9	34.615
	1	17	65.385
Cl	1	25	96.154
	2	1	3.846

**(c) Correlation matrix - Pearson correlation coefficients**

Variables	Ngr	Sv	Vol	CCl4	Dp	Vel
Ngr	1	0.563	-0.344	-0.019	0.285	0.127
Sv	0.563	1	-0.160	0.042	0.127	0.373
Vol	-0.344	-0.160	1	-0.175	-0.392	-0.320
CCl4	-0.019	0.042	-0.175	1	0.023	0.228
Dp	0.285	0.127	-0.392	0.023	1	0.691
Vel	0.127	0.373	-0.320	0.228	0.691	1

**(d) Eigenvalues and percentages of factors**

	F1	F2	F3	F4	F5	F6	F7	F8	F9
Eigenvalue	1.734	1.471	1.062	0.701	0.456	0.234	0.190	0.055	0.008
Variability (	29.336	24.887	17.963	11.860	7.716	3.951	3.220	0.928	0.139
Cumulative	29.336	54.224	72.187	84.047	91.762	95.713	98.933	99.861	100.000

**(e) Correlations between variables and factors**

	F1	F2	F3	F4	F5	F6	F7	F8	F9
Cntm	0.488	0.698	0.438	0.350	0.247	0.201	0.152	0.052	0.004
Sv	0.710	0.063	0.379	0.047	0.029	0.030	0.017	0.001	0.004
Vol	0.523	0.048	0.225	0.041	0.157	0.002	0.004	0.001	0.000
CCl4	0.014	0.661	0.020	0.264	0.022	0.001	0.017	0.000	0.000
Dp+V	0.240	0.137	0.043	0.215	0.172	0.173	0.028	0.018	0.003
Cl	0.000	-0.042	-0.038	-0.129	-0.013	-0.015	-0.049	-0.052	0.000

**(f) Lg and RV coefficients****Lg coefficients:**

	Cntm	Sv	Vol	CCI4	Dp+V	Cl	MFA
Cntm	1.785	0.611	0.194	0.185	0.661	0.193	1.601
Sv	0.611	1.078	0.092	0.001	0.096	0.025	1.028
Vol	0.194	0.092	1.000	0.031	0.151	0.002	0.759
CCI4	0.185	0.001	0.031	1.000	0.031	0.003	0.702
Dp+V	0.661	0.096	0.151	0.031	1.033	0.096	0.542
Cl	0.193	0.025	0.002	0.003	0.096	1.000	0.128
MFA	1.601	1.028	0.759	0.702	0.542	0.128	2.358

**RV coefficients:**

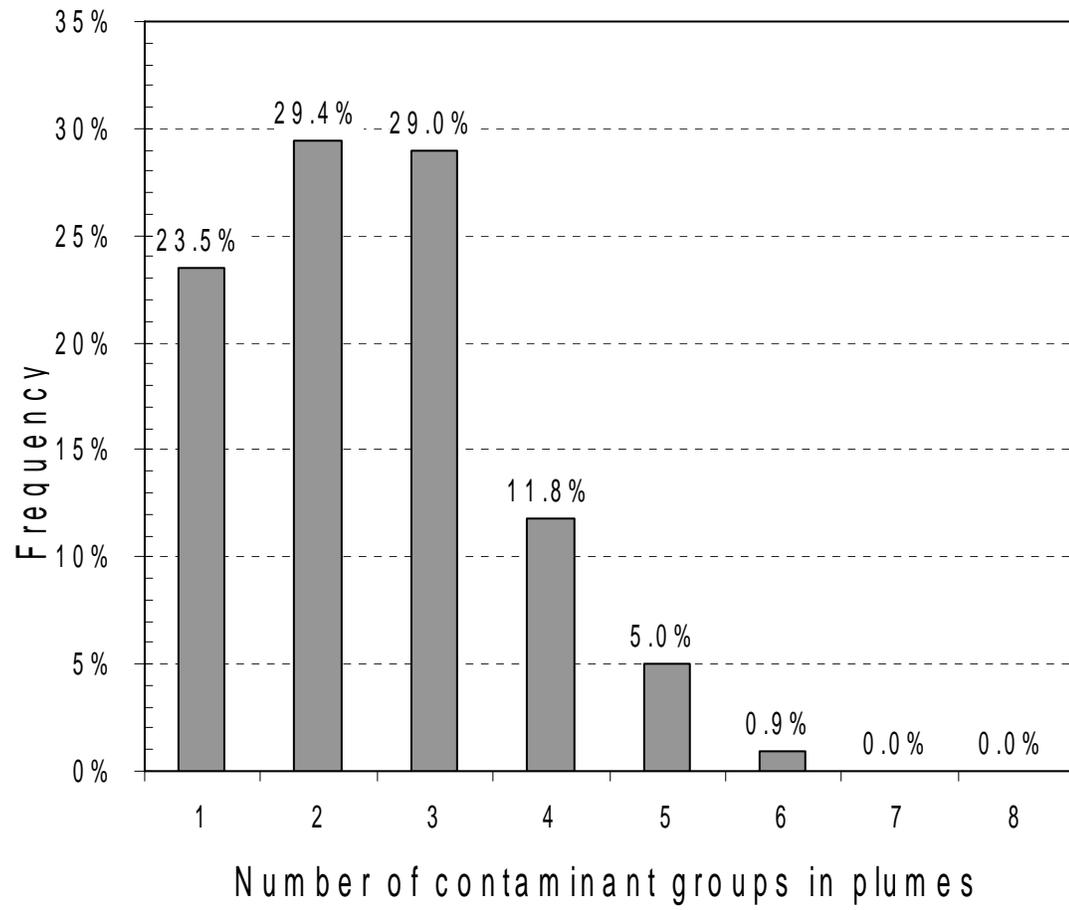
	Cntm	Sv	Vol	CCI4	Dp+V	Cl	MFA
Cntm	1.000	0.440	0.145	0.139	0.487	0.144	0.780
Sv	0.440	1.000	0.089	0.001	0.091	0.024	0.645
Vol	0.145	0.089	1.000	0.031	0.149	0.002	0.494
CCI4	0.139	0.001	0.031	1.000	0.031	0.003	0.457
Dp+V	0.487	0.091	0.149	0.031	1.000	0.094	0.347
Cl	0.144	0.024	0.002	0.003	0.094	1.000	0.083
MFA	0.780	0.645	0.494	0.457	0.347	0.083	1.000

**(g) Factors corresponding to cluster centroids (k-means clustering)**

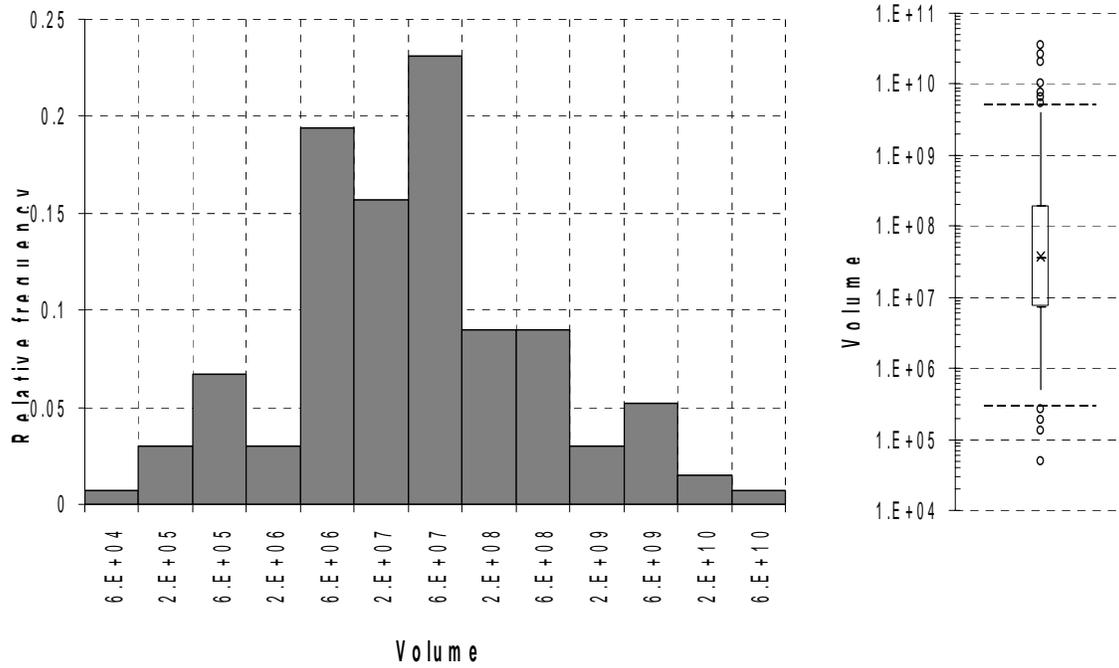
Cluster	F1	F2	F3
1	1.535	1.135	0.003
2	-1.038	0.143	1.177
3	-1.108	0.644	0.118
4	1.327	-0.953	0.890
5	-0.397	-0.544	-1.548

**(h) Classification of plumes into 5 clusters (numbers are plume codes given in Table S1)**

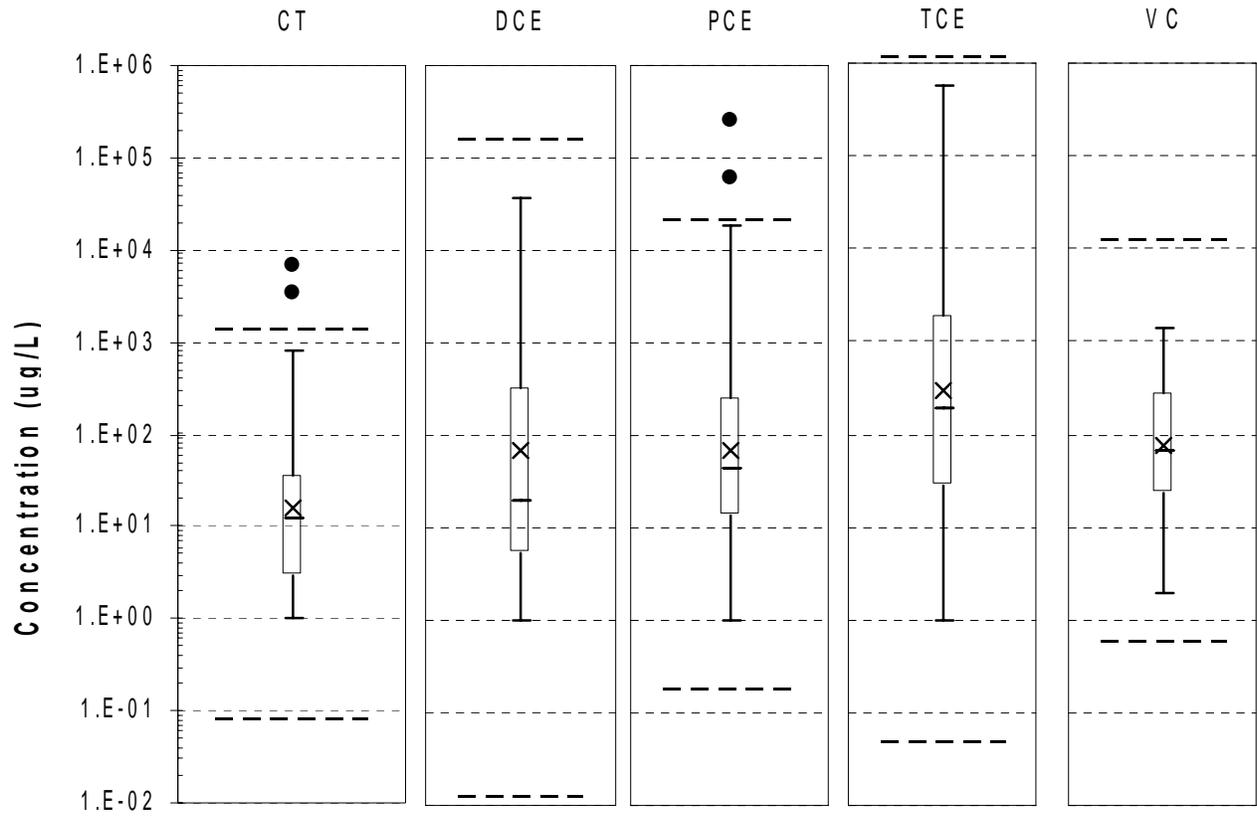
Cluster	1	2	3	4	5
	26	37	44	57	197
	27	41	53	58	200
		49	54	193	203
		81	202	194	204
				205	206
				212	207
				214	211
				216	219



**Figure S1. Frequency of occurrence of contaminant groups in groundwater plumes.**

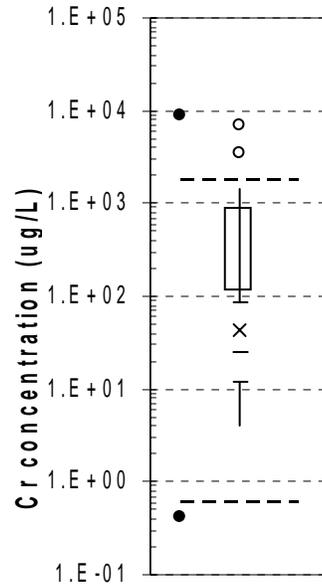


**Figure S2. (a) Relative frequency of plume volumes: bin values shown are midpoints of log of volume (in  $m^3$ ); (b) Box plot of log plume volumes. The mean is labeled as “x,” the median as “–“, the whiskers are shown as  $Q1-1.5(Q3-Q1)$  and  $Q3+1.5(Q3-Q1)$ , and the outliers are shown by open circles.**

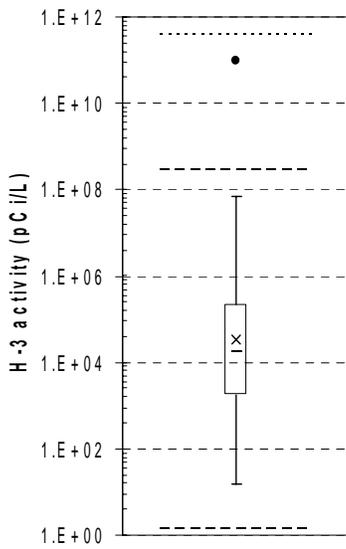
**(a) Chlorinated Hydrocarbons**

## (b) Metals and radioisotopes

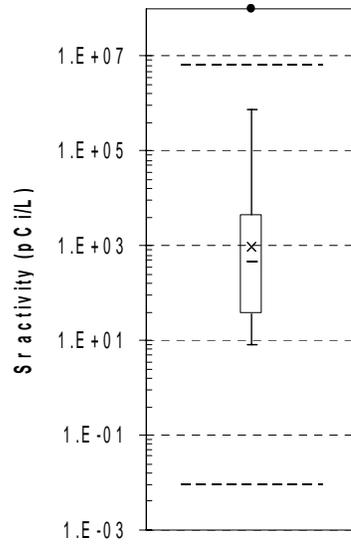
Cr



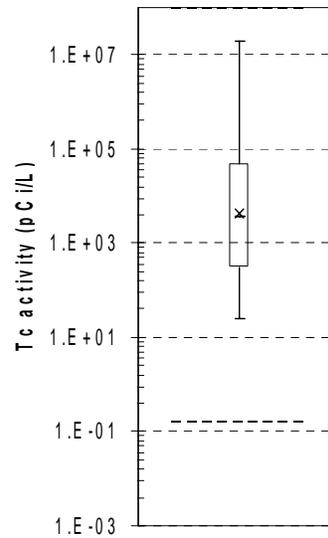
H-3



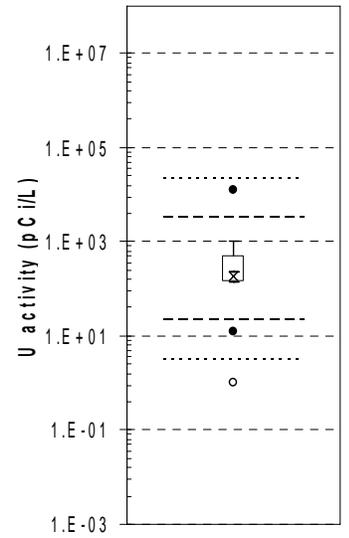
Sr



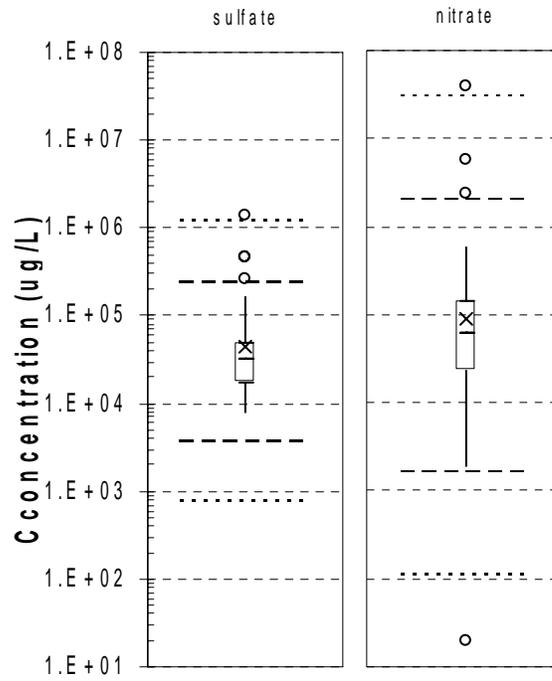
Tc



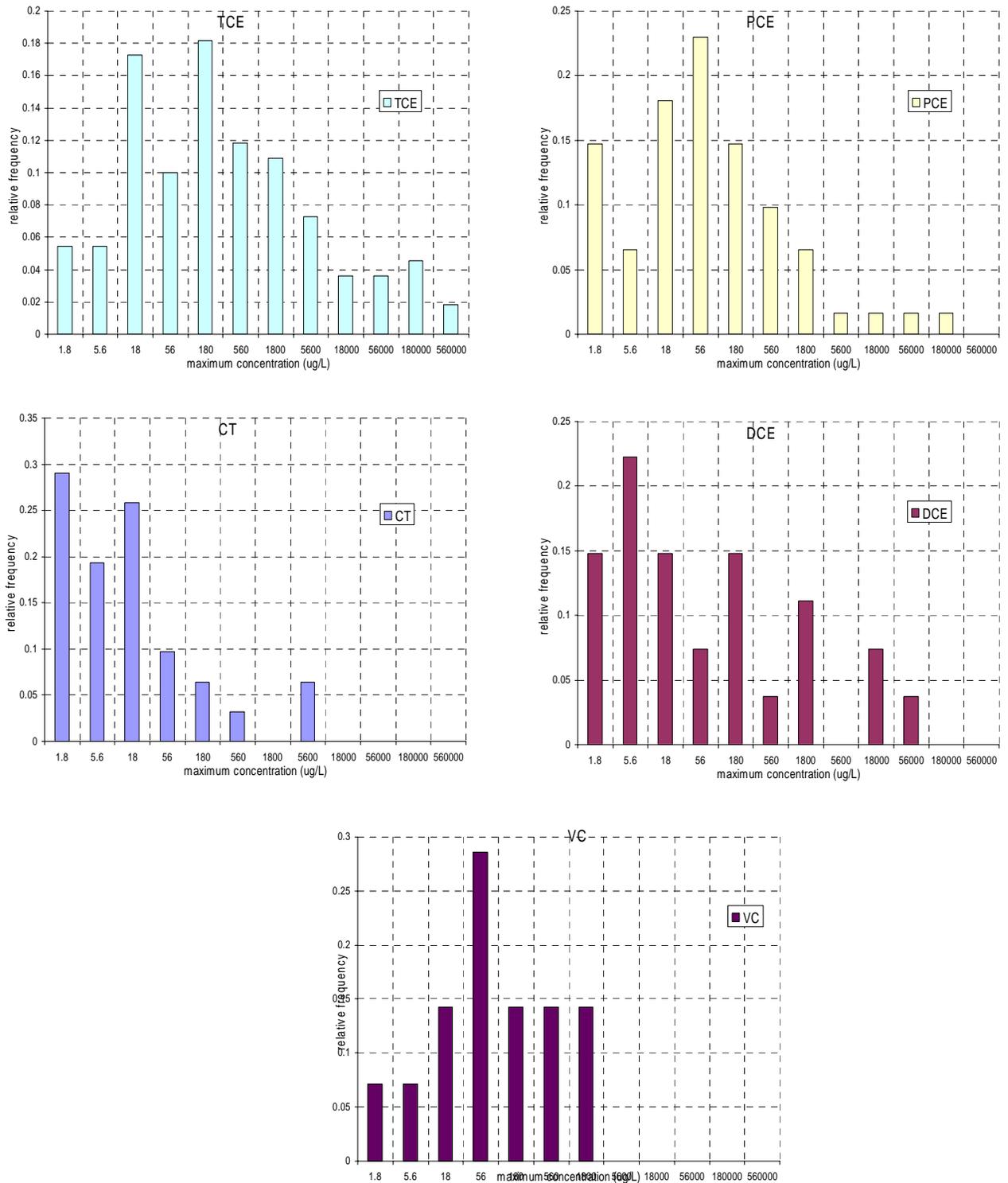
U



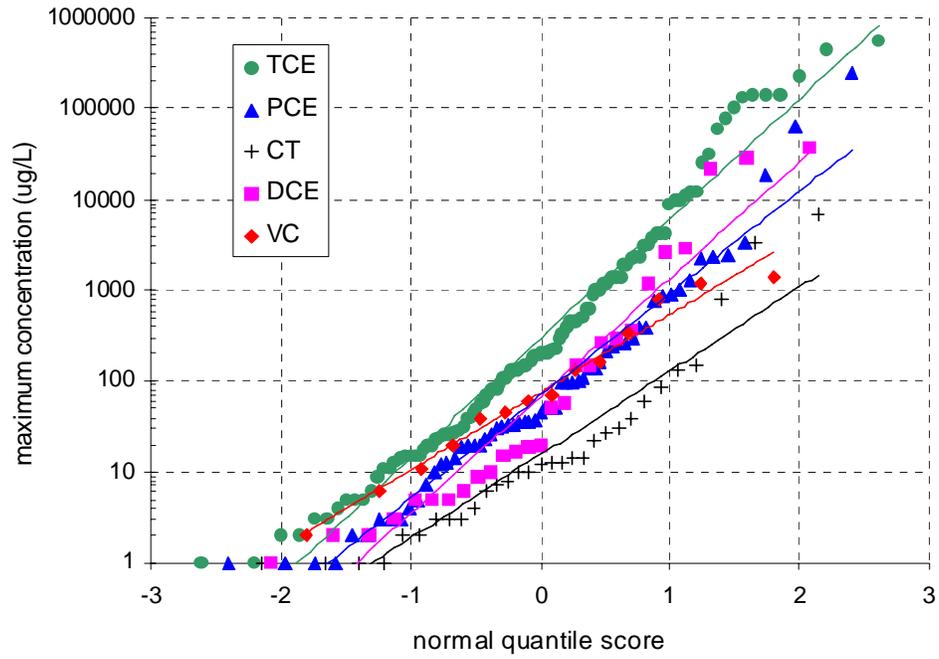
## (c) Sulfates and nitrates



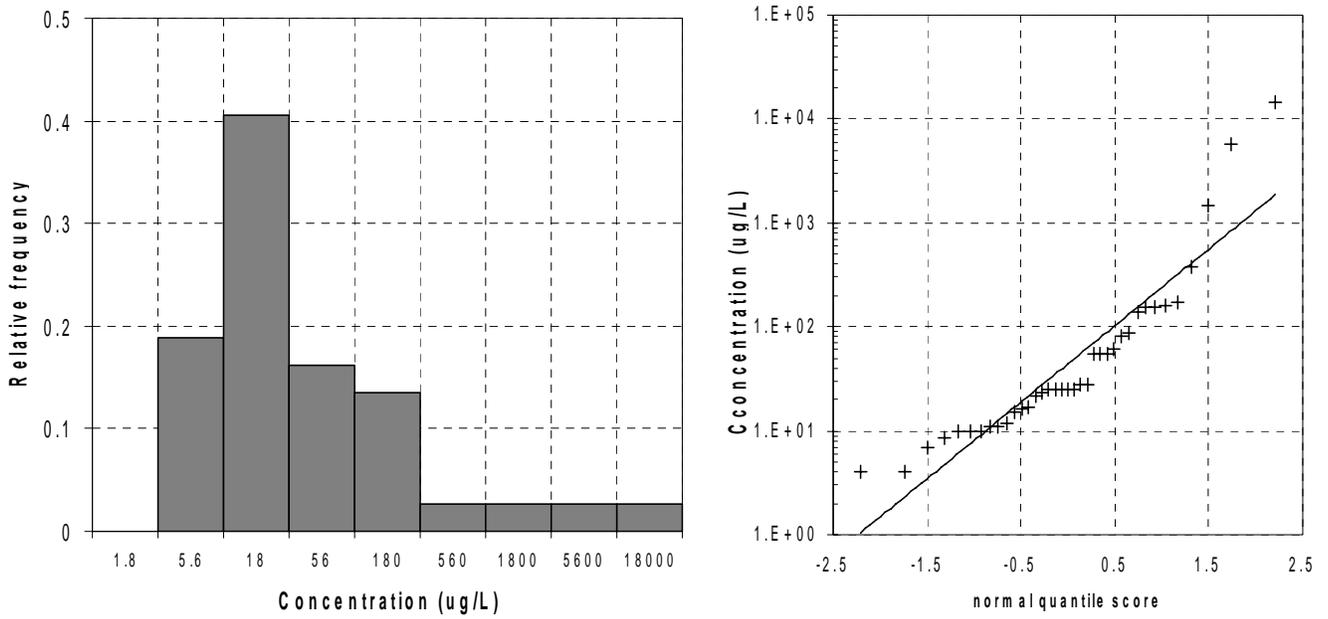
**Figure S3. Box-and-whiskers plots of maximum concentrations of contaminants: the mean is shown by a symbol “x”, the median by a symbol “-”, the whiskers are shown as  $Q1-1.5(Q3-Q1)$  and  $Q3+1.5(Q3-Q1)$ , and the outliers are shown by open circles. Solid circles are minimum and maximum concentrations from Riley and Zachara (1992).**



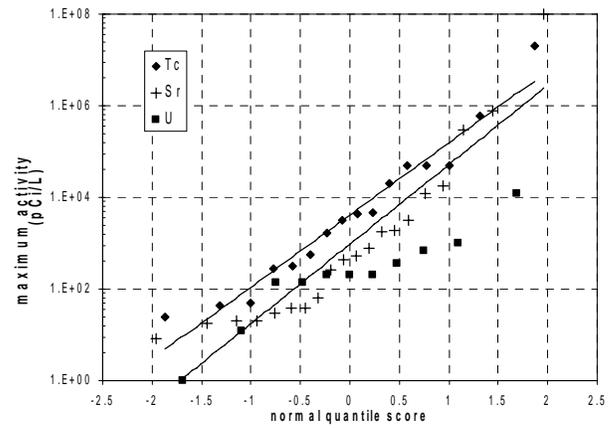
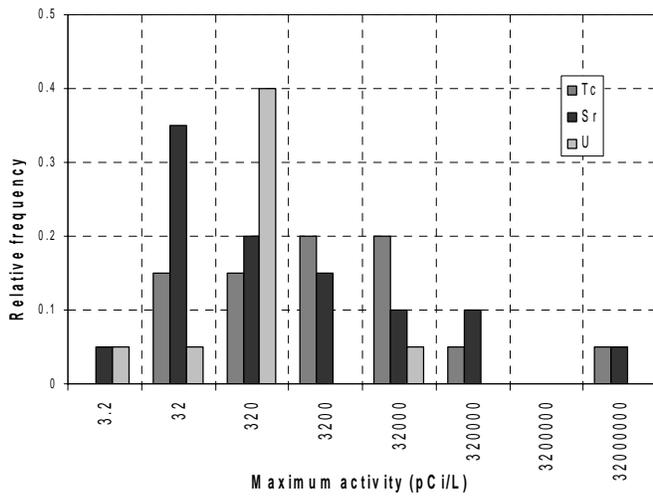
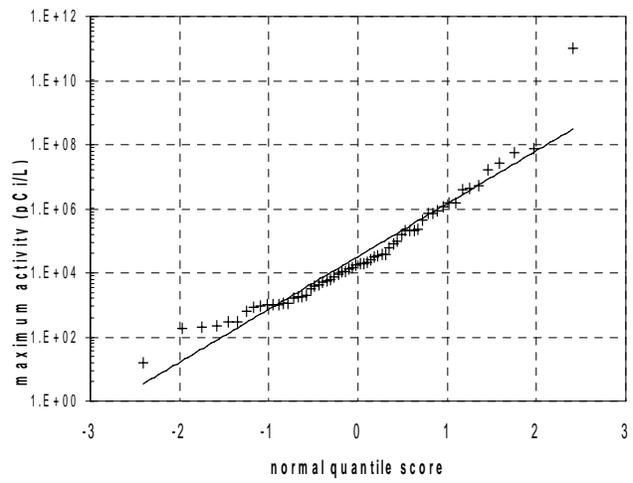
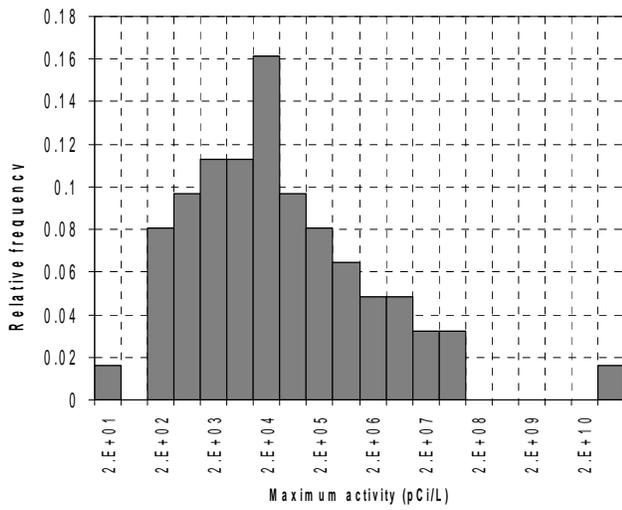
**Figure S4. Relative frequency of the maximum concentrations of chlorinated hydrocarbons. Note bin values are midpoints in log space.**



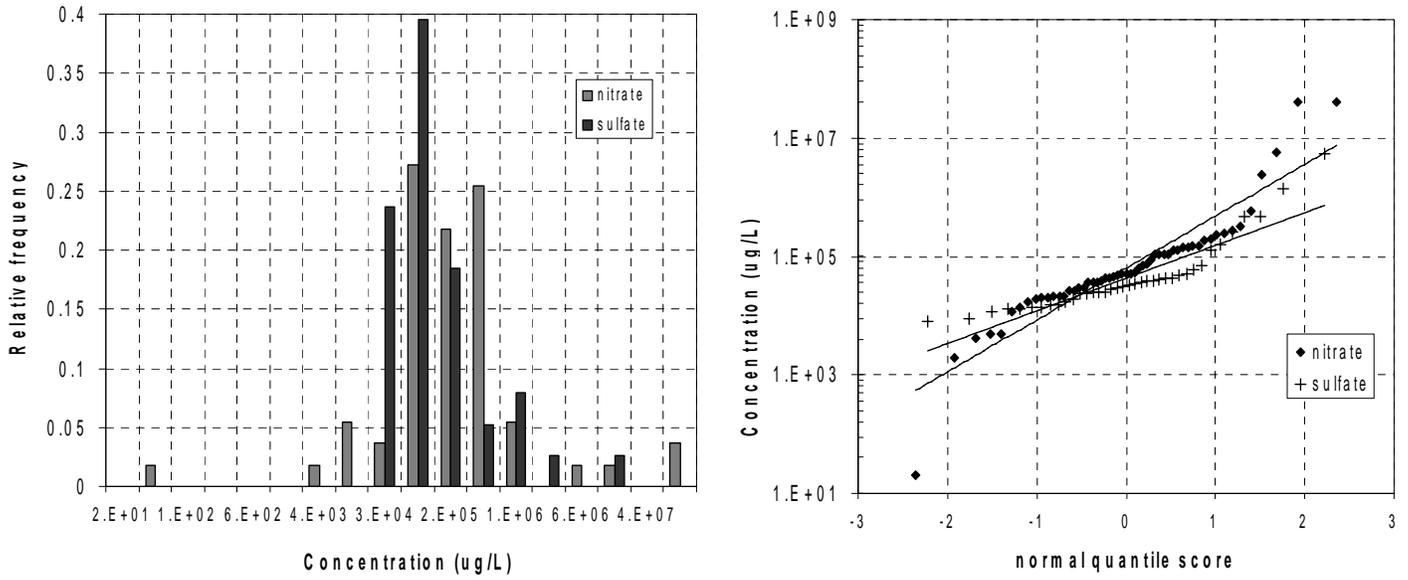
**Figure S5. Plots of a normal quantile score vs. maximum concentrations of chlorinated hydrocarbons.**



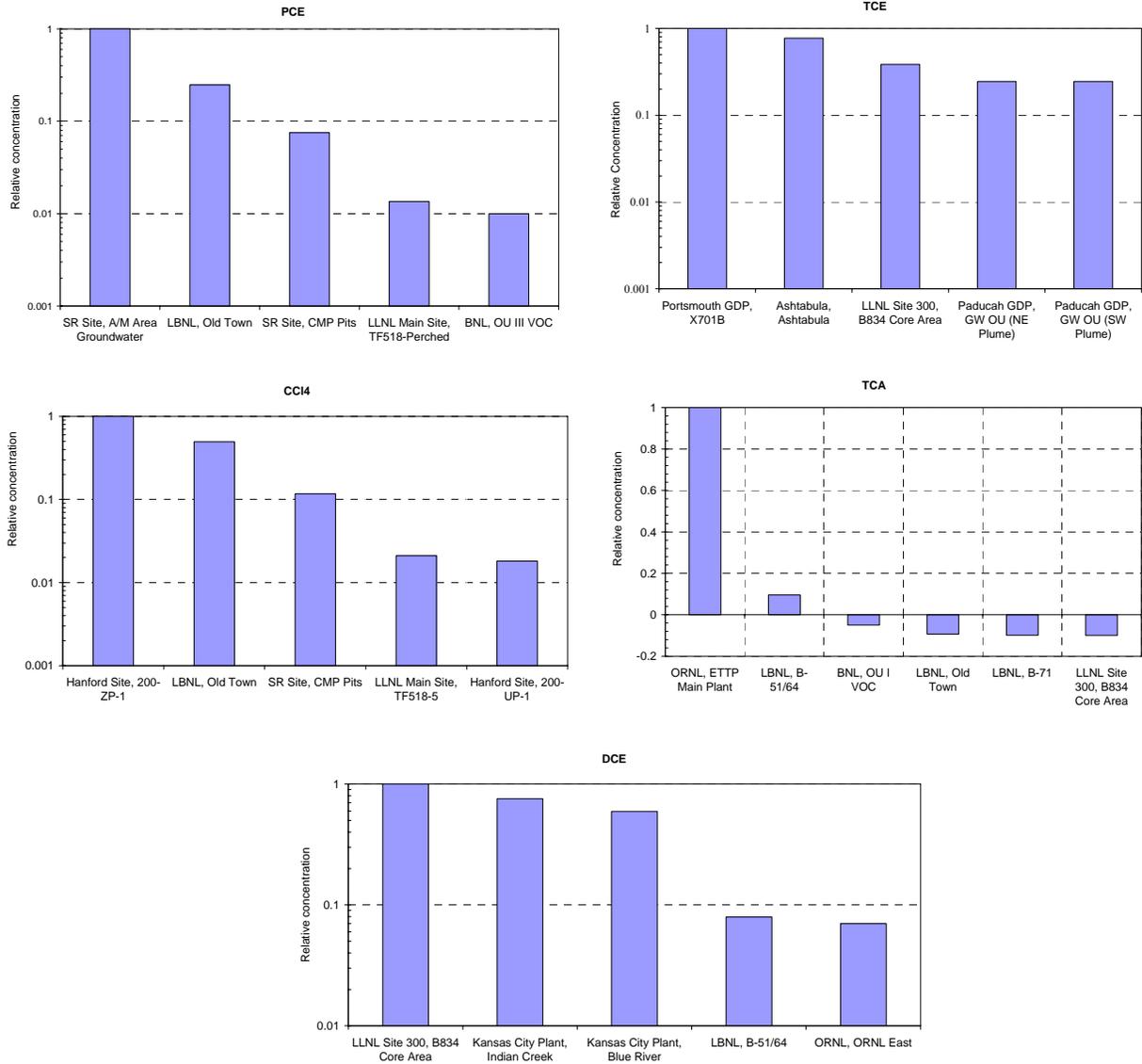
**Figure S6. Relative frequency and a normal quantile score vs. maximum Cr concentrations. Bin values are midpoints in log space.**



**Figure S7. Relative frequency and a normal quantile score vs. maximum  $^3\text{H}$ , Sr, Tc, and U concentrations. Bin values are midpoints in log space.**



**Figure S8. Relative frequency and a normal quantile score vs. maximum concentrations of nitrates and sulfates. Bin values are midpoints in log space.**



**Figure S9. Relative concentration for chlorinated hydrocarbons. Five largest estimates for each contaminant are shown.**

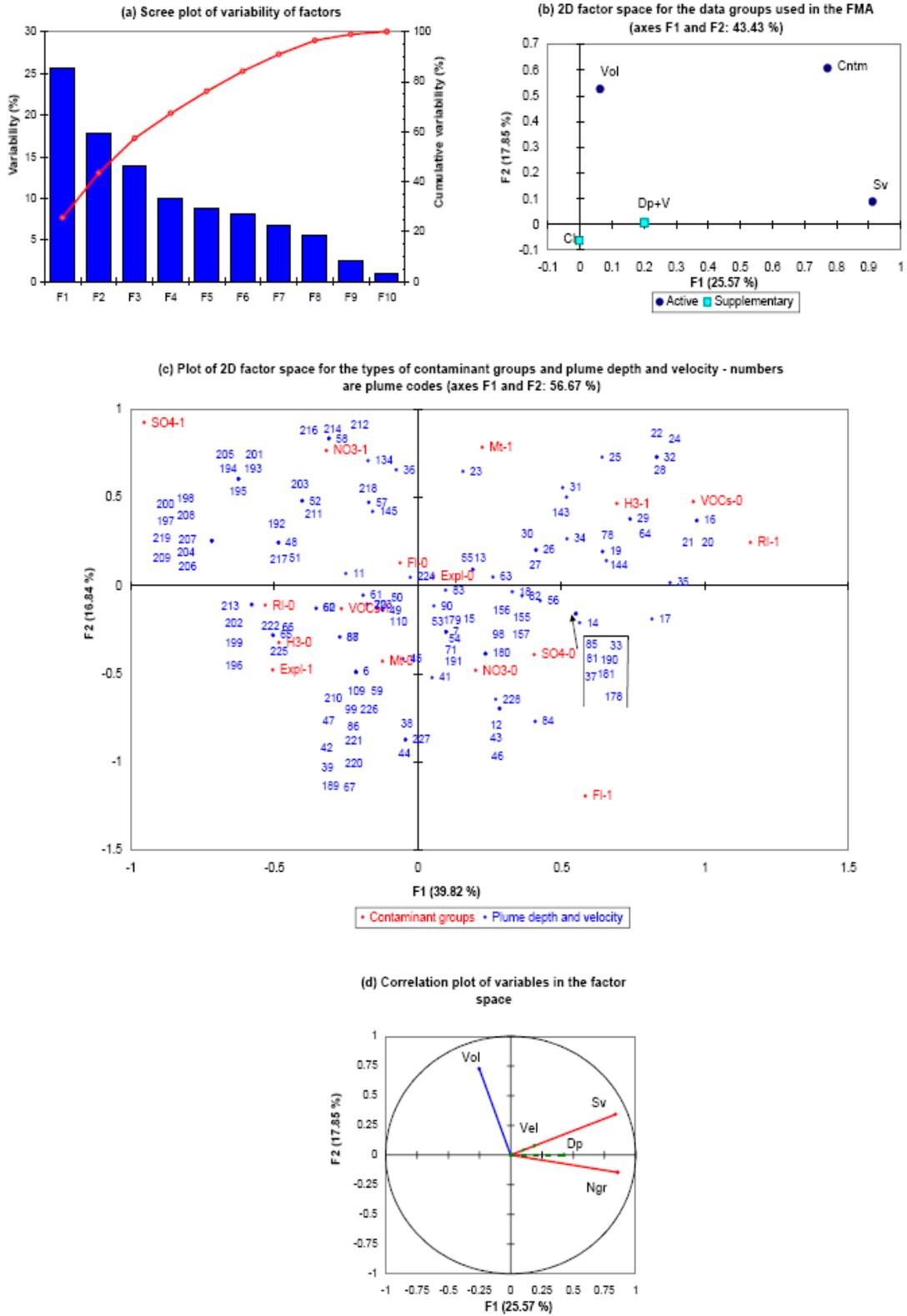


Figure S10. Results of MFA for groundwater plume characteristics (numbers are plume codes - see Table S1)

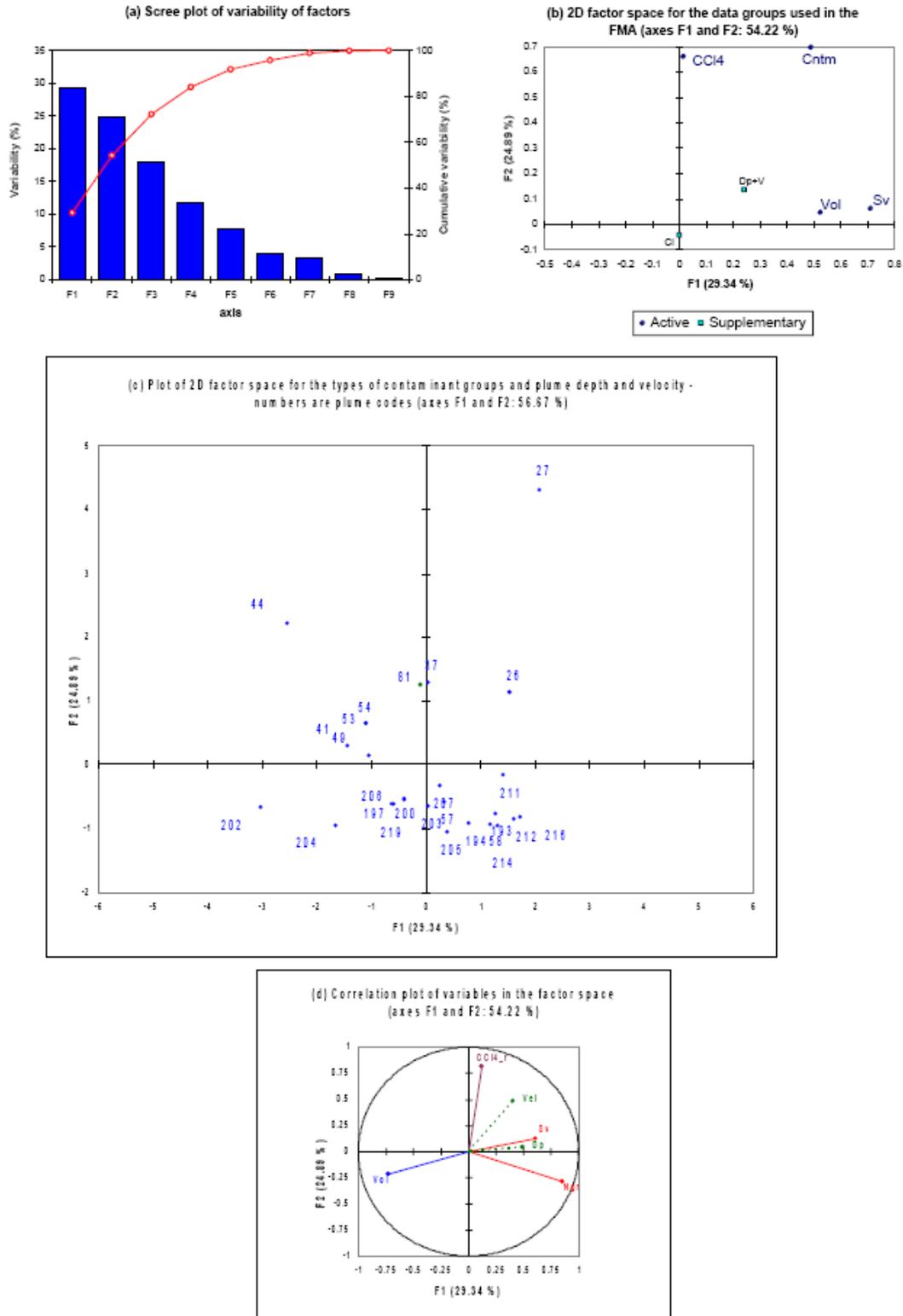


Figure S11. Results of MFA for data groups including CCl<sub>4</sub> concentrations

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