Chemical Contaminants on DOE Lands and Selection of Contaminant Mixtures for Subsurface Science Research

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Preface

This report identifies individual contaminants and contaminant mixtures that have been measured in the ground at 91 waste sites at 18 U.S. Department of Energy (DOE) facilities within the weapons complex. The inventory of chemicals and mixtures was used to identify generic chemical mixtures to be used by DOE's Subsurface Science Program in basic research on the subsurface geochemical and microbiological behavior of mixed contaminants (DOE 1990a and b). The generic mixtures contain specific radionuclides, metals, organic ligands, organic solvents, fuel hydrocarbons, and polychlorinated biphenyls (PCBs) in various binary and ternary combinations. The mixtures are representative of in-ground contaminant associations at DOE facilities that are likely to exhibit complex geochemical behavior as a result of intercontaminant reactions and/or microbiologic activity stimulated by organic substances. Use of the generic mixtures will focus research on important mixed contaminants that are likely to be long-term problems at DOE sites and that will require cleanup or remediation.

The report provides information on the frequency of associations among different chemicals and compound classes at DOE waste sites that require remediation. For example, radionuclides such as uranium, plutonium, strontium, and cobalt were found, in some cases, to be disposed of with organic substances (e.g., organic acids, completing agents, and solvents) that could influence radionuclide geochemical behavior and subsurface transport. Knowledge of the types of chemicals that coexist in waste sites is important to remediation for various reasons:

- The efficiency of many biotic and abiotic treatment processes for soil and ground-water contaminants is affected by the presence of co-contaminants.
- Multiple contaminant species may be treated simultaneously and more effectively by specific aboveground or in-ground techniques if the nature of the contaminant association is understood in advance.
- Certain types of chemical mixtures may require special precautions or the development of new remediation strategies or techniques.
- In-ground remediation activities may selectively mobilize certain mixtures of chemical constituents to air or ground water, thereby increasing environmental risk; or some mixtures may be stabilized, thus reducing environmental impact.

The report provides quantitative information on the frequency of occurrence of binary, ternary, and higher order contaminant mixtures in the 91 waste sites. This quantitative information may be used to refine or guide the development of new above-ground and in situ remediation strategies that can be used throughout the weapons complex.

Scientists who are interested in participating in DOE's Subsurface Science Program are encouraged to review this document and the Program Overview (U.S. Department of Energy 1990b) for information about DOE's research interests and as a basis for collaboration with current investigators. Additional information about DOE's research under the Subsurface Science Program can be obtained by writing Dr. Frank Wobber, DOE's Program Manager; further details on research in Co-Contaminant Chemistry can be obtained from Dr. John Zachara, Geosciences Department, Pacific Northwest Laboratory, P.O. Box 999, Richland, WA 99352.

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Summary

This document summarizes a review of monitoring and restoration reports from 91 waste sites at 18 U.S. Department of Energy (DOE) facilities. The review was conducted to identify (1) inorganic and organic contaminants found within soil and ground water at DOE waste sites, (2) their concentration ranges, and (3) their frequency of occurrence as single compounds and as binary, ternary, quaternary, and higher order contaminant mixtures. Fuel hydrocarbons, chlorinated hydrocarbons, radionuclides, metals, inorganic anions, and ketones were the contaminant classes most frequently measured in the ground at DOE facilities. The chlorinated hydrocarbon, fuel hydrocarbon, radionuclide(s), metal(s), and ketone reported in ground water most frequently were trichloroethylene, toluene, tritium/uranium, lead/chromium, and acetone, respectively,

Contaminants in waste sites were frequently mixed; binary contaminant mixtures were reported at 64 percent of the waste sites, and ternary mixtures were observed at 49 percent of the sites, The most common binary contaminant mixture was that of metals and radionuclides. Twelve other common pairings included metals, anions, radionuclides, chlorinated hydrocarbons, polychlorinated biphenyls (PCBs), and ketones in various combinations. Mixtures of contaminants that could interact with each other and modify each other's subsurface geochemical behavior were disposed of together in DOE waste sites. For example, mixtures of radionuclides and metals with organic ligands (organic acids or aminocarboxylic chelating agents) that could lead to mobile aqueous complexes in soil and ground water were observed at 19 waste sites. Organic solvents (chlorinated hydrocarbons and ketones) that can mobilize sparingly soluble hydrophobic organic compounds were disposed of with PCBs at 15 waste sites. Furthermore, organic substances that can modify metal ion/radionuclide speciation by stimulating subsurface microflora were disposed of to the ground with metal- and radionuclide-containing wastes.

Information on the contaminants occurring most frequently and on their observed in-ground combinations was used to identify a series of generic chemical mixtures that can be used in basic research on co-contaminant geochemistry and microbiology. The generic mixtures represent compound class combinations that (1) are expected, based on observations in the literature, to exhibit different types of co-contaminant interactions and (2) are known to exist in the subsurface environment at DOE sites. These mixtures include—

- Chlorinated hydrocarbons and fuel hydrocarbons.
- Metals/anions and radionuclides.
- Organic solvents and PCBs.
- Metals/radionuclides and organic acids.
- Metals/radionuclides and completing agents.
- Metals/radionuclides and ketones.
- Metals/radionuclides, organic acids/complexing agents, and organic solvents.
- Metals/radionuclides and natural organic substances.

These mixtures all have equal priority for research, based on the frequency of their occurrence, their likelihood to influence contaminant dynamics, and the extent of research knowledge. This document provides guidance on how to select elements or compounds from the generic mixtures for research.

The review and the process of mixture selection were limited by the data base on chemical constituents in DOE waste sites. Nonregulated chemical contaminants often were not included in monitoring and chemical characterization efforts at DOE sites. Consequenty, data were insufficient to define the true frequency of occurrence and environmental concentrations of many important co-contaminants, including various organic complexing agents that could significantly affect radionuclide mobility.

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Acronyms

ANL	Argonne National Laboratory
BNL	Brookhaven National Laboratory
BTEX	benzene/toluene/ethylbenzene/xylene
BTX	benzene/toluene/xylene
CMP	chemicals, metals, and pesticides
DOE	U.S. Department of Energy
DDT	dichlorodiphenyltrichloroethane
DTPA	diethylenetriamine pentaacetic acid
EDTA	ethylenediamine tetraacetic acid
EPA	U.S. Environmental Protection Agency
FMPC	Fernald, Feed Materials Production Center
GAO	U.S. Government Accounting Office
HMX	octahydro- 1,3,5,7-tetranitro- 1,3,5,7-tetraazozine
HS	Hanford Site
ICPP	Idaho Chemical Processing Plant
INEL	Idaho National Engineering Laboratory
KCP	Kansas City Plant
LANL	Los Alamos National Laboratory
LLNL	Lawrence Livermore National Laboratory
MCL	maximum contaminant level
MCLG	maximum contaminant level goal
MND	Mound
NTA	nitriloacetic acid
NTS	Nevada Test Site
OHER	Office of Health and Environmental Research
ORNL	Oak Ridge National Laboratory
PCB	polychlorinated biphenyl
PCE	perchloroethylene
PETN	2,2,-Bis [(nitroxy) methyl-] 1,3-propanediol-dinitrate
PGDP	Portsmouth Gaseous Diffusion Plant
pH	opposite log of the hydrogen ion activity
PNTX	Pantex Plant
PP	Pinellas Plant
ppb	parts per billion
ppt	parts per thousand
PUREX	plutonium-uranium extraction process
RCRA	Resource Conservation and Recovery Act
RDX	hexahydro-1,3,5-trinitro-1,3,5-triazine
redox	geochemical reaction involving the transfer of an electron
REDOX	reduction-oxidation extraction process
RFP	Rocky Flats Plant
SNLA	Sandia National Laboratory, Albuquerque
SNLL	Sandia National Laboratory, Livermore
SRP	Savannah River Plant
TAN	Test Area North
TCE	trichloroethylene
TNX	Testing and Experiment
TRA	Test Reactor Area
2,4-D	2,4-dichlorophenoxyacetic acid

Introduction

The U.S. Department of Energy (DOE) recognizes the severity of environmental quality problems at its facilities (DOE 1989, 1990a). It has pledged to assist in the cleanup of these sites through (1) direct remediation/restoration activities and (2) basic research to improve understanding of contaminant behavior in subsurface environments and to develop new concepts for remediation. DOE's Subsurface Science Program (DOE 1990b) is part of this commitment to address subsurface contamination issues at DOE facilities. The Subsurface Science Program involves basic research on hydrologic, microbiologic, and geochemical mechanisms that operate in subsurface environments and that control contaminant migration, persistence, and ease of remediation. Part of the research within the Subsurface Science Program is focused on understanding the subsurface geochemical behavior of chemical mixtures (Co-Contaminant Chemistry Subprogram) as a basis for (1) improving the ability to forecast contaminant migration and (2) establishing new techniques to mobilize, immobilize, or degrade in-ground chemical contaminants on DOE lands.

This report was written as a source document for the Subsurface Science Program, with emphasis on the Co-Contaminant Chemistry Subprogram. It provides information on the types of chemical contaminants and mixtures found on DOE lands and guidance on which of these contaminants and mixtures should be emphasized in basic research that targets subsurface contaminants at DOE facilities. Specifically, the report includes the following:

- Review of the types of contaminants that have reportedly been disposed of to the ground at 18 DOE facilities and that have been analytically determined to be present in soils, sediments, and ground waters at the sites.
- Identification of the types of inorganic and organic contaminants that have been mixed in the ground through disposal activities and of the frequency of occurrence of different chemical mixtures at 91 DOE waste sites.
- Evaluation of which chemical mixtures reported on DOE lands warrant research because of scientific uncertainty regarding the implications of intercontaminant interactions to contaminant geochemistry and transport.
- Development of a set of appropriate and defensible chemical mixtures to be used in research into co-contaminant chemistry.

Use of the generic chemical mixtures will focus subsurface science research on priority contaminants and the real co-contaminant issues at DOE facilities.

Background

DOE performs its mission through the operation of research and production facilities, including the 18 facilities that form the basis of this report. The DOE facilities occupy a total area of approximately 2,800 square miles (mi^2) (7,280 square kilometers (km^2)) within the contiguous United States (DOE 1986; Table 1; Figure 1). Activities conducted at DOE facilities have included multidisciplinary research; enrichment (e.g., uranium) and production (e.g., plutonium and tritium) of nuclear materials; spent-fuel reprocessing; development, testing, and fabrication of nuclear and non-nuclear weapons; construction and testing of nuclear reactors; and the management of various radioactive wastes and spent fuels.

Some wastes at DOE facilities are stored in tanks (e.g., high-level waste) or in the ground in a retrievable form (e.g., transuranic waste) awaiting additional treatment before permanent subsurface disposal (DOE 1987). However, most wastes (by volume) have been disposed of to the ground surface, ponds, cribs, basins, pits, piles, injection wells, and landfills, leading to subsurface contamination. Subsurface contamination is also the result of leaks from process sewer lines, fuel and hazardous waste underground storage tanks, and breached drums of buried chemicals and wastes. In the early days of DOE operations, environmental disposal was common and was believed to have limited long-term implications. However, many of the individual chemical constituents in the

Table 1. **Sizes of DOE Research and Defense Production Facilities and Number of Waste Sites Considered**

Facility	Abbreviation	Size		No. of Sites
		mi^2	km^2	
Argonne National Laboratory	ANL	2.7	7.0	2
Brookhaven National Laboratory	BNL	8.2	21.3	4
Fernald, Feed Materials Production Center	FMPC	1.9	4.9	11
Hanford Site	HS	558.0	1,450.0	7
Idaho National Engineering Laboratory	INEL	894.0	2,324.4	6
Kansas City Plant	KCP	0.2	0.5	7
Lawrence Livermore National Laboratory	LLNL			12
Main Site		1.3	3.4	
Site 300		10.2	26.5	
Los Alamos National Laboratory	LANL	43.5	113.1	3
Mound	MND	0.5	1.3	2
Nevada Test Site	NTS	965.0	2,509.0	6
Oak Ridge National Laboratory	ORNL	16.0	41.6	9
Pantex Plant	PNTX	15.9	41.3	3
Pinellas Plant	PP	0.2	0.5	1
Portsmouth Gaseous Diffusion Plant	PGDP	5.8	15.1	4
Rocky Flats Plant	RFP	10.2	26.5	3
Sandia National Laboratory, Albuquerque	SNLA	11.6	30.2	1
Sandia National Laboratory, Livermore	SNLL	0.6	1.6	1
Savannah River Plant	SRP	300.0	780.0	9

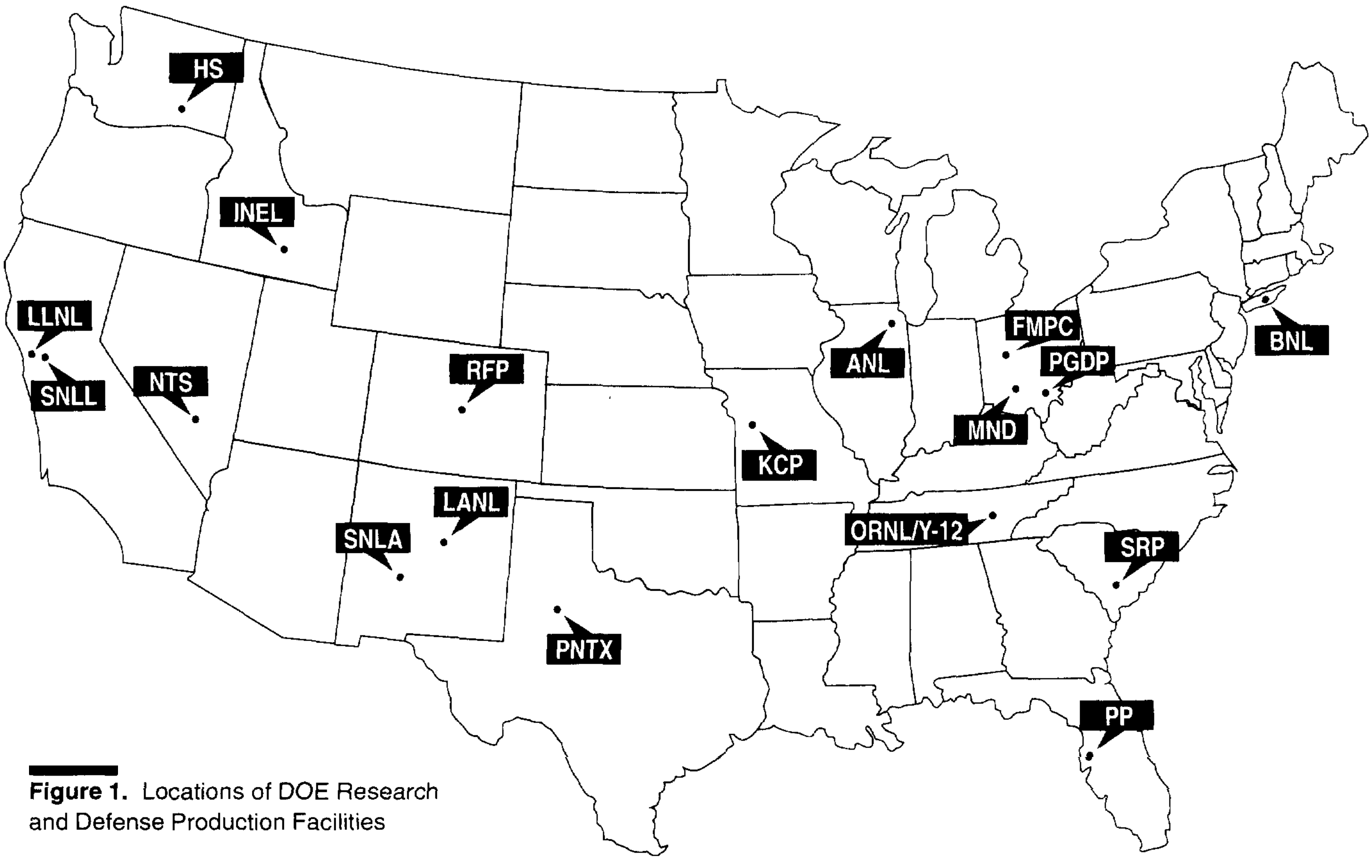

Figure 1. Locations of DOE Research and Defense Production Facilities

wastes are now of health concern, and they either are regulated under Federal and State statutes or are currently under evaluation for possible regulatory control (Federal Register 1985a and b, 1989, 1990).

More than 3,000 inactive waste sites have been identified at DOE facilities (GAO 1988a and b), and the total costs of environmental compliance and cleanup in the 1988-1989 time frame have been estimated to have been in the range of $60 to $90 billion (GAO 1988a, DOE 1988). The extent and complexity of contamination by hazardous and mixed hazardous wastes at DOE facilities vary with the facility's mission, size, and waste-management practices, At one extreme are large facilities with multiple activities and a complex history of waste-disposal practices (e.g., Hanford, Oak Ridge National Laboratory, and Savannah River Plant). Activities at these facilities were chemically intensive; i.e., large amounts of chemical agents were manipulated in day-to-day operations, and complex chemical processes involving inorganic and organic reagents, solvents, and catalysts were used to recover radioactive elements from spent fuels or to produce or fabricate fuels and target elements. Over the decades of operation, the compositions of waste streams and wastes disposed of to the subsurface environment changed as processes were modified or new processes came on line (Stenner et al. 1988b, Christensen and Gordon 1983, Rogers et al. 1989a and b). These facilities produced and received high-level, transuranic, and low-level wastes that were disposed of to the ground (DOE 1987).

At the other extreme are small facilities with limited activities and less complex subsurface contamination problems (e.g., fewer waste sites). For example, at the Pinellas Plant, effluent emissions to public sewer systems are controlled, the amount of radioactive material used in production processes is minimal, and liquid and solid wastes are stored and subsequently shipped offsite for disposal (Klein 1988). At another small establishment (Kansas City Plant), all processes involve nonradioactive materials, so mixed hazardous and radioactive waste problems in the subsurface environment are not a concern (Brown 1988).

Even though many waste sites have been identified, the extent and complexity of subsurface contamination at

DOE facilities are still largely unknown as a result of several factors. For example, the completencess of records describing quantities and types of chemicals disposed of at individual waste sites varies, It has been suggested that record purges may have occurred at some DOE futilities. At some sites, a disparity exists between the chemicals reported to have been disposed of (according to historical records) and those analytically determined to be in the underlying ground waters. Also, the facilities have different schedules for implementing compliance/remediation activities at waste sites. Another f factor is the compliance-driven nature of environmental monitoring programs. Unregulated chemicals have not been routinely monitored; only in the past 5 years have programs begun to monitor an expanded list of organic chemicals.

Published information has documented that the chemical composition of waste sites at DOE facilities is complex. with individual contaminant concentrations in soils/sediments ranging from trace (parts per billion (ppb)) to percent (parts per hundred) levels. Soils and sediments are contaminated with radionuclides (e.g., uranium, plutonium, cesium, thorium, strontium, tritium and technetium). metals (e. g.. chromium, mercury, and lead), and anions (e.g., nitrate. fluoride, and cyanide). Reports of codisposal of inorganic and radioactive contaminants with the following contaminants are common: (1) chlorinated stolvents such as trichlomethylene, tetrachloroethylene, and carbon tetrachloride; (2) fuel hydrocarbons such as benzene, toluene, xylenes, and polycyclic aromatic hydrocarbons; (3) plasticizers such as phthalates: (4) polychlorinated biphenyls (PCBs); (5) alkyl phosphates: (6) conventional explosives such as hexahydro- 1,3.5-trinitro- 1,3.5-triazine (RDX), octahydro-1.3,5.7-tetranitro-1,3,5,7-tetraazozine (HMX), and trinitrotoluene; (7) complexing agents such as ethylenediamine letraacetic acid (EDTA) and associated degradation products; (8) organic acids such as oxalic and citric: (9) pesticides: and (10) other miscellaneous materials and liquids such as coal fly ash, scintillation fluids, low-level waste debris, and pharmaceutical wastes. These compound classes have been reported in ground waters at concentrations ranging from trace (ppb) to parts per thousand (ppt) levels. In the case of radionuclides, radioactivity in ground waters has been reported in concentration ranges from picocuries per liter (pCi/L) or less up to millicuries per liter (mCi/L).

Approach to the Co-Contaminant Review and the Selection of Generic Mixtures

The review began with the collection of source documents that describe the history of disposal and/or the measurement of concentrations of chemical contaminants in soil and subsurface sediments and in ground water at selected DOE facilities (Figure 2). Most source documents were environmental monitoring and site characterization reports or contractor/subcontractor remedial investigation and feasibility study assessments. Approximately 100 documents published from 1980 to 1990 were reviewed.

The data base defined by these documents has limits. Monitoring programs at DOE sites have had to deal with a large number of waste streams and sites, and the chemicals have often been present in complex environmental and waste matrices. Because most monitoring programs at DOE sites have been directed most recently at environmental compliance, the most frequently analyzed chemicals have been regulated constituents (i. e., priority pollutants defined by the U.S. Environmental Protection Agency (EPA)). As a result, other chemical contaminants (e.g., several of those listed as Appendix IX* constituents and those not listed at all) that were

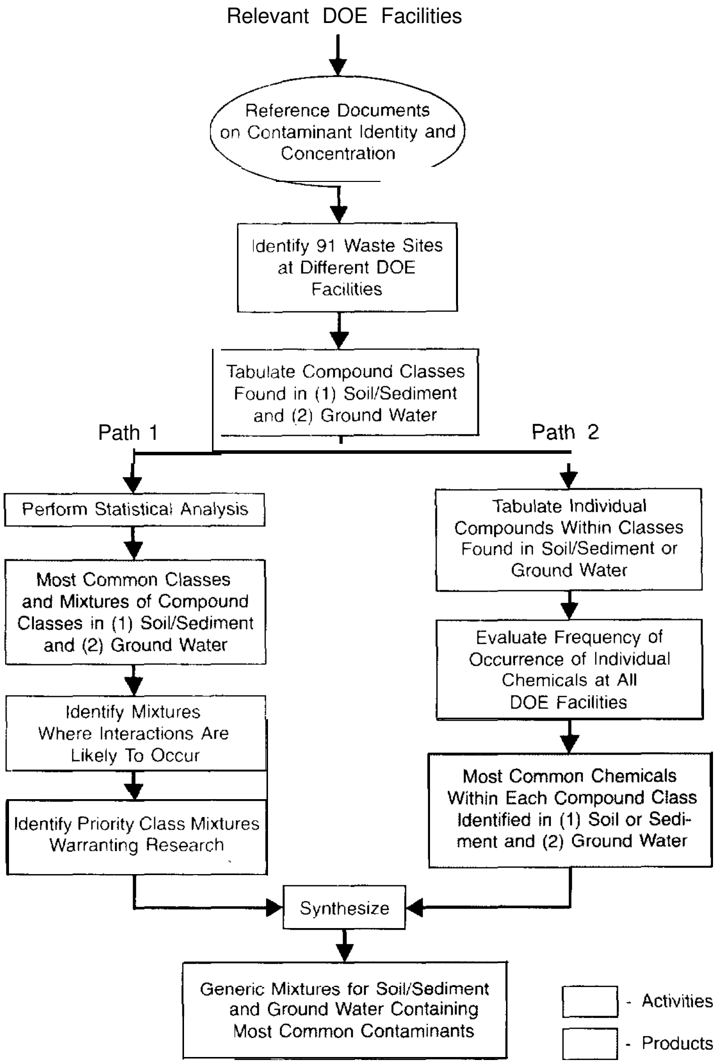

Figure 2. Approach Taken To Identify Chemical Mixtures on DOE Lands and To Establish Generic Chemical Mixtures for Subsurface Science Research

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*Appendix IX is a list of approximately 250 chemicals that require monitoring and that provide an indication of ground-water pollution under/adjacent to Resource Conservation and Recovery Act (RCRA) waste sites. If any of these chemicals are detected, the EPA Regional Administrator can set ground-water protection standards and require corrective action. Monitoring of chemicals outside of the Appendix IX list can be required by the Administrator if, for example, a particular chemical is a known product or a known or suspected by-product produced at the site (*Federal Register* 1986, 1987).

disposed of to the ground have been analyzed more selectively or less frequently. The boundaries of the data base are discussed in more detail in Section 10.

After these reports were evaluated, 91 individual waste sites (listed in Table 3 on pages 10-13) at the 18 DOE facilities were identified (based on their large size or location, the nature or concentration of contaminants, or their priority for cleanup) for comprehensive evaluation. Generally, these 91 sites represent those whose chemical characterization data or historical disposal records are sufficient to identify which chemical compounds were disposed of to the ground and/or currently exist in the ground. The central objective of identifying the types of contaminants that are mixed in the ground at the DOE facilities required that inventories be established for important contaminant types at each waste site.

The reports were then used to identify the classes of organic and inorganic compounds in soil or subsurface sediments and ground water and the frequency of their occurrence. The evaluation considered the 13 classes of elements/chemical compounds listed in Table 2. These classes include constituents regulated under Federal statutes (e.g., chromium, nitrate. trichloroethylene, benzene, and PCB), constituents unique to DOE (e.g., technetium. plutonium, and tritium), organic compounds and complexing agents (e.g., oxalic acid and EDTA) that may modify metal ion and radionuclide transport in the subsurface environment, and unlisted chemicals that are subject to potential future environmental regulation (e.g., bis-2-ethylhexylphthalate).

Following the evaluation of compound classes, two independent paths of evaluation were taken (Figure 2) to identify priority-class mixtures warranting research (Path 1) and the most common contaminants in soils, sediments, and ground water within each compound class (Path 2). The information generated from the completion of steps within each pathway was then used to identify generic mixtures for basic research.

In the first step of Path 1, a statistical analysis was performed to determine the frequency of occurrence (across the 91 waste sites) of compound class combinations (combinations of two, three, four, and five compound classes). This analysis identified the most common types of contaminant mixtures based on available data. Next, a brief literature review was performed to identify the mixtures in which intercontaminant chemical reactions (i. e., complexation and cosolvation) are expected to cause complex subsurface behavior that cannot be predicted with current scientific understanding. The seven compound class mixtures that exhibited the greatest potential for co-contaminant interactions and that appeared with the greatest frequency at the 91 waste sites were identified as priorities warranting research.

Table 2. Compound Classes and Selected Representative Constituents

Compound Class	Representative Constituents	Class Number[1]
Metals	Lead, chromium, mercury	1
Anions	Nitrate, fluoride, cyanide	2
Radionuclides	Tritium, plutonium, technetium	3
Chlorinated hydrocarbons	Trichloroethylene	4
Fuel hydrocarbons	Benzene, toluene, xylenes	5
Phthalates	Bis-2-ethylhexylphthalate	6
PCBs	Arochlor 1248, Arochlor 1260[2]	7
Explosives	HMX, RDX, trinitrotoluene	8
Ketones	Acetone, methyl ethyl ketone	9
Pesticides	Chlordane,[3] lindane, 4,4'-DDT[4]	10
Alkyl phosphates	Tributyl phosphate	11
Complexing agents	EDTA, DTPA,[5] NTA[6]	12
Organic acids	Oxalic acid, citric acid	13

[1] These numbers refer to specific compound classes in tables in Appendices B and C.

[2] Arochlor 1248 and 1260 consist of a mixture of different individual PCBs.

[3] Mixture of different chlorinated compounds.

[4] Dichlorodiphenyltrichloroethane.

[5] Diethylenetriamine pentaacetic acid.

[6] Nitriloacetic acid.

Table 3. Tabulation of Compound Classes Reported in 91 Waste Sites and Associated Ground Waters at 18 DOE Facilities

	Compound Classes				
Facility/Site	**Metals**	**Anions**	**Radionuclides**	**Chlorinated Hydrocarbons**	**Fuel Hydrocarbons**
Argonne National Laboratory-East					
317/319 Landfill	G[2]	G	G	G	-
Sanitary Landfill	G	G	G	-	-
Brookhaven National Laboratory					
Waste Management Area	-	-	G	G	G
Former Landfill	-	-	G	G	G
Current Landfill	-	-	G	G	G
Filter Beds	G	G	G	G	-
Feed Materials Production Center (Fernald)					
Pit 1 (Covered)	G	G	S1,[3] S2,[4] G	S2, G	S2, G
Pit 2 (Covered)	G	G	S1, S2, G	G	S2, G
Pit 3 (Covered)	S2, G	G	S1, S2, G	G	G
Pit 4 (Covered)	S2, G	S2, G	S1, S2, G	S2, G	S2, G
Pit 5	S2, G	G	S1, S2, G	G	G
Pit 6	S2, G	G	S1, S2, G	S2, G	G
Fly Ash Disposal Area	S2	-	S1, S2	-	-
Burn Pit	S2, G	G	S2, G	S2, G	G
Clear Well	S2, G	G	S2, G	G	G
North Lime Sludge Pond	-	G	G	-	-
Hanford Site					
300 Area Ponds	S1, S2, G	S1, S2, G	S1, S2, G	S1, S2, G	-
300 Area Trenches	S1, S2, G	S1, S2, G	S1, S2, G	S1, S2, G	S1
216 B Trenches	G	S1, G	S1, G	-	-
116 H Trenches/Cribs/Basins	S1, G	G	S1, G	G	-
116 D Trenches/Cribs	S1	G	S1, G	-	-
116 B/C Trenches/Cribs/Basins	S1, G	G	S1, G	-	-
116 K Trenches/Cribs/Basins	S1	G	S1, G	-	-
Idaho National Engineering Laboratory					
Radioactive Waste Management Complex	S1, S2, G	S1	S1, S2, G	S1, G	S1, G
Test Area North (TAN)	G	-	-	G	-
Test Reactor Area (TRA) Warm Waste Pond	S1, S2, G	S2, G	S1, G	S1, G	-
TRA Disposal Well	S1	-	-	-	-
Idaho Chemical Processing Plant (ICPP) Deep Disposal Well	-	S1, G	S1, G	-	-
Naval Reactors Facility	-	G	-	G	-
Kansas City Plant					
Tank Farm Area	-	-	-	G	-
Old Railroad Dock Area	-	-	-	S2, G	-
North Lagoon	-	-	-	S2	-
Indian Creek Outfall	S2	-	-	-	S2
Oil House	S2	-	-	S2	S2
Department 27 Area	S2	-	-	S2	-
Sanitary Sewer Lift Station	S2	-	-	-	S2
Lawrence Livermore					
Area West of LLNL	G	-	-	S2, G	-
Building 518 Area	-	-	-	S1, S2, G	S2
Building 612 Yard/ Building 514 Area	-	-	-	S2, G	-
Building 403 Area	-	-	-	G	S1, S2, G
East Traffic Circle Landfill	-	-	-	G	-
Taxi Strip/Old Salvage Yard Areas	-	-	-	G	-
Bldg 834/854 Complexes (Site 300)	-	-	-	S2, G	
West Firing Area (Site 300)	-	-	-	G	
Building 850 (300 Area)	-	-	G	-	-
Building 829 Burn Pit (300 Area)	-	-	-	S2, G	-
806/807 Waste Water Lagoon Complex (300 Area)	G	G	-	-	G
East Firing Area (300 Area)	-	G	-	-	-

The first step of path 2 involved tabulation of individual compounds or elements within each compound class that were identified in soils, sediments, and ground water at the 18 DOE facilities. For a compound or element to be listed, at least one facility must have reported measurements of concentration in sediment or ground water. The frequency of occurrence of each of the individual compounds or elements at each of the DOE facilities was then determined for each of the 13 compound classes. The frequency distribution was used to identify those individual compounds or elements that were most commonly observed in either soil/subsurface sediment or ground water.

The results from Paths 1 and 2 were merged in a synthesis activity (Figure 2) that led to the identification of the generic co-contaminant mixtures. The procedure used to identify the generic mixtures is best illustrated by the following example, Path 1 might identify the compound classes designated by A and D as a priority compound class mixture (AD) because they were frequently mixed in waste sites and because they react with one another to form complexes that are weakly reactive with mineral surfaces and are consequently mobile in ground water. Path 2 may determine that the most common chemical constituents reported within each of these compound classes at the 18 DOE facilities are the chemical components a, b, and c in class A and x, y, and z in class D. The generic class mixture representing AD would then be some combination of the chemical components a, b, c, x, y, and z, such as a, b, c, and z. Use of the mixture for research would be well justified, given chemical properties of the classes, the type of chemical interaction or reaction that occurs between them, and the reported chemical components in the waste sites.

The proposed generic chemical mixtures are a reference point for the selection of relevant chemical compounds for co-contaminant chemistry research. Investigators may decide to use the generic mixtures without change, or the proposed generic mixtures may be changed or augmented by investigators who wish to span the chemical properties of some set of chemical contaminants to develop free energy relationships for a certain geochemical phenomenon or reaction. The generic mixture provides the investigator with a reference point that is defensible, given the nature of contamination on DOE lands.

Compound Classes								
Ketones	Phthalates	PCB	Explosives	Pesticides	Alkyl Phosphates	Complexing Agents	Organic Acids	Other[1]
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
G	-	S2	-	S2	-	-	-	G(a,b,e,j)
G	G	-	S2	-	S2	-	-	-
G	-	S2	-	-	-	-	-	G(a,b,e,j)
G	-	S2	-	S2	-	-	-	G(a,b,e,j)
G	-	S2	-	-	-	-	-	G(a,b,e,j)
G	-	S2	-	-	-	-	-	G(a,b,e,j)
-	-	S2	-	-	-	-	-	-
G	-	S2	-	-	-	-	-	G(a,b,e,j)
G	-	S2	-	-	-	-	-	G(a,b,e,j)
-	S2	S2	-	S2	-	-	-	-
S2	S2	S2	-	-	S2	-	-	-
S1	S2	-	-	-	S1	-	-	S1(a,b,f,g,h,j)
-	-	-	-	-	-	-	S1	-
-	-	-	-	-	-	-	S1	-
-	-	-	-	-	-	-	S1	-
-	-	-	-	-	-	-	S1	-
-	-	-	-	-	-	-	-	-
-	-	S1	-	-	S1	S1	S1	S1(b,f,i)
G	-	-	-	-	-	-	-	-
S1, S2	S2	S2	-	S2	-	-	G	S2(a,c)
-	-	-	-	-	S1	-	G	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	S2	-	-	-	-	-	-
-	-	S1, S2, G	-	-	-	-	-	-
-	-	S2	-	-	-	-	-	-
S2	-	S2	-	-	-	-	-	-
-	-	S2	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	S2	-	-	-	-	-
-	-	-	S2, G	-	-	-	-	-
-	-	-	-	-	-	-	-	-

Table 3. Tabulation of Compound Classes Reported in 91 Waste Sites and Associated Ground Waters at 18 DOE Facilities (Continued)

Facility/Site	Metals	Anions	Radionuclides	Chlorinated Hydrocarbons	Fuel Hydrocarbons
Los Alamos National Laboratory					
Material Disposal Area T (TA-21)	-	S1	S1, S2	-	-
Area L (TA-54)	S1, S2	S1, S2	-	S1, S2	S1, S2
Area G (TA-54)	-	-	S1	-	-
Mound					
Area B/Areas 2 and 18	-	-	S2	G	-
Area I/Area 3	-	-	S1	-	-
Nevada Test Site					
Chesire	G	G	G	-	-
Nash	-	G	S2	-	-
Faultless	G	G	G	-	-
Bourbon	-	-	G	-	-
Bilby	-	-	S2, G	-	-
Cambrick	-	-	S2, G	-	
Oak Ridge/Y-12					
S-3 Ponds	G	S1, G	S1, G	G	G
Chestnut Ridge Security Pits	G	-	-	G	-
New Hope Pond	S2, G	-	S2, G	G	-
Chestnut Ridge Sediment Disposal Basin	G	-	-	G	-
S-2 Pond	S1, G	S1, G	S1	G	-
Bear Creek Burial Grounds	S1, G	-	S1, G	S1, G	S1, G
Rogers Quarry (Fly Ash Disposal)	G	G	-	-	-
Oil Land Farm	-	-	-	G	S1
Low-Level Waste Burial Grounds	-	-	G	-	-
Pantex Plant					
Chemical Burn Pit	-	-	-	-	S2
Building 12-35	G	G	G	S2, G	S1, S2
Building 16-1	G	G	G	S2	S1, S2, G
Pinellas Plant					
East Pond Area	G	-	-	G	G
Portsmouth Facility					
X-701B Holding Pond	G	-	S1, S2, G	G	-
X-616 Chromium Sludge Surface Impoundments	S1, G	-	S2, G	-	-
X-231B Oil Plots	G	-	S1, S2	G	-
X-749 Low Level Radioactive Waste Landfill	G	S1	S1	G	-
Rocky Flats Plant					
881 Hillside Area	S2, G	-	S2, G	S2, G	-
903 Pad, Mound and East Trenches	G	-	S2, G	S2, G	-
Combined Phase II-Final Measure	S2, G	S2, G	S2, G	S2, G	S2, G
Sandia National Laboratories, Albuquerque					
Chemical Waste Landfill	S2	-	-	S2	S2
Sandia National Laboratories, Livermore					
Fuel Oil Spill	G	-	-	-	S1, S2, G
Savannah River					
M-Area Settling Basin	S1, S2, G	S1, S2, G	S1, S2, G	S1, S2, G	-
CMP Pit 1	G	S1, G	G	S1, G	S1
CMP Pit 2	G	G	G	S1, G	-
TNX Seepage Basins	S1, G	S1, G	S1, G	-	-
200F/200H Seepage Basins	S1, S2, G	S1, G	G	G	S1
SRP Seepage Basins	S1, G	S1, G	G	S1, G	-
Radioactive Waste Burial Grounds	S1	-	S1	-	-
Coal Pile Runoff Basins	S1, G	G	G	G	-
Metallurgical Lab Basin	G	S1, G	-	S1, G	S1

[1] Other compound classes indentified are indicated as follows:

a. phenols	c. nitrites	e. haloforms	g. amines	i. nitro compounds
b. alcohols	d. esters	f. ethers	h. aldehydes	j. sulfur-containing compounds

Ketones	Phthalates	PCB	Explosives	Pesticides	Alkyl Phosphates	Complexing Agents	Organic Acids	Other[1]
-	-	-	-	-	-	-	S1	S1(b,d,g,j) S2(b,c,f)
S2	S1	S1	-	-	S1	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
S1	-	-	S1	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
G	G	-	-	-	-	-	-	G(j)
-	-	-	-	-	-	-	-	-
G	S2	S2	-	-	-	-	-	-
G	-	-	-	-	-	-	-	-
G	G	-	-	-	S1	-	-	S1,(b,f)G(a)
G	-	S2	-	-	-	S1	-	-
-	-	-	-	-	-	-	-	-
-	-	S1	-	-	-	-	-	-
-	-	-	-	-	-	G	-	-
S1,S2	-	-	S1	-	-	-	-	-
S2	-	-	G	-	-	-	-	-
S2	-	-	G	-	-	-	-	-
G	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-
S2	-	-	-	-	-	-	-	
-	-	-	-	-	-	-	-	-
S2	-	-	-	-	-	-	-	S1(a,g,h,i,j)
-	-	-	-	-	-	-	-	
-	-	-	-	G	-	-	-	-
-	-	-	S1	-	-	-	-	-
-	-	-	S1	S1,G	-	-	-	-
-	-	-	-	-	S1	S1	S1	-
G	G	-	-	S1,G	-	-	-	S1(a) G(a,c,d,j)
-	-	-	-	G	-	-	-	-
-	-	-	S1	-	-	-	-	S1(f)
-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-

[2]G Published data are available on concentrations of contaminants in ground water below or adjacent to the site.

[3]S1 Documentation indicates contaminant-class disposal at the site. May include information on quantities disposed

[4]S2 Published data are available on concentrations of contaminants in soils/sediments at the site.

SECTION 4

Identification of the Most Common Contaminant Classes

Table 3 on pages 10-13 identifies the 18 DOE facilities and 91 waste sites that were included in this assessment and summarizes information on the distribution of compound classes in soils/sediments and ground waters at the waste sites. The table includes compound classes that were reportedly disposed of to the site (S 1) and those that have been measured in soil or sediment (S2) * or in ground water (G). These data were incorporated into a computerized data base (Appendix B, Tables B-1 and B-2) that was used for identifying the most common contaminant classes.

Frequency of Compound-Class Occurrence in Soils/Sediments

Soil and sediment analyses, if complete, can provide a good assessment of the total chemical composition of wastes and contaminants disposed of to the ground. However, over time and exposure to the environment, soils and sediments tend to become enriched in immobile, recalcitrant species and depleted in species that have been degraded or transported to ground water.

The compound classes most commonly reported in sediments (by facility) were fuel hydrocarbons, followed by chlorinated hydrocarbons, metals, and radionuclides (Figure 3a). Less commonly reported compound classes included anions, ketones, and PCBs. Organic acids, phthalates, explosives, alkyl phosphates, complexing agents, and pesticides were reported at only two to five facilities.

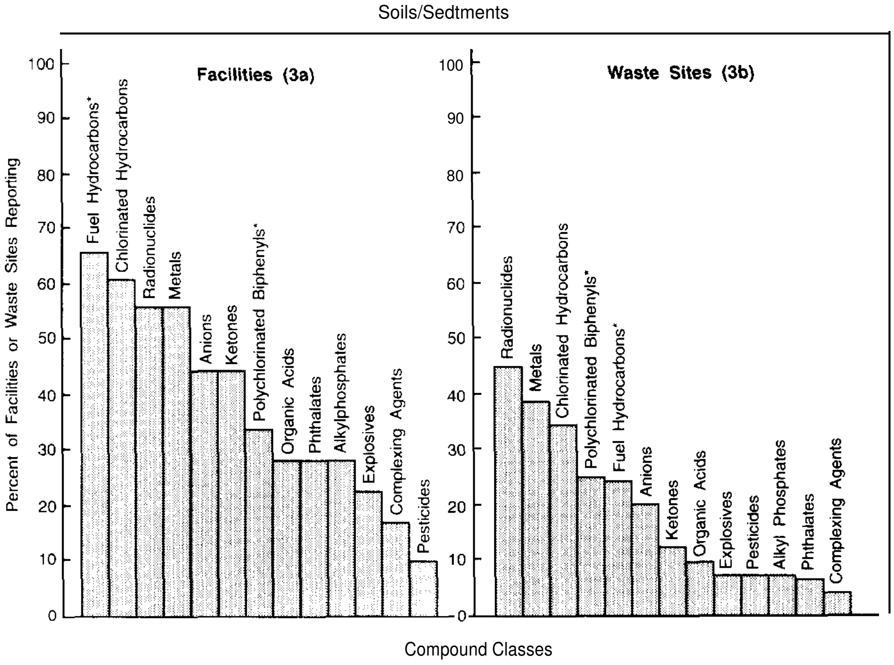

Figure 3. Distribution of Compound Classes in Soils/Sediments at 18 DOE Facilities and 91 Waste Sites

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*Here and throughout the report, the terms "soil" and "sediment" are used in their most general meanings. Soil refers to near-surface geologic material influenced by plant and microbiological activity (A-B horizons). Sediment refers to unconsolidated geologic material collected from below the soil zone (i.e., C horizon and vadose and saturated zones). No attempt was made to differentiate between contaminant analyses performed in surface soil (A-B horizon), subsoil (C horizon), or vadose/saturated zone materials. Analyses tabulated under the heading of soil/sediment are simply total chemical measurements performed in unconsolidated solid-phase materials of terrestrial origin.

In contrast to the trend for the DOE facilities in Figure 3a, when the waste sites were evaluated as a single population (Figure 3b), radionuclides were the most frequently reported class. Although fuel hydrocarbons were reported for all the facilities (Figure 3a), they appeared localized to a smaller subset of waste sites. In contrast, PCBs appear to be facility specific. (Note the changes in order ranking of these two compound classes, marked by asterisks, in facility/waste site components in Figure 3.)

Frequency of Compound-Class Occurrence in Ground Water

Compounds detected in ground water are those that were disposed of to the ground and subsequently transported through the soil and vadose zone by water or, in select instances, by nonaqueous liquids such as organic solvents. These compound classes are generally those that exhibit high solubility in and low attenuation from the carrier fluid phase.

The compound classes most commonly reported for ground waters of the 18 facilities (Figure 4a) were metals and chlorinated hydrocarbons, followed by radionuclides, anions, fuel hydrocarbons, and ketones. Reported with less frequency were phthalates, explosives, and organic acids. The least commonly reported classes of compounds in ground water (pesticides, PCBs, and complexing agents) each occurred at only one facility. The distribution of compound classes was similar for the 91 waste sites (Figure 4b).

Although alkyl phosphates have been reported in soil, none of the 18 DOE facilities reported their presence in ground water. This observation contrasts with waste-site inventories that document significant quantities of these compounds disposed of to the ground at DOE facilities. For example, at least 275,900 kilograms (kg) of alkyl phosphates were disposed of to the ground at the Hanford Site (Stenner et al. 1988a; Appendix E). Some of the classes reported less frequently (phthalates, organic acids, explosives, akyl phosphates, and chelating agents) are not currently listed by EPA as a priority pollutant; therefore, they have commanded little attention in monitoring programs driven by the Federal regulatory process.

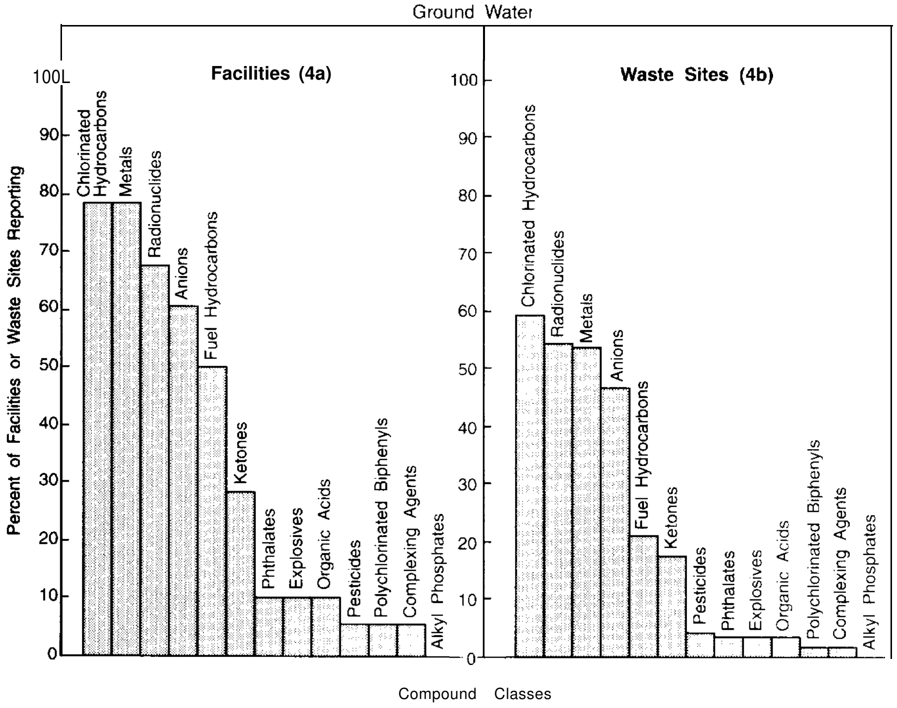


Figure 4. Distribution of Compound Classes in Ground Water at 18 DOE Facilities **and 91** Waste Sites

Frequency of Occurrence of Contaminant Class Combinations

The frequency of occurrence of specific mixtures of two-, three-, four-, and five-compound classes within the 91 waste sites was determined by a computerized manipulation of the data base. This activity was central to the identification of the generic chemical mixtures for research (discussed in Sections 8 and 9) because it showed which compound classes were most frequently mixed in DOE disposal sites. Complete tabulation of the results of this assessment is provided in Appendix C, and selected results are described in this section. Mixtures of two, three, and four contaminants were observed at 59, 45, and 30 of the 91 sites, respectively.

Soils and Sediments

The most frequently reported binary (two-compound) compound-class mixture in soils/sediments was metals and radionuclides. Eleven other commonly reported binary mixtures included metals, anions, radionuclides, chlorinated hydrocarbons, fuel hydrocarbons, and PCBs in various combinations (Table 4). The frequency of occurrence for these 12 combinations ranged from 10 to 25 waste sites and 5 to 11 facilities. Radionuclides were most frequently found in association with metals, PCBs, anions, and chlorinated hydrocarbons. Neutral organic compounds (i.e., chlorinated hydrocarbons, fuel hydrocarbons, and PCBs) occurred as mixtures with one another (Table C-1) and with ketone solvents with relatively high frequency (Table 4). Binary mixtures of metals and radionuclides with organic complexing agents and solvents were reported but were rare (Table C-1). At a minimum, organic acids, complexing agents, alkyl phosphates, and organic solvents were each disposed of with metals and radionuclides at 3 to 10 waste sites (Table C-1).

The most common ternary (three-compound) contaminant mixtures reported in soils/sediments contained metals, anions, radionuclides, chlorinated and fuel hydrocarbons, and PCBs in various combinations (Table 4). The most ubiquitous ternary mixture components were metals, chlorinated hydrocarbons, and radionuclides. The frequency of occurrence for the ternary mixtures was lower than that observed for binary mixtures (Table 4). The most frequent combination (metals, radionuclides, and PCBs) was observed at 13 waste sites. Neutral organic contaminants, such as chlorinated and fuel hydrocarbons and PCBs, were observed in combination at seven sites, and ternary combinations of the neutral compounds with ketone solvents were reported at five sites. Metals, radionuclides, and inorganic anions were reported together at nine sites, and various ternary combinations of metals, anions, radionuclides, organic acids, complexing agents, and alkyl phosphates were observed at three to five sites.

Mixtures of four or more compound classes were relatively infrequent (Tables 4, C-3, and C-4). The most common components of these mixtures were metals, inorganic anions, radionuclides, and chlorinated hydrocarbons. Significant combinations included mixtures of (1) metals, inorganic anions, radionuclides, and alkyl phosphates; (2) metals, inorganic anions, radionuclides, and organic acids; (3) metals, radionuclides, alkyl phosphates, and organic acids; and (4) chlorinated hydrocarbons, fuel hydrocarbons, PCBs, and pesticides.

Table 4. Combinations of Compound Classes of Contaminants Reported Most Frequently in Soils/Sediments and Ground Waters at DOE Facilities

Soils/Sediments			Ground Water		
Class	No. of Sites[1]	No. of Facilities[2]	Class	No. of Sites[1]	No. of Facilities[2]
Metals, radionuclides	25	7	Metals, chlorinated hydrocarbons	38	12
Metals, PCBs	18	6	Metals, radionuclides	36	11
Metals, chlorinated hydrocarbons	16	9	Metals, anions	33	11
Radionuclides, PCBs	15	4	Anions, radionuclides	33	10
Chlorinated hydrocarbons, fuel hydrocarbons	15	11	Radionuclides, chlorinated hydrocarbons	32	10
Anions, radionuclides	14	8	Anions, chlorinated hydrocarbons	26	9
Radionuclides, chlorinated hydrocarbons	14	6	Chlorinated hydrocarbons, fuel hydrocarbons	17	7
Chlorinated hydrocarbons, PCBs	13	6	Metals, fuel hydrocarbons	16	8
Metals, anions	12	7	Metals, ketones	16	5
Metals, fuel hydrocarbons	11	9	Radionuclides, fuel hydrocarbons	16	6
Anions, chlorinated hydrocarbons	11	6	Chlorinated hydrocarbons, ketones	16	5
Fuel hydrocarbons, PCBs	10	5	Anions, fuel hydrocarbons	12	5
Metals, radionuclides, PCBs	13	4	Metals, anions, radionuclides	29	10
Metals, chlorinated hydrocarbons, fuel hydrocarbons	8	8	Metals, radionuclides, chlorinated hydrocarbons	29	10
Metals, radionuclides, chlorinated hydrocarbons	11	6	Metals, anions, chlorinated hydrocarbons	25	9
Metals, chlorinated hydrocarbons, PCBs	10	6	Anions, radionuclides, chlorinated hydrocarbons	23	9
Metals, anions, radionuclides	9	6	Metals, chlorinated hydrocarbons, ketones	16	5
Metals, anions, chlorinated hydrocarbons	9	6	Radionuclides, chlorinated hydrocarbons, fuel hydrocarbons	15	5
Radionuclides, chlorinated hydrocarbons, PCBs	9	4	Metals, radionuclides, fuel hydrocarbons	13	5
Metals, fuel hydrocarbons, PCBs	7	5	Metals, chlorinated hydrocarbons, fuel hydrocarbons	12	5
Anions, radionuclides, chlorinated hydrocarbons	7	5	Metals, anions, fuel hydrocarbons	12	5
Anions, chlorinated hydrocarbons, fuel hydrocarbons	7	6	Metals, radionuclides, ketones	12	3
Radionuclides, chlorinated hydrocarbons, fuel hydrocarbons	7	5	Anions, radionuclides, fuel hydrocarbons	11	4
Metals, anions, radionuclides, chlorinated hydrocarbons	7	5	Metals, anions, radionuclides, chlorinated hydrocarbons	23	9
Metals, radionuclides, chlorinated hydrocarbons, PCBs	7	4	Metals, radionuclides, chlorinated hydrocarbons, fuel hydrocarbons	12	4
Metals, anions, radionuclides, alkyl phosphates	5	4	Metals, radionuclides, chlorinated hydrocarbons, ketones	12	3
Metals, anions, chlorinated hydrocarbons, fuel hydrocarbons	5	5	Metals, anions, radionuclides, fuel hydrocarbons	11	4
Metals, anions, chlorinated hydrocarbons, PCBs	5	4	Metals, anions, chlorinated hydrocarbons, ketones	11	3
Metals, radionuclides, chlorinated hydrocarbons, fuel hydrocarbons	5	5	Metals, chlorinated hydrocarbons, fuel hydrocarbons, ketones	11	3

[1] Number of waste sites (out of 91) reporting specific class combination.

[2] Number of facilities (out of 18) reporting specific class combination.

Ground Water

The most frequently reported binary compound-class mixture in ground water (Table 4) was metals and chlorinated hydrocarbons; this mixture was present at 38 waste sites and at 12 facilities. Other important binary mixtures were metals and radionuclides, metals and anions, anions and radionuclides, radionuclides and chlorinated hydrocarbons, and anions and chlorinated hydrocarbons. All of these pairs were reported at more than 25 percent of the waste sites and at least 50 percent of the facilities (Table 4). Because PCBs, alkyl phosphates, complexing agents, and organic acids were infrequently reported in DOE-site groundwaters, they were not found as mixtures with other contaminants in ground water. The absence of data on alkyl phosphates, complexing agents, and organic acids is due to several factors, including (1) the site-specific nature of the constituents, (2) the lack of regulation, and (3) limitations of the analytical measurement technique. Ketones appeared frequently as a binary mixture with metals, radionuclides, or chlorinated hydrocarbons; fuel hydrocarbons appeared frequently with chlorinated hydrocarbons. (See Table C-5 for details on minor pairings.)

Ternary compound-class mixtures including metals, radionuclides, chlorinated hydrocarbons, and anions in various combinations occurred at 23 percent of the waste sites and 50 percent of the facilities (Table 4). Other ternary mixtures were observed with less frequency (Tables 4 and C-6).

The most common quaternary (four-compound) combination in ground water contained metals, anions, radionuclides, and chlorinated hydrocarbons; it occurred at 23 percent of the waste sites and at 50 percent of the facilities (Table 4). Other important quaternary mixtures included ketones in various combinations with (1) metals, radionuclides, and chlorinated hydrocarbons; (2) metals, chlorinated hydrocarbons, and fuel hydrocarbons; or (3) metals, anions, and chlorinated hydrocarbons. (See Table C-7 for details on minor combinations of four-compound classes.)

Quinternary (five-compound) compound-class mixtures were limited to 9 to 10 waste sites at 2 to 3 facilities (Table C-8); these mixtures were composed of combinations of metals, anions, radionuclides, chlorinated hydrocarbons, fuel hydrocarbons, and ketones.

Identification of the Most Frequently Occurring Chemicals

This section provides information on (1) the types of chemical compounds within each class that have been reported in soil/sediment and ground water at the 18 DOE facilities and (2) their frequency of occurrence. This report is not intended to account for why or how certain chemical constituents have been mobilized to ground water. The transport and attenuation process has been complex, involving various multicomponent geochemical reactions, microbiologic activity, mass transfer by water and nonaqueous fluids, and the possible contribution of mobile colloidal material. Many of the species that exist in ground waters at DOE sites, including chlorinated and fuel hydrocarbons, chromate, and technetium, are relatively mobile in subsurface systems. However, other constituents, such as cobalt, lead, and plutonium, exhibit highly variable mobility depending on the aqueous chemical (hydrogen ion activity (pH) and oxidation-reduction (redox) potential) and mineralogic properties of the subsurface environment. The soil and subsurface geochemical properties at DOE facilities span a wide range because the facilities are located in all major geographic regions of the country (Figure 1). Because of such variety, the attenuation of specific chemical constituents at different sites may vary by many orders of magnitude. Furthermore, acids, bases, and other chemical agents that were often added to waste disposal areas could modify subsurface behavior. Approximately 100 individual chemicals or mixtures (or measurements of chemicals) have been reported in sediments and ground water on DOE lands (Table D-1); specific details on the sites where these contaminants were measured and other pertinent geochemical factors may be found in the references listed in Appendix A. For information on the chemical processes in which some of these chemicals were used, see Cleveland (1979, pp. 461–586), McFadden (1980), or Appendix E, where selected operations performed at the Hanford Site are discussed.

Metals and Inorganic Anions

The most commonly reported metals in ground water (Figure 5) were lead, chromium, arsenic, and zinc. Nitrate was the most commonly reported anion. More than 50 percent of all facilities reported that 9 of the 12 species listed in Figure 5 were present in ground water. Most of the metals and anions reported in Figure 5 are common constituents of wastes associated with reactor operations (e.g., chromium and lead), irradiated fuel processing (e.g., nitrate, chromium, cyanide, and fluoride), uranium recovery (nitrate), fuel fabrication (chromium, nitrate, and copper), fuel production (mercury), and isotope separation (mercury) (Evans et al. 1990, Rogers et al. 1989, Stenner et al. 1988a).

The same 12 inorganic species were also reported in soil/sediments (Figure 5), although less information was available on the sediment concentrations. The most frequently reported metals were copper, chromium, zinc, mercury, arsenic, and cadmium. Consistent with the extensive use of nitric acid and nitrate salts in nuclear fuels reprocessing and fabrication (Stenner et al. 1988a), the most commonly reported anion was nitrate.

Radionuclides

The frequency of occurrence of radionuclides common to reactor operations and nuclear fuels production, fabrication, and waste reprocessing is described in Figure 6. The radionuclides reported most frequently from ground water at more than 50 percent of the facilities were tritium, uranium, and strontium. In soil/sediments, uranium, plutonium, and cesium were most common.

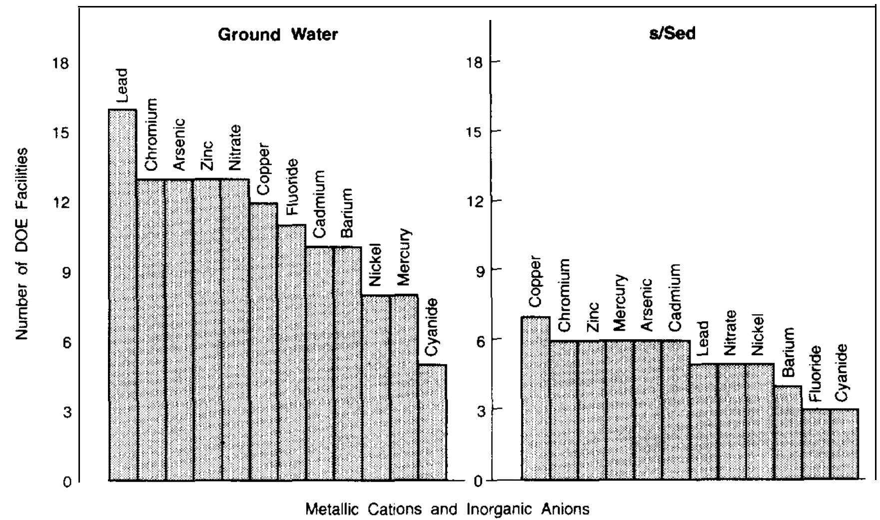


Figure 5. Frequency of Occurrence of Selected Metals and Inorganic Anions in Ground Water and Soils/Sediments at DOE Facilities

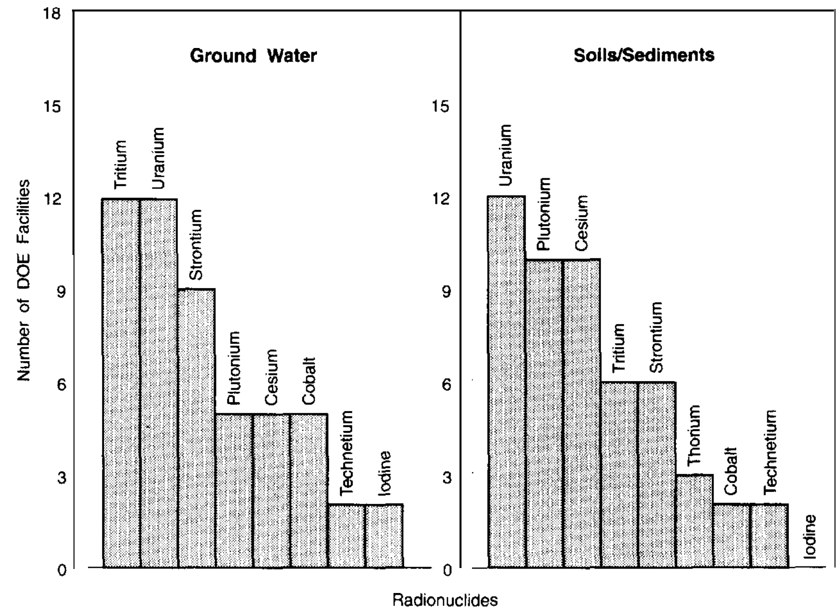


Figure 6. Frequency of Occurrence of Selected Radionuclides in Ground Water and Soils/Sediments at DOE Facilities

Radionuclides reported with less frequency include cobalt, technetium, thorium, and iodine. In some cases, their presence may reflect problems at specific facilities, as do the presence of iodine-129 at Hanford; technetium-99 at Hanford (Evans et al. 1990) and Portsmouth (Roger et al. 1989, Evans et al. 1990); and thorium-228, 230, and 232 at Fernald (Solow and Phoenix 1987). Other radionuclides, including americium-241 and neptunium-237, have been identified in soils/sediments at DOE waste sites that were not included in this review (e.g., Corbo et al. 1986). Many knowledgeable personnel involved in chemical processing activities at Hanford and other production sites have stated categorically that the frequency of occurrence of such elements as neptunium and americium in soils and sediments is higher than their absence from this review would indicate.

Chlorinated Hydrocarbons

Nineteen chlorinated hydrocarbons were identified in ground waters at DOE facilities (Figure 7). Some of these compounds are abiotic transformation products (Vogel et al. 1987) of chemicals that were used as solvents and decreasing agents in nuclear fuels reprocessing and fabrication (Christensen and Gordon 1983, Stenner et al. 1988a). The most commonly reported constituents (occurring at more than 50 percent of the facilities) were trichloroethylene; 1,1,1 -trichloroethane and 1,2-dichloroethylene; and tetrachloroethylene, 1,1 -dichloroethane, and chloroform.

Fifteen chlorinated hydrocarbon constituents were identified in soils/sediments at DOE sites (Figure 7). The most commonly reported constituents (occurring at 50 percent or more of the facilities) were trichloroethylene, 1,1,1 -trichloroethane, tetrachloroethylene, and dichloromethane.

Fuel Hydrocarbons

The fuel hydrocarbon constituents in ground water reported most frequently were toluene, xylene, benzene, and ethylbenzene (Figure 8). Low-solubility hydrophobic polyaromatic hydrocarbons (i.e., chrysene and benz(a)anthracene) were observed in the ground water at only one site.

The fuel hydrocarbons found in soil/sediment included those found in ground water (Figure 8) and many sparingly soluble polyaromatic hydrocarbons (e.g., phenanthrene, anthracene, and fluoranthene) that are unlikely to be mobilized to ground water in appreciable concentrations. The aromatic hydrocarbons of higher molecular weight were associated with only two to four facilities. Toluene was the most commonly reported aromatic constituent, followed by xylenes and ethylbenzene. Likely sources of the high-molecular-weight hydrocarbons are coal and coal wastes (fly ash) derived from the operation of coal-fired electric power- and steam-generating plants located at many of the facilities (Rogers et al. 1989, Solow and Phoenix 1987, Dennison et al. 1989, Stenner et al. 1988b). Sources of components of lower molecular weight include gasoline and other petroleum-derived fuels stored in leaking aboveground or belowground storage tanks (Dresen et al. 1986, Roy F. Weston, Inc. 1989).

Ketones

The most frequently reported ketones in ground water were acetone, methyl ethyl ketone, and methyl isobutyl ketone (Figure 9). Acetone was also the most commonly reported ketone in soil/sediment, followed by methyl ethyl ketone (Figure 9). Ketones were frequently used in nuclear fuels reprocessing. For example, methyl isobutyl ketone was the preferred solvent used at Hanford in processing to separate uranium and plutonium from fission products (Stenner et al. 1988a).

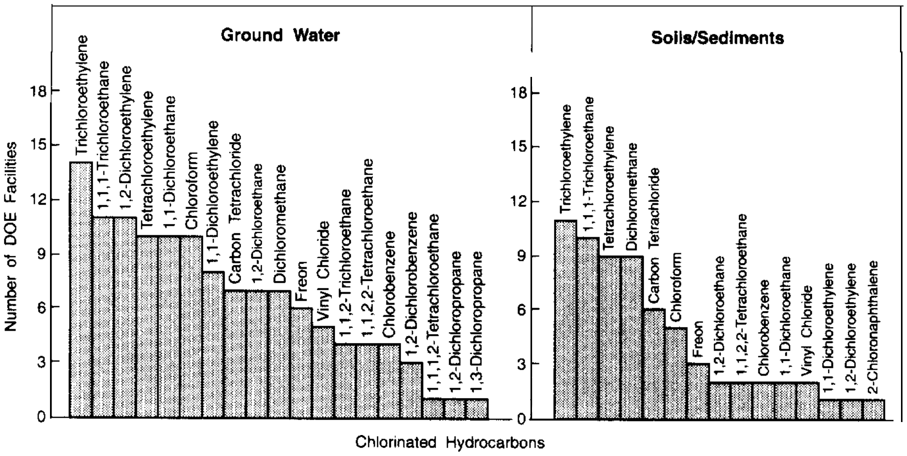
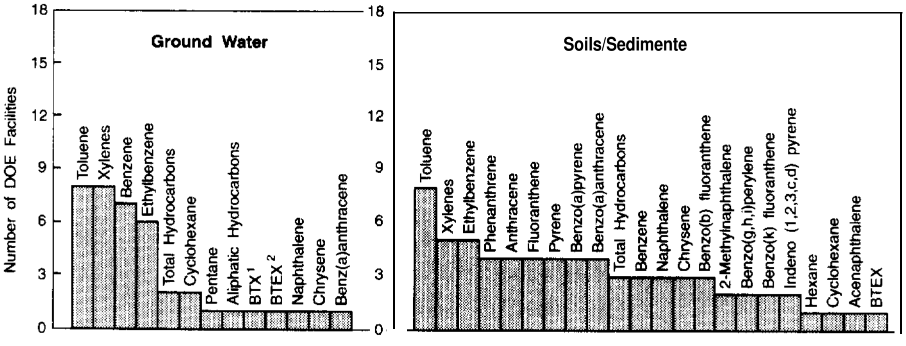


Figure 7. Frequency of Occurrence of Chlorinated Hydrocarbons in Ground Water and Soils/Sediments at DOE Facilities



[1] Total Benzene/Toluene/Xylene

[2] Total Benzene/Toluene/Ethylbenzene/Xylene

Figure 8. Frequency of Occurrence of Fuel Hydrocarbons in Ground Water and Soils/Sediments at DOE Facilities

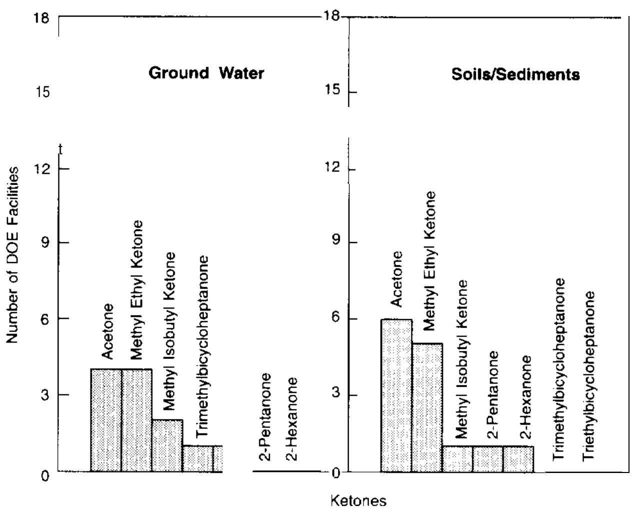


Figure 9. Frequency of Occurrence of Ketones in Ground Water and Soils/Sediments at DOE Facilities

Other Chemicals and Compounds

Table 5 lists chemical constituents within those compound classes that have been reported with less frequency at the 91 waste sites. Within Table 5, compound classes are listed by frequency of occurrence, with the phthalates being most common. Bis-2-ethylhexylphthalate was the most frequently observed phthalate, and possible regulation of this constituent, along with butylbenzyl-phthalate, in drinking water is being considered *(Federal Register 1989,* 1990). Pesticides, many of which are regulated constituents, are routinely monitored as part of monitoring programs at the DOE facilities. However, pesticides are rarely observed at levels above detection limits. The organic acids include paraffinic derivatives (e.g., palmitic and hexadecanoic acid) that originate from thermal decomposition of hydrocarbon solvents used in nuclear fuels reprocessing and fabrication (Toste et al. 1988) and benzoic acid that results from the decomposition of organic material in low-level waste debris (Toste and Lechner-Fish 1989).

Historical records show that some of the minor classes of compounds (e.g., chelating agents and organic acids) may be far more common than is suggested by the monitoring and characterization data from the 91 waste sites. For example, records document the disposal of the chelating agent EDTA or diethylenetriamine pentaacetic acid (DTPA) at waste sites at Hanford, Savannah River, Oak Ridge, and INEL (Table 6). Disposal of large quantities of organic compounds (e.g., oxalic and citric acid) (Tables 6 and E- 1) and alkyl phosphates (Table E- 1) that may facilitate metal/radionuclide migration in the subsurface environment has also been reported. These organic chemical agents have not generally been analyzed during characterization activities at DOE waste sites.

Table 5. Chemical Constituents Reported for Less Frequently Observed Compound Classes

Class/ Constituent	Number of Facilities: Ground Water	Number of Facilities: Soils/ Sediments
Phthalates		
Bis-2-ethylhexylphthalate	5	3
Di-n-octylphthalate	2	2
Di-n-butylphthalate	2	2
Butylbenzylphthalate	1	3
Diethylphthalate	2	2
PCBs		
Total PCB	1	2
Arochlor 1016	1	1
Arochlor 1242	1	2
Arochlor 1248	—	4
Arochlor 1254	1	2
Arochlor 1260	1	4
Explosives		
HMX	1	1
RDX	1	1
Trinitrotoluene	—	1
PETN^2	1	—
Pesticides		
Heptachlor epoxide	1	—
Endosulfan-1	1	2
Chlordane	1	2
Endrin	—	1
Lindane	2	—
Methoxvchlor	1	—
Toxaphene	1	—
2.4-D	1	
Fenthion	1	—
Aldrin	1	1
Benzenehexachloride	1	2
Heptachlor	1	—
Dicamba	1	—
4,4' DDT	1	2
Ethyl parathion	—	1
Malathion	1	—
Methyl parathion	—	1
Dieldrin	—	1
Endosulfan-2	—	1

Table 5. Chemical Constituents Reported for Less Frequently Observed Compound Classes (Continued)

Class/ Constituent	Number of Facilities[1]	
	Ground Water	Soils/ Sediments
Alkyl Phosphates		
Tributyl phosphate	—	1
Chelating Agents		
EDTA	1	—
Organic Acids		
Palmitic acid	1	—
Hexadecanoic acid	—	1
Benzoic acid	1	—
Other		
Acetonitrile	—	1
N-nitrosodiphenyl amine	1	—
Triethylsilanol	1	
2,4,5-Trichlorophenol	1	
2-Methylphenol	1	1
Acrylonitrile	1	
Bromoform	2	—
2,4-Dinitrophenol	—	1
P-chloro-m-cresol	—	1
2,4-Dimethylphenol	—	1
3,3'-Dichlorobenzidine	1	—
Cyclohexane	2	—
Vinyl acetate	1	—
Isopropyl alcohol	2	1
2-Propylfuran	1	—
Trimethylsilanol	1	—
Tetrahydrofuran	1	1
Butanol	1	1
Carbon disulfide	1	1
4-Chlorophenyl-phenylether	—	1
Ethanol	—	1
2-Methyl-2-propanol	—	1
Dioxane	—	1

[1] Number of DOE facilities reporting measurements of this compound or parameter in ground water and/or soils/sediments.

[2] PETN=2,2-Bis(nitroxy)methyl-1,3-propanediol-dinitrate.

Table 6. Chelating Agents/Organic Acids at DOE Waste Sites

Facility/Site	ChelatingAgent	Organic Acid
Hanford Site		
a. 100 Area	—	Sodium oxalate[1]
b. 200 Area	—	Sodium oxalate[2]
c. 300 Area	EDTA[3]	Ammonium citrate[3]
		Oxalic acid[3]
		Hexadecanoic acid[3]
INEL		
a. Radioactive Waste Management Complex	EDTA[4]	Organic acids[4]
b. ICPP	—	Organic acids[5]
c. TRA	—	Organic acids[6]
Oak Ridge		
a. Bear Creek Burial Grounds	EDTA[7]	Phthalic acid[8]
b. Low-Level Waste Trenches/Pits	EDTA[8]	Phthalic acid[8]
Savannah River		
a. Old Testing and Experiment (TNX) Basins	DTPA[9]	Formic acid[9]
		Oxalic acid[9]

[1] 19,300 kg disposed to trenches, cribs, and basins (see Appendix A, Hanford; Stenner et al. 1988a).

[2] 134,000 kg disposed to trenches, cribs, and basins (see Appendix A, Hanford; Stenner et al. 1988a).

[3] From 1943 to 1974, wastes generated from fuel fabrication processes and containing these chemicals were discharged to North and South Process Ponds (see Appendix A, Hanford; Weakley 1958; DOE 1990c; Loe 1967). For example, autoclave solutions of ammonium citrate (13 lb/90 gal H_2O—17.3 ppt) and EDTA (0.8 lb/90 gal—1.1 ppt) were periodically disposed of to the ponds (see Appendix A, Hanford; Clemans 1988).

[4] A total of 1,287 gal of Versene (solution containing EDTA) and 1,287 gal of organic acids were listed as disposed to Pit 9 (see Appendix A; EG&G, Idaho 1990a). Liquids (series 744 sludge) transferred from Rocky Flats Plant to INEL for disposal and containing these constituents were first solidified in Portland cement prior to transport (see Appendix A, INEL; Virgil 1989).

[5] Organic acids tentatively identified in ICPP waste effluent and ground water (see Appendix A; Leenheer and Bagby 1982).

[6] Organic acids tentatively identified in ground water (see Appendix A, INEL; Leenheer and Bagby 1982)

[7] Listed as being disposed to Burial Ground A - South (see Appendix A, Oak Ridge/Y-12; Walter et al. 1990).

[8] EDTA in ground water near Pit 7 at concentration level of 3.7×10^{-7} M (87 ppb). In addition to palmitic and phthalic acid, several unknown dicarboxylic acids were detected (see Appendix A, Oak Ridge/Y-12; Means et al. 1978).

[9] Listed as being disposed to Old TNX Seepage Basin (See Appendix A, Savannah River Plant, Christensen and Gordon 1983).

Concentration Ranges and Regulatory Compliance

Table 7 summarizes the concentration ranges observed in ground water and soils/sediments for the most commonly reported constituents in seven compound classes. The table also lists current guidelines for regulatory compliance in water. This information is provided (1) to display the high levels of contamination that occur for certain constituents, (2) to identify the constituents most in need of environmental remediation because their concentrations significantly exceed guidelines, and (3) to provide guidance on what concentration ranges are appropriate for co-contaminant chemistry research relevant to DOE sites. It is important to note that, although the upper concentrations of many constituents in Table 7 are quite high, these concentrations typically represent isolated analyses in small, highly contaminated areas.

Metals and Anions

The highest concentrations reported for metal ions in ground water were for zinc, followed by mercury and lead. At the lower ends of the ranges, constituent concentrations in ground water were below regulatory guidelines by a factor of 10 to 1,000. At the higher ends, reported ground-water levels exceeded regulatory guidelines by as much as 10^2 to 10^5. Nitrate has been reported in ground water at concentrations as high as 10 percent, which exceeds regulatory standards by 10^4, In soils/sediments, levels of four metals (lead, chromium, zinc, and mercury) have exceeded one ppt.

Radionuclides

Federal guidelines for the regulation of radionuclides in water include the National Interim Drinking Water Regulations (EPA 1976) and DOE's derived concentration guides. The interim drinking water regulations are more stringent by a factor of 10 to 100. Tritium has exceeded both guidelines in ground water, as has strontium. Uranium has exceeded the interim drinking water regulations by as much as a factor of 10; cesium has exceeded the interim drinking water regulations but not the DOE guidelines. Although significant levels of plutonium in soils/sediments have been reported, the reported concentrations in ground water are below regulatory guidelines. consistent with the strong attenuation noted for most valence states of plutonium on subsurface sorbents (Sanchez et al. 1985) or in subsurface environments (Rai et al. 1980, Cowan et al. 1985).

Chlorinated Hydrocarbons

The highest concentrations of chlorinated hydrocarbon constituents reported for ground water were for dichloromethane and trichloroethylene, followed by tetrachloroethylene. At the low end of the concentration ranges in ground water, constituent concentrations below regulatory guidelines by a factor of 10 to 100 have been reported. At the high end, the observed concentrations exceed the existing regulatory guidelines by as much as a factor of 10^5 (i.e., trichloroethylene). In soils and sediments, levels of three compounds (trichloroethylene, 1,2-dichloroethylene, and tetrachloroethylene) have exceeded one ppt.

Table 7. Concentration Ranges[1] and Guidelines for Regulation of Most Frequently Reported Constituents in Ground Water and/or Soils and Sediments at DOE Facilities[2]

Class/Constituent	Ground Water	Soils/Sediment	Guidelines
Metals			
Lead	0.56 to 120,000	1,000 to 6,900,000	[3]0; [4]50; [5]5
Chromium	0.42 to 9,010	5.1 to 3,950,000	[3]100; [4]50; [5]100
Arsenic	0.3 to 32,100	100 to 102,000	[4]5
Zinc	1 to 697,000	150 to 5,000,000	[6]5,000
Copper	1 to 3,300	30 to 550,000	[3]1,300; [5]1,300
Mercury	0.08 to 216,900	0.1 to 1,800,000	[3]2; [4]2; [5]2
Cadmium	0.005 to 7,600	100 to 345,000	[3]5; [4]10; [5]5
Anions			
Nitrate	2.6 to 100,000,000	30 to 1,480,000	[3,4,5]10,000
Radionuclides			
Tritium	[7]3.3 to 20,900,000,000	[7]7.8 to 124,000,000	[8]20,000; [9]2,000,000
Uranium	[10]0.001 to 11,700,000 [7]0.02 to 22,700	[11]0.2 to 16,000 [12]0.06 to 18,700	— [9]500 to 600
Strontium	[7]0.05 to 231,000	[13]0.02 to 540,000	[8]8; [9]1,000
Plutonium	[7]0.0009 to 12.8	[13]0.00011 to 3,500,000	[9]300 to 400
Cesium	[7]0.0027 to 1,830	[13]0.02 to 46,900	[8]200; [9]3,000
Chlorinated Hydrocarbons			
Trichloroethylene	0.2 to 870,000	0.2 to 12,000,000	[4]5
1,1,1-Trychloroethane	0.2 to 16,600	1 to 200,000	[4]200
1,2-Dichloroethylene	0.7 to 50,000	10 to 1,000,000	[3,5]70(cis); [3,5]100(trans)
Tetrachloroethylene	0.18 to 272,000	1.3 to 2,045,000	[3]0; [5]5
1,1-Dichloroethane	0.3 to 7,800	27,000 to 84,000	—
Chloroform	0.3 to 2,070	0.3 to 1,300	—
Dichloromethane	0.29 to 2,400,000	6 to 890	[3]0; [5]5
Fuel Hydrocarbons			
Benzene	0.01 to 46,000	0.3 to 310,000	[4]5
Toluene	0.19 to 26,000	0.3 to 2,000,000	[3]2,000; [5]2,000
Xylenes	1 to 14,000	0.3 to 2,800,000	[3]10,000; [5]10,000
Ethylbenzene	1.5 to 540	0.7 to 70,000	[3]700; [5]700
Ketones			
Acetone	3 to 24,500	13 to 350,000	—
Methyl ethyl ketone	4 to 1,500	9 to 470	—
Phthalates			
Bis-2-ethylexylphthalate	2 to 1,050	200 to 57,000	[3]0; [5]4

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[1] Micrograms per liter (µg/L) and micrograms per kilogram (µg/kg) unless otherwise indicated.

[2] Concentration data synthesized from references listed in Appendix A.

[3] Proposed U.S. EPA Maximum Contaminant Level Goals (MCLG, µg/L) in drinking water.

[4] Existing U.S. EPA Maximum Contaminant Level (MCL, µg/L) in drinking water.

[5] Proposed U.S. EPA MCL (µg/L) in drinking water.

[6] Nonenforceable U.S. EPA secondary level standard (µg/L) based on taste, odor, or appearance guidelines.

[7] Picocuries per liter (pCi/L).

[8] National Interim Drinking Water Regulations, Table IV-2A (EPA 1976). Derived Guidelines (pCi/L) based on 4 millirem annual dose to target organ.

[9] DOE-derived concentration guides (pCi/L) based on effective dose limit not to exceed 100 millirem/year. Derived from DOE Order 5480.1A (Jaquish and Bryce 1990).

[10] Micrograms per liter (µg/L).

[11] Micrograms per gram (µg/g).

[12] Picocuries per gram (pCi/g).

[13] Picocuries per kilogram (pCi/kg).

Fuel Hydrocarbons

Benzene, toluene, and xylenes are the fuel hydrocarbon constituents with the highest reported concentrations in ground water, followed by ethylbenzene. Maximum concentrations reported for soils/sediments were approximately 10 to 100 times higher than what was reported for ground water. In ground water, benzene has exceeded regulatory guidelines by a factor of 1,000. Proposed guidelines for toluene and xylenes have been exceeded by factors of as much as 13 and 1.4, respectively.

Ketones

Concentration ranges for acetone in ground water and soils/sediments were 3 to 24,000 µg/L and 13 to 350,000 µg/g, respectively. For methyl ethyl ketone, concentration ranges in ground water and sediments were 4 to 1,500 µg/L and 200 to 57,000 µg/g, respectively. Neither of these chemicals is a priority pollutant, but both are listed as Appendix IX constituents.

Phthalates

The EPA has proposed an MCL of 4 µg/L for bis-2-ethylhexylphthalate. This concentration level has been exceeded in ground water at DOE facilities by factors exceeding 100. Concentrations of this chemical in soils/sediments ranged from 200 to 57,000 µg/g.

Identification of Priority Class Mixtures for Subsurface Science Research

Section 5 documented that many compound class mixtures exist in the ground at DOE facilities and waste sites. The existence of these mixtures is significant in that certain components within these mixtures may undergo chemical interactions that either facilitate or retard their environmental dissemination and transport. These intercontaminant reactions are termed "co-contaminant interactions." Within DOE's Subsurface Science Program, the Co-Contaminant Chemistry Subprogram is performing research on the geochemical behavior of contaminant mixtures. Such research is necessary because (1) co-contaminant interactions are generally less understood than the geochemical behavior of the individual compounds, (2) co-contaminant interactions may explain cases of enhanced contaminant mobility at DOE sites (Means et al. 1978, Killey et al. 1984, Olsen et al. 1986), and (3) an enhanced understanding of co-contaminant interactions may be useful in identifying improved concepts for in situ remediation of contamination around DOE waste sites (DOE 1990b).

Not all contaminants interact when present in mixtures. In fact, co-contaminant interactions may be significant to the surface geochemical behavior of only a subset of the mixtures identified in Table 4 and Appendix C. The objectives of this section are to (1) define and document the types of co-contaminant interactions that may be significant on DOE lands, given the mixtures identified in Section 5 and Appendix C, and (2) identify, based on current scientific understanding, which of these mixtures are likely to exhibit co-contaminant interactions.

Nature of Co-Contaminant Interactions

Research has shown that the following co-contaminant interactions can alter the geochemical behavior of individual contaminants when those contaminants are present in mixtures: competitive sorption, cosolvation, aqueous complexation, and cosorption. These interactions are not well understood with respect to the dynamics of contaminant mixtures in the subsurface environment, and their investigation forms the basis of co-contaminant chemistry research in the DOE Subsurface Science Program (DOE 1990b). In the paragraphs that follow, these co-contaminant interactions are defined and briefly discussed within the context of DOE contamination problems.

Competitive Sorption Aqueous solutes with similar chemical properties sorb to the same types of surface sites on solid materials. In subsurface materials, the most important surface sites for sorption are fixed-negative-charge sites on layer-lattice silicates, hydroxylated sites on iron and aluminum oxides or minerals containing these components, surface lattice or kink sites on salt-type minerals such as calcium carbonate, hydrophobic domains on or within organic material, and carboxylated sites on organic material (Sposito 1984, Curtis et al. 1986, Kent et al. 1988). When solute mixtures contact sorbing mineral surfaces, surface sites can become saturated with adsorbed solutes (Zachara et al. 1987, Cowan et al. 1991), and the individual contaminants are forced to compete for surface sites. Competitive sorption effects have been observed for a number of solute combinations relevant to DOE, including metal cations and anions (Cavallaro and McBride 1978, Bowman et al. 1981, Elrashidi and O'Connor 1982, Zachara et al. 1989) and ionogenic organic compounds (Zachara et al.1987, Jafvert et al. 1990). Competitive sorption has not generally been observed for hydrophobic organic compounds in contact with high-organic-carbon soil materials (Chiou et al. 1983), but it may occur to a limited extent in mineral-dominated sorbents (MacIntyre and de Fur 1985). The magnitude of competitive sorption for hydrophobic organic chemicals, metal ions, or radionuclides is not yet predictable. Competition generally leads to suppression of the sorption of the more weakly binding constituents and enhanced subsurface mobility.

Competitive sorption effects may therefore be expected in mixtures of contaminants that have similar physiochemical properties, such as (1) metallic cations and cationic radionuclides; (2) anionic metals, anionic radionuclides, and anionic organic solutes, and (3) neutral organic compounds in contact with low-carbon subsurface sorbents.

Cosolvation At high concentrations (ppt), dissolved organic substances such as ketone or alcohol solvents alter the thermodynamic properties of water (i.e., dielectric constant and interfacial tension) and its solvating properties for both minor inorganic and organic solutes by functioning as a co-solvent (Popovych and Tomkins 1981). Solvation/desolvation reactions contribute significantly to the overall energetics, magnitude, and kinetics of both solution and surface reactions. Therefore, cosolvation can exert a major influence on a variety of reactions, including aqueous complexation, solubility, and sorption, that control contaminant concentrations in the subsurface environment.

When present at very high (percentage) concentration levels, miscible solvents such as alcohols and ketones increase the solubility of hydrophobic organic compounds (Pinal et al. 1990) and markedly decrease their sorption (Rao et al. 1985 and 1990, Nkedi-Kizza et al 1985, Walters and Guiseppi-Elie1988). A result is an increase in the mobility of the organic contaminant (Nkedi-Kizza et al. 1989). The presence of organic solvents alters the thermodynamic properties of ionic inorganic solutes (Esteso et al. 1989, Reynolds and Davis 1990) and depresses the sorption of ionogenic organic compounds that sorb in competition with inorganic ions (Zachara et al. 1988). The presence of miscible organic solvents in water affects the solubility of inorganic and mineral solids (Popovych and Tomkins 1981), sorption and ion exchange of inorganic solutes (Fessler and Strobel 1963, Moody and Thomas 1968, El-Prince and Babcock 1975, Sheet and Fuller 1986), and surface properties of mineral material (Loeppert et al. 1979). Only limited experimental data represent either the effects of cosolvents on the sorption of metal ions or radionuclides or their complexes with organic ligands.

Cosolvation effects may be expected in contaminant mixtures of (1) water-soluble organic substances/solvents with sparingly soluble organic contaminants, such as PCBs, if the water-soluble component reaches a concentration of I percent and (2) weakly hydrated cations, such as cesium, or anionic and cationic metals and radionulides with alcohol or ketone solvents.

Aqueous Complexation Two or more aqueous species can associate in solution to form a complex. Thus complexes can form between inorganic and organic cations and anions (ligands), between ionogenic and neutral organic compounds (such as between PCBs and a humic substance or anionic surfactant), and between neutral organic compounds (such as between PCBs and a nonionic surfactant). Aqueous complexation leads to enhanced contaminant solubility (see Chiou et al. 1987, Kile and Chiou 1989 on organic solutes). The sorption and transport behavior of aqueous complexes of inorganic ions may be vastly different from those of the parent ions (Elliot and Huang 1979, Elliot and Denneny 1982, Nelson et al. 1985, LaFlamme and Murray 1987, Huang et al. 1988, Chairidchai and Ritchie 1990). For instance, aqueous complexation will often render a relatively reactive, immobile constituent significantly more mobile (Hunter et al. 1988). Uranium may be cited as an example because complexation by carbonate will significantly depress its sorption at intermediate and higher pH levels (Hsi and Langmuir 1985). In addition to such inorganic ligands as bicarbonate, sulfate, and phosphate, organic complexing agents (such as organic acids, amino carboxylic acids, and natural organic compounds) function as important mobilizing agents for many cationic metals and radionuclides on DOE lands and in ground water (Means et al. 1978, Cleveland and Rees 1981, Killey et al. 1984, Olsen et al. 1986, Hanson et al. 1990, Helm and Curtiss 1990). Some radionuclides form particularly strong complexes with natural organic matter and natural organic ligands (Nelson et al. 1985, Moulin et al. 1987, Cacheris and Choppin 1987, Kim et al. 1989). The effects of aqueous complexation may be most significant in mixtures in which organic waste materials from extraction and decontamination activities (i.e., organic acids, aminocarboxylic acids, and alkylated phosphates) were combined with metal and radionuclide cations.

Cosorption Certain process-related organic chemicals present in DOE waste materials, as well as a variety of natural organic compounds such as humic substances, contain multiple functional groups (i.e., carboxylate groups and hydrophobic domains). These polyfunctional compounds (1) form strong complexes with certain dissolved contaminants (Nelson et al. 1985, Gauthier et al, 1987, Helm and Curtiss 1990) and (2) can sorb to surfaces of mineral or organic particles in the subsurface environment (Jardine et al. 1989, Murphy et al. 1990). Unoccupied sites on these surface-associated, polyfunctional organic substances may bind or cosorb contaminants in competition with the underlying solid substrate. Hydrophobic organic compounds (Keoleian and Curl 1989, Murphy et al. 1990), metal cations (Davis 1984, Zachara et al. 1991), and radionuclides (Ho and Miller 1985, Allard et al. 1989) may be cosorbed to mineral-bound humic substances. Smaller multifunctional organic ligands (Davis and Leckie 1978), surfactants (Rea and Parks 1990), and certain inorganic ligands (Benjamin and Leckie 1982) can also promote cosorption of inorganic ions to mineral surfaces.

Cosorption effects may be encountered in mixtures of metal ions and/or radionuclides with polyfunctional complexing agents, organic acids, or natural organic substances found in subsurface environments at DOE sites.

Compound-Class Mixtures Likely To Exhibit Co-Contaminant Interactions

This section identifies the compound-class mixtures documented in Section 5 that are likely to undergo significant co-contaminant interactions in the subsurface. This analysis was based on the assumption that the co-contaminant interactions discussed in the previous subsection are important ones that occur at DOE sites. Experimentation or additional literature review may reveal that other co-contaminant interactions are also significant.

The compound-class mixtures observed on DOE lands (Table 4 and Appendix C) whose subsurface geochemical behavior may be influenced by co-contaminant interactions are summarized in Table 8. Several chemical interactions, though not discussed previously, may occur in the compound-class mixtures. These interactions include co-precipitation, solid phase modification, solvent-surface interactions, and phase transfer. Co-precipitation is the formation of a mixed solid phase, in this case one involving both metal ion and radionuclide constituents, that behaves as a thermodynamic entity distinct from the homogeneous solid phases of the individual constituents (Sposito 1984). Solid phase modification is the dissolution of mineral solids/sorbents (e. g., iron oxides) by strong organic chelating agents and organic acids (Chang and Matijevic 1983, Blesa et al. 1984). Solvent-surface interactions involve the alteration of the surface properties and sorptivity of a solid phase for contaminants as a result of the presence of a water-soluble organic agent, such as a ketone (Loeppert et al. 1979). Phase transfer is the partitioning of contaminant species between liquid phases in a biphasic co-contaminant mixture, such as in a mixture of water and trichloroethylene.

An attempt was made to assign research priorities to these mixtures (Table 9), using the following criteria: (1) frequency of observation, (2) probability of the co-contaminant interaction affecting migration, (3) extent of research information available on the interaction, and (4) importance of the site where the mixture has been reported and priority of that site for cleanup. These criteria were given a three-point ranking (3, 2, and 1, with 3 being the highest priority).

Table 8. Compound-Class Mixtures Expected To Exhibit Co-Contaminant Interactions

Compound-Class Mixtures	Co-Contaminant Interaction
1. Chlorinated hydrocarbons-fuel hydrocarbons	Competitive sorption, cosolvation, phase transfer
2. Metals-radionuclides	Competitive sorption, co-precipitation
3. Chlorinated hydrocarbons/fuel hydrocarbons/ketones-PCBs	Cosolvation
4. Metals/radionuclides-organic acids	Aqueous complexation, cosorption, competitive sorption, solid phase modification
5. Metals/radionuclides-complexing agents	Aqueous complexation, cosorption, precipitation, competitive sorption, solid phase modification
6. Metals/radionuclides-ketones	Cosolvation, solvent-surface interactions
7. Metals/radionuclides-organic acids/complexing agents-ketones/chlorinated hydrocarbons	Cosolvation, solvent-surface interactions, phase transfer

Table 9. Prioritization of Generic Mixtures for Research

Mixture[1]	Frequency of Observation[2]	Probability of Effect[2,3]	Scientific Uncertainty[2,4]	Site Importance[2,5]	Priority Ranking
1	3	2	2	3	2.50
2	3	2	2	3	2.50
3	2	2	2	2	2.00
4	1	3	3	2	2.25
5	1	3	3	2	2.25
6	2	2	3	2	2.25
7	1	2	3	2	2.00

[1] Numbers 1 through 7 as shown in Table 8.

[2] Priority ranking: 3=high, 2=medium, and 1=low.

[3] A qualitative assessment of whether co-contaminant interactions in the mixture are expected to cause a significant modification of individual component behavior based on knowledge of contaminant concentrations and the strength of the co-contaminant interaction.

[4] A subjective appraisal of the status of scientific knowledge. A rating of high (3) indicates limited knowledge on which to base quantitative environmental predictions.

[5] Sites such as Hanford, Savannah River, Oak Ridge, Fernald, and Rocky Flats were considered most important in this assessment because of the magnitude of their in-ground contaminant inventories, acreage of contaminated land, and priority for cleanup. A rating of high (3) indicates the mixture was observed at multiple waste sites on more than one of these facilities.

The scoring for probability of effect and scientific uncertainty was subjective. An overall priority ranking was calculated by giving each criterion equal weight (Table 9). Using this approach, mixtures of (1) chlorinated and fuel hydrocarbons and (2) metals and radionuclides were given highest priority, followed by (3) mixtures of metals and radionuclides with organic acids, chelating agents, and ketones. However, the priority rankings for all the mixtures are similar, indicating that research on all the mixtures is warranted.

Chemical Mixtures for Subsurface Science Research

Information on the most frequent chemical constituents observed within each compound class (Figures 5 through 9) was integrated with information on those compound class mixtures believed to have potential for co-contaminant interactions (Table 8) to yield seven generic mixtures for subsurface science research (Table 10). Each generic mixture represents a menu of compounds or elements whose importance to DOE is justified by their high frequency of occurrence within the 91 DOE waste sites evaluated. The list does not suggest that all compounds identified within each generic mixture should be used within a given study or by a single investigator. Rather, the investigator can choose from among these compounds to establish a defensible compound mixture for research into the subsurface behavior of contaminant mixtures found on DOE sites. The generic mixtures can also be augmented with additional inorganic or organic constituents, at the discretion of individual investigators, to test specific scientific hypotheses or to broaden the range of chemical properties spanned by a mixture. No attempt has been made to rank either the generic mixtures or the specific species within the mixtures according to perceived priority for research.

Description of Generic Chemical Mixtures

Chlorinated hydrocarbons and fuel hydrocarbons were chosen as a mixture to be used in research on competitive sorption between hydrophobic solutes and cosolvation in subsurface materials representative of DOE sites. These phenomena may be studied with binary, ternary, and higher order compound mixtures, with probe compounds selected from both individual classes, to suit the hypotheses and objectives of the individual investigator. The data for ground water in Table 7 suggest that co-contaminant studies are warranted over a wide concentration range, beginning at trace levels and extending to concentrations near the aqueous solubility of the compounds. The reported high concentrations of certain compounds in soils/sediments (i.e., trichloroethylene, tetrachloroethylene, toluene, xylene) indicate the probable existence of free organic liquid (i.e., trichlorethylene (TCE) or fuel) in the pore space. This observation suggests that studies of phase transfer between the liquid organic phase and water are warranted for dissolved organic constituents present in either phase.

Metal ions and radionuclides were disposed of together at many waste sites and were selected as a generic mixture to evaluate multispecies sorption and coprecipitation. As shown in Table 10, a variety of metals and radionuclides can be justified for research based on frequency of occurrence. The recommended research subjects are binary, and possibly also ternary and quaternary, mixtures of cationic metals and radionuclides for studying (1) competitive sorption on subsurface mineral phases and heterogeneous mineral material and (2) coprecipitation both in homogeneous solution and in subsurface material. Cation mixtures must be carefully selected, based on firm scientific hypotheses and knowledge of the chemistry of the metal ion. For example, mixtures of lead and thorium, zinc and cobalt, and barium and strontium/cesium represent logical binary mixtures because similarities in chemical behavior exist within each of these compound pairings. Mixtures of anionic contaminants should focus on the competitive

Table 10. Generic Chemical Mixtures for Subsurface Science Research

Compound-Class Mixtures		Compound-Class Components
Mixture 1		
Chlorinated hydrocarbons	⇨	Trichloroethylene, tetrachloroethylene, chloroform, carbon tetrachloride, chlorobenzene
with		
Fuel hydrocarbons	⇨	Toluene, benzene, ethylbenzene, cyclohexane
Mixture 2		
2a. Cationic metals	⇨	Lead, zinc, copper, barium
with		
Radionuclides	⇨	Thorium, uranium, plutonium, cobalt, cesium/strontium
2b. Anionic metals	⇨	Chromate, arsenite/arsenate, cyanide, fluorine
with		
Radionuclides	⇨	Pertechnetate
Mixture 3		
Chlorinated hydrocarbons	⇨	Trichloroethylene, tetrachloroethylene
or		
Fuel hydrocarbons	⇨	Toluene, benzene
or		
Ketones	⇨	Acetone, methyl ethyl ketone
with		
PCBs	⇨	Arochlor 1248
Mixture 4		
Metals	⇨	Lead, chromium (III), chromium (VI)
or		
Radionuclides	⇨	Uranium, plutonium, strontium, cobalt
with		
Organic acids	⇨	Oxalic, citric, formic, phthalic
Mixture 5		
Metals	⇨	Lead, mercury
or		
Radionuclides	⇨	Uranium, plutonium, strontium, cobalt
with		
Complexing agents	⇨	EDTA, DTPA, NTA, tributylphosphate
Mixture 6		
Metals	⇨	Lead, mercury
or		
Radionuclides	⇨	Uranium, cesium/strontium
with		
Ketones	⇨	Acetone, methyl ethyl ketone, methy isobutyl ketone
Mixture 7		
Metals or Radionuclides	⇨	Lead, cobalt, uranium, plutonium, strontium
with		
Organic acids or Complexing agents	⇨	EDTA, oxalate/citrate, tributylphosphate
with		
Ketones or Chlorinated hydrocarbons	⇨	Acetone, trichloroethylene
Mixture 8		
Metals or Radionuclides	⇨	Lead, cobalt, uranium, plutonium, strontium
with		
Natural organic substances	⇨	Humic and fulvic substances, low-molecular-weight organic acids

influence of trace (i.e., arsenic and chromium) and major (i.e., fluorine and cyanide) anion contaminants on pertechnetate (TcO^4) sorption. Concentrations of the metal ions and some of the radionuclides in both ground water and soil/sediment are quite high (Table 7), indicating that research is needed on both adsorption and solubility reactions in metal/radionuclide mixtures.

According to the reports, PCBs were frequently disposed of with chlorinated hydrocarbons, fuel hydrocarbons, or ketones at DOE sites, causing concern that these compounds could facilitate PCB migration through cosolvation. Therefore, mixtures of these components in various combinations offer an excellent opportunity to investigate hypotheses regarding complex cosolvation effects on the solubility and sorption of hydrophobic solutes. It is important to note that the ketones, which are miscible in water, may enhance the solubility and aqueous concentrations of both the chlorinated and fuel hydrocarbons (which are partially miscible solvents) as well as the PCBs.

Metals and radionuclides were disposed of with both organic acids and chelating agents at a number of DOE waste sites. As shown in Table 10. generic mixtures can be justified for lead, uranium, plutonium, strontium, cobalt, and chromium in contact with organic acids (mixture 4) and complexing agents (mixture 5).

From these series (mixtures 4 and 5), various combinations of cations and organic ligands can be established for investigating (1) the influence of aqueous complexation on metal/radionuclide sorption, (2) the sorption and microbiologic degradation of organic-metal/radionuclide complexes, and (3) other scientific issues related to solubility and adsorption behavior of cation-ligand complexes. The recommended research focus is on specific cation/organic ligand pairs or multispecies combinations that can be justified based on the charge and stability constants of the resulting complexes. For example, UO_2^{2+}-oxalate (log $K_{ML}=6.36$) and Co^{2+}-EDTA* (log $K_{ML}= 17.2$) are complexes with high stability constants and reasonable frequencies of occurrence, two factors that justify research into their geochemical behavior. For chromium, experimentation for both the chromium(III) and chromium(VI) valence states in contact with organic acids is needed to evaluate aqueous complexation and competitive sorption effects, respectively. Choice of an appropriate and environmentally relevant metal/radionuclide-ligand concentration ratio is a major consideration in the use of mixtures 4 and 5 in Table 10 because that ratio may determine whether the metals and radionuclides exhibit metal or ligand-like behavior. Unfortunately. the concentration range data in Table 7 are inadequate to estimate the metal/radionuclide-to-ligand ratios that may exist in the ground at DOE sites.

Mixtures of metals/radionuclides and ketone solvents at DOE waste sites were also reported with some frequency. The ketones vary in their water solubility, ranging from miscible (acetone) to relatively insoluble (methyl isobutyl ketone). Hydration/dehydration reactions and solvation forces exert a strong influence on metal ion/radionuclide interfacial reactions on subsurface mineral sorbents. Therefore, the presence of dissolved solvents such as ketones that change the solvating properties of water may be expected to influence metal ion or radionuclide subsurface behavior. Mixture 6 was proposed to evaluate such phenomena. Experiments are expected to commence with one metal ion and one of the ketone solvents varying over a wide range in aqueous concentration. These simple mixtures could be contacted with subsurface minerals or materials with varying properties to test hypotheses regarding cosolvation effects on different sorption mechanisms, such as ion exchange or surface coordination. Subsequent studies could focus on the comparative effects of the different ketone solvents and competitive sorption from different cosolvent mixtures.

The final proposed generic mixture of DOE contaminants is a complex ternary mixture containing metals/radionuclides, organic acids/complexing agents, and ketones/chlorinated hydrocarbons (Table 10). This mixture would allow evaluation of the influence of organic solvents, which are present as dissolved and free-phase components, on the subsurface geochemical behavior of organic ligand-metal/radionuclide complexes. Neutral complexes could partition into free-phase organic solvents, while miscible solvent components could alter the stability constants, interfacial behavior, and microbiologic stability of inorganic-organic complexes in

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*Although the short half-life of ^{60}Co (5.27 years) lowers its overall priority as a long-term contaminant at DOE sites, its documented mobility in selected waste sites and its emission of high-energy gamma radiation make it a relevant and important radionuclide for DOE research.

the aqueous phase. The complexity of the potential co-contaminant interactions mandates that research be initiated with just simple ternary mixtures of one compound from each class, in which the organic compounds and the metal or radionuclide have all been selected based on their known chemical properties and a valid hypothesis of behavior. For example, the mixture uranium, tributylphosphate, and acetone or methyl isobutyl ketone and the mixture cobalt, EDTA, and acetone can be justified from this standpoint.

Another mixture that is fundamental to the understanding and prediction of contaminant mobilization and migration at DOE sites is one with cationic and anionic metals and radionuclides in combination with natural organic compounds (Table 10, mixture 8). Natural organic substances, derived primarily from plant remains, are ubiquitous in soils, subsoils, and ground water at many DOE facilities. Natural organic substances modify the subsurface behavior of both inorganic and organic contaminants by (1) complexation and cosorption with cationic constituents and (2) competitive sorption with anionic metals and radionuclides. Research on these mixtures containing natural organic material is warranted because many of the details regarding metal/radionuclide interaction with natural organic substances and their influence on other geochemical reactions are not well understood. The recommended initial research using this mixture should target (1) the interactions of a single metal or radionuclide ion with one or more natural organic substances and (2) the effect of such interaction on sorption or solubility reactions. The natural organic substances and their concentrations should be justifiable within the context of geochemical conditions on DOE sites; they could include such materials as humic and fulvic acid reference samples from the International Humic Substances Society and/or natural, fractionated, or extracted organic matter from DOE-site soils, subsoils, or ground water, with their attendant site saturation by indigenous ions such as Fe^{3+} or $A1^{3+}$.

Uses for the Generic Mixtures

The generic chemical mixtures in Table 10 were primarily selected for research into the subsurface geochemical behavior of mixed contaminants (i.e., co-contaminant chemistry research as defined by DOE (1990b)). However, the mixtures also represent defensible experimental materials for research into subsurface microbiological stability, transformation, and degradation of mixed contaminants (i.e., biodegradation/microbial physiology research as defined by DOE (1990b)). The chemical mixtures could also be used to study such phenomena as—

- Degradation rates of chlorinated or fuel hydrocarbons in complex, multisolute mixtures.
- Effects of aqueous complexation with metals and radionuclides on the rate of microbiologic degradation of organic acids and complexing agents.
- Influence of sorption to the solid phase on the rate of microbiologic degradation of metal/radionuclide-bound organic ligands.
- Effects of dissolved or free-phase organic solvents on the rates of microbial degradation of organic contaminants or the valence transformations of polyvalent metals or radionuclides.

SECTION 10

Boundaries of the Co-Contaminant Analysis

The characterization data used in this report came from only 3 percent of the waste sites that exist on DOE lands (91 out of approximately 3,000). Although these 91 waste sites were deemed important with respect to their size and priority for cleanup at the larger facilities (i.e., Hanford, Savannah River Plant, Oak Ridge National Laboratory), they may or may not be representative of DOE's entire waste complex. Equally important, however, is the fact that some chemical mixtures that exhibit strong interactions (i.e., chelating/complexing agents and metals/radionuclides) may occur infrequently but still, in fact, may be significant factors at a large number of sites when the total waste site population of 3,000 is considered.

The collection of data on the identities and concentrations of chemical constituents in DOE waste sites has been driven primarily by regulatory concerns. As a result, analyses have not been performed for many other important chemical agents that have been disposed of to the ground. For example, data on the subsurface concentrations of important organic substances (such as chelating agents, organic acid complexants, and alkyl phosphates) are limited. However, records at many of the sites, although incomplete, indicate the disposal of large quantities of these chemical agents to the ground (see Tables 6 and E-I). Therefore. the lack of subsurface concentration data for chelating and complexing agents results not from their absence but from the fact that they are unregulated chemicals and are not routinely measured as part of environmental compliance programs at DOE facilities. The limitations of available analytical measurement techniques influence the acquisition of data for such substances. DOE recognizes the limitations of existing monitoring programs and is taking steps to strengthen them. The improvements include incorporation of measurements, using methodologies with documented sensitivity, for organic chemical agents that have been disposed of to the ground and exhibit potential to mobilize metal ions or radionuclides.

Two other factors have also affected the breadth of the data base and the comprehensiveness of this assessment. Many of the organic chemical agents used in chemical processing on DOE lands and disposed of to the ground pose challenges for environmental measurement and analysis. As a result, past analysis and measurement methodologies may not be sensitive or precise enough to accurately measure, monitor, or even detect the presence of these constituents in environmental samples with complex chemical matrices. Finally, the identity and concentrations of elements in weapons-testing sites and the environmental concentrations of certain radionuclides have been labeled "classified" by the Federal Government and either are not or have not been accessible for scientific review.

The assessment performed in this report can be expanded as additional data are obtained on the nature and concentrations of chemical contaminants on DOE lands. Meanwhile, the generic chemical mixtures identified in Section 9 are justified for research, given existing data, and this justification is not likely to change with new information. Basic research on the subsurface behavior of these mixtures will provide DOE with a much needed understanding of complex co-contaminant geochemical interactions to improve predictions of subsurface migration and develop better restoration techniques.

SECTION 11

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*Chemical data in this reference summarize data compiled from other references under the Rocky Flats Plant listing. Data cited in this report for Rocky Flats Plant were taken from this reference.

Appendix B

Compound-Class Distributions

The tables in this appendix present the frequency of occurrence of the compound classes at the 18 DOE facilities and 91 waste sites.

Table B-1. Distribution of Compound Classes in Soils as a Function of Facility and Individual Waste Site

Facility	No. of Waste Sites[1]	Distribution (by % of Waste Sites)[2] of Compound Classes[3]												
		1	2	3	4	5	6	7	8	9	10	11	12	13
Argonne National Laboratory	2	0	0	0	0	0	0	0	0	0	0	0	0	0
Brookhaven National Laboratory	4	0	0	0	0	0	0	0	0	0	0	0	0	0
Fernald	11	72	9	90	45	27	9	100	0	0	36	0	0	0
Hanford Site	7	85	42	100	28	14	28	14	0	28	0	28	0	71
Idaho National Engineering Laboratory	6	50	50	50	33	16	16	33	0	16	16	33	16	16
Kansas City Plant	7	57	0	0	57	42	0	71	0	14	0	0	0	0
Lawrence Livermore National Laboratory	12	0	0	0	41	16	0	0	16	0	0	0	0	0
Los Alamos National Laboratory	3	33	66	66	33	33	33	33	0	33	0	33	0	33
Mound	2	0	0	100	0	0	0	0	50	50	0	0	0	0
Nevada Test Site	6	0	0	50	0	0	0	0	0	0	0	0	0	0
Oak Ridge National Laboratory	9	33	22	44	11	22	11	33	0	0	0	11	11	0
Pantex Plant	3	0	0	0	66	100	0	0	33	100	0	0	0	0
Pinellas Plant	1	0	0	0	0	0	0	0	0	0	0	0	0	0
Portsmouth Gaseous Diffusion Plant	4	25	25	100	0	0	0	0	0	0	0	0	0	0
Rocky Flats Plant	3	66	33	100	100	33	0	0	0	33	0	0	0	0
Sandia National Laboratory, Albuquerque	1	100	0	0	100	100	0	0	0	100	0	0	0	100
Sandia National Laboratory, Livermore	1	0	0	0	0	100	0	0	0	0	0	0	0	0
Savannah River Plant	9	66	66	33	55	33	0	0	33	0	22	11	11	11

[1] Number of waste sites evaluated at a specific facility.

[2] Percent of waste sites at a specific facility reporting a specific compound class.

[3] Compound-class index:

1 = metals
2 = anions
3 = radionuclides
4 = chlorinated hydrocarbons
5 = fuel hydrocarbons
6 = phthalates
7 = polychlorinated biphenyls
8 = explosives
9 = ketones
10 = pesticides
11 = alkyl phosphates
12 = complexing agents
13 = organic acids

Table B-2. Distribution of Compound Classes in Ground Waters as a Function of Facility and Individual Waste Site

Facility	No. of Waste Sites[1]	Distribution (by % of Waste Sites)[2] of Compound Classes[3]												
		1	2	3	4	5	6	7	8	9	10	11	12	13
Argonne National Laboratory	2	100	100	100	50	0	0	0	0	0	0	0	0	0
Brookhaven National Laboratory	4	25	25	100	100	75	0	0	0	0	0	0	0	0
Fernald	11	72	90	81	72	72	0	0	0	72	0	0	0	0
Hanford Site	7	71	100	100	42	0	0	0	0	0	0	0	0	0
Idaho National Engineering Laboratory	6	50	50	50	66	16	0	0	0	16	0	0	0	33
Kansas City Plant	7	0	0	0	28	0	0	14	0	0	0	0	0	0
Lawrence Livermore National Laboratory	12	16	16	16	66	16	0	0	8	0	0	0	0	0
Los Alamos National Laboratory	3	0	0	0	0	0	0	0	0	0	0	0	0	0
Mound	2	0	0	0	50	0	0	0	0	0	0	0	0	0
Nevada Test Site	6	33	50	83	0	0	0	0	0	0	0	0	0	0
Oak Ridge National Laboratory	9	77	33	44	77	22	22	0	0	55	0	0	11	11
Pantex Plant	3	66	66	66	33	33	0	0	66	0	0	0	0	0
Pinellas Plant	1	100	0	0	100	100	0	0	0	100	0	0	0	0
Portsmouth Gaseous Diffusion Plant	4	100	0	50	75	0	0	0	0	0	0	0	0	0
Rocky Flats Plant	3	100	33	100	100	33	0	0	0	0	0	0	0	0
Sandia National Laboratory, Albuquerque	1	0	0	0	0	0	0	0	0	0	0	0	0	0
Sandia National Laboratory, Livermore	1	100	0	0	0	100	0	0	0	0	0	0	0	0
Savannah River Plant	9	88	88	77	77	0	11	0	0	11	44	0	0	0

[1] Number of waste sites evaluated at a specific facility.

[2] Percent of waste sites at a specific facility reporting a specific compound class.

[3] Compound-class index:

1 = metals
2 = anions
3 = radionuclides
4 = chlorinated hydrocarbons
5 = fuel hydrocarbons

6 = phthalates
7 = polychlorinated biphenyls
8 = explosives
9 = ketones
10 = pesticides

11 = alkyl phosphates
12 = complexing agents
13 = organic acids

Frequency of Compound-Class Mixtures

The tables in this appendix present the frequency of occurrence of mixtures of compound classes at the 18 DOE facilities and 91 waste sites.

Table C-1. Frequency of Occurrence at DOE Facilities of the Most Commonly Reported Pairs of Compound Classes in Soils/Sediments

Class Combinations	Number of Waste Sites[1]	Facility Frequency of Occurrence[2]
Metals, radionuclides	25	Savannah River(3), Oak Ridge(3), Hanford(6), Portsmouth(1), Rocky Flats(2), Fernald(8), INEL(2)
Metals, PCBs	18	Oak Ridge(2), Hanford(1), Kansas City(4), Fernald(8), INEL(2), Los Alamos(1)
Radionuclides, PCBs	15	Oak Ridge(2), Hanford(1), Fernald(10), INEL(2)
Chlorinated hydrocarbons, fuel hydrocarbons	15	Savannah River(2), Oak Ridge(1), Hanford(1), Rocky Flats(1), Sandia-Albuquerque(1), Pantex(2), Lawrence Livermore(1), Kansas City(1), Fernald(3), INEL(1), Los Alamos(1)
Metals, chlorinated hydrocarbons	14	Savannah River(2), Oak Ridge(1), Hanford(2), Rocky Flats(2), Sandia-Albuquerque(1), Kansas City(2), Fernald(3), Los Alamos(1)
Anions, radionuclides	14	Savannah River(2), Oak Ridge(2), Hanford(3), Portsmouth(1), Rocky Flats(1), Fernald(1), INEL(3), Los Alamos(1)
Radionuclides, chlorinated hydrocarbons	14	Savannah River(1), Oak Ridge(1), Hanford(2), Rocky Flats(3), Fernald(5), INEL(2)
Chlorinated hydrocarbons, PCBs	13	Oak Ridge(1), Hanford(1), Kansas City(3), Fernald(5), INEL(2), Los Alamos(1)
Metals, anions	12	Savannah River(4), Oak Ridge(1), Hanford(2), Rocky Flats(1), Fernald(1), INEL(2), Los Alamos(1)
Metals, fuel hydrocarbons	11	Savannah River(1), Oak Ridge(1), Hanford(1), Rocky Flats(1), Sandia-Albuquerque(1), Kansas City(3), Fernald(1), INEL(1), Los Alamos(1)
Anions, chlorinated hydrocarbons	11	Savannah River(4), Hanford(2), Rocky Flats(1), Fernald(1), INEL(2), Los Alamos(1)
Fuel hydrocarbons, PCBs	10	Oak Ridge(2), Kansas City(3), Fernald(3), INEL(1), Los Alamos(1)
Chlorinated hydrocarbons, ketones	9	Hanford(2), Rocky Flats(1), Sandia-Albuquerque(1), Pantex(2), Kansas City(1), INEL(1), Los Alamos(1)
Anions, fuel hydrocarbons	8	Savannah River(3), Hanford(1), Rocky Flats(1), Fernald(1), INEL(1), Los Alamos(1)
Radionuclides, organic acids	8	Savannah River(1), Hanford(5), INEL(1), Los Alamos(1)
Metals, alkyl phosphates	7	Savannah River(1), Oak Ridge(1), Hanford(2), INEL(2), Los Alamos(1)
Metals, organic acids	7	Savannah River(1), Hanford(4), Sandia-Albuquerque(1), INEL(1)
Radionuclides, fuel hydrocarbons	7	Oak Ridge(1), Hanford(1), Rocky Flats(1), Fernald(3), INEL(1)
Metals, ketones	6	Hanford(2), Sandia-Albuquerque(1), Kansas City(1), INEL(1), Los Alamos(1)
Anions, alkyl phosphates	6	Savannah River(1), Oak Ridge(1), Hanford(2), INEL(1), Los Alamos(1)
Fuel hydrocarbons, ketones	6	Hanford(1), Sandia-Albuquerque(1), Pantex(3), Los Alamos(1)
Metals, phthalates	5	Oak Ridge(1), Hanford(2), INEL(1), Los Alamos(1)
Anions, PCBs	5	Hanford(1), Fernald(1), INEL(2), Los Alamos(1)
Anions, organic acids	5	Savannah River(1), Hanford(2), INEL(1), Los Alamos(1)
Radionuclides, ketones	5	Hanford(2), Rocky Flats(1), INEL(1), Mound(1)
Radionuclides, alkyl phosphates	5	Savannah River(1), Oak Ridge(1), Hanford(2), INEL(1)
Chlorinated hydrocarbons, pesticides	5	Savannah River(1), Fernald(3), INEL(1)
Phthalates, PCBs	5	Oak Ridge(1), Hanford(1), Fernald(1), INEL(1), Los Alamos(1)
PCBs, pesticides	5	Fernald(4), INEL(1)
Anions, phthalates	4	Hanford(2), INEL(1), Los Alamos(1)
Anions, ketones	4	Hanford(2), INEL(1), Los Alamos(1)
Radionuclides, phthalates	4	Oak Ridge(1), Hanford(2), INEL(1)
Radionuclides, pesticides	4	Fernald(3), INEL(1)
Chlorinated hydrocarbons, phthalates	4	Hanford(2), INEL(1), Los Alamos(1)
Chlorinated hydrocarbons, alkyl phosphates	4	Hanford(2), INEL(1), Los Alamos(1)
Fuel hydrocarbons, pesticides	4	Savannah River(1), Fernald(3)
Phthalates, ketones	4	Hanford(2), INEL(1), Los Alamos(1)
PCBs, ketones	4	Hanford(1), Kansas City(1), INEL(1), Los Alamos(1)
Metals, pesticides	3	Savannah River(1), Fernald(1), INEL(1)
Metals, complexing agents	3	Savannah River(1), Oak Ridge(1), INEL(1)
Anions, pesticides	3	Savannah River(1), Fernald(1), INEL(1)
Radionuclides, complexing agents	3	Savannah River(1), Oak Ridge(2), INEL(1)

Table C-1. Frequency of Occurrence at DOE Facilities of the Most Commonly Reported Pairs of Compound Classes in Soils/Sediments (Continued)

Chlorinated hydrocarbons, explosives	3	Savannah River(2), Lawrence Livermore(1)
Chlorinated hydrocarbons, organic acids	3	Hanford(1), Sandia-Albuquerque(1), INEL(1)
Fuel hydrocarbons, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Fuel hydrocarbons, organic acids	3	Hanford(1), Sandia-Albuquerque(1), INEL(1)
Phthalates, alkyl phosphates	3	Hanford(2), Los Alamos(1)
PCBs, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Alkyl phosphates, organic acids	3	Savannah River(1), Hanford(1), INEL(1)

[1] Number of waste sites (out of 91) reporting specific class combination.

[2] Facility frequency of occurrence is the frequency at which a particular class combination appears at a particular DOE facility.

Table C-2. Frequency of Occurrence at DOE Facilities of the Most Commonly Reported Combinations of Three Compound Classes in Soils/Sediments

Class Combinations	Number of Waste Sites[1]	Facility Frequency of Occurrence[2]
Metals, radionuclides, PCBs	13	Oak Ridge(2), Hanford(1), Fernald(8), INEL(2)
Metals, radionuclides, chlorinated hydrocarbons	11	Savannah River(1), Oak Ridge(1), Hanford(2), Rocky Flats(2), Fernald(3), INEL(2)
Metals, chlorinated hydrocarbons, PCBs	10	Oak Ridge(1), Hanford(1), Kansas City(2), Fernald(3), INEL(2), Los Alamos(1)
Metals, anions, radionuclides	9	Savannah River(2), Oak Ridge(1), Hanford(2), Rocky Flats(1), Fernald(1), INEL(2)
Metals, anions, chlorinated hydrocarbons	9	Savannah River(2), Hanford(2), Rocky Flats(1), Fernald(1), INEL(2), Los Alamos(1)
Radionuclides, chlorinated hydrocarbons, PCBs	9	Oak Ridge(1), Hanford(1), Fernald(5), INEL(2)
Metals, chlorinated hydrocarbons, fuel hydrocarbons	8	Oak Ridge(1), Hanford(1), Rocky Flats(1), Sandia-Albuquerque(1), Kansas City(1), Fernald(1), INEL(1), Los Alamos(1)
Metals, fuel hydrocarbons, PCBs	7	Oak Ridge~~(1), Kansas~~ City(3), Fernald(1), INEL(1), Los Alamos(1)
Anions, radionuclides, chlorinated hydrocarbons	7	Savannah River(1), Hanford(2), Rocky Flats(1), Fernald(1), INEL(2)
Anions, chlorinated hydrocarbons, fuel hydrocarbons	7	Savannah River(2), Hanford(1), Rocky Flats(1), Fernald(1), INEL(1), Los Alamos(1)
Radionuclides, chlorinated hydrocarbons, fuel hydrocarbons	7	Oak Ridge(1), Hanford(1), Rocky Flats(1), Fernald(3), INEL(1)
Chlorinated hydrocarbons, fuel hydrocarbons, PCBs	7	Oak Ridge(1), Kansas City(1), Fernald(3), INEL(1), Los Alamos(1)
Metals, anions, fuel hydrocarbons	6	Savannah River(1), Hanford(1), Rocky Flats(1), Fernald(1), INEL(1), Los Alamos(1)
Metals, anions, alkyl phosphates	6	Savannah River(1), Oak Ridge(1), Hanford(2), INEL(1), Los Alamos(1)
Metals, radionuclides, organic acids	6	Savannah River(1), Hanford(4), INEL(1)
Metals, chlorinated hydrocarbons, ketones	6	Hanford(2), Sandia-Albuquerque(1), Kansas City(1), INEL(1), Los Alamos(1)
Metals, anions, PCBs	5	Hanford(1), Fernald(1), INEL(2), Los Alamos(1)
Metals, radionuclides, fuel hydrocarbons	5	Oak Ridge(1), Hanford(1), Rocky Flats(1), Fernald(1), INEL(1)
Metals, radionuclides, alkyl phosphates	5	Savannah River(1), Oak Ridge(1), Hanford(2), INEL(1)
Anions, radionuclides, alkyl phosphates	5	Savannah River(1), Oak Ridge(1), Hanford(2), INEL(1)
Anions, radionuclides, organic acids	5	Savannah River(1), Hanford(2), INEL(1), Los Alamos(1)
Anions, chlorinated hydrocarbons, PCBs	5	Hanford(1), Fernald(1), INEL(2), Los Alamos(1)
Radionuclides, fuel hydrocarbons, PCBs	5	Oak Ridge(1), Fernald(3), INEL(1)
Chlorinated hydrocarbons, fuel hydrocarbons, PCBs	5	Hanford(1), Sandia-Albuquerque(1), Pantex(2), Los Alamos(1)
Metals, anions, phthalates	4	Hanford(2), INEL(1), Los Alamos(1)
Metals, anions, ketones	4	Hanford(2), INEL(1), Los Alamos(1)
Metals, radionuclides, phthalates	4	Oak Ridge(1), Hanford(2), INEL(1)
Metals, chlorinated hydrocarbons, phthalates	4	Hanford(2), INEL(1), Los Alamos(1)
Metals, chlorinated hydrocarbons, alkyl phosphates	4	Hanford(2), INEL(1), Los Alamos(1)
Metals, phthalates, PCBs	4	Oak Ridge(1), Hanford(1), INEL(1), Los Alamos(1)
Metals, phthalates, ketones	4	Hanford(2), INEL(1), Los Alamos(1)
Metals, PCBs, ketones	4	Hanford(1), Kansas City(1), INEL(1), Los Alamos(1)
Anions, radionuclides, fuel hydrocarbons	4	Hanford(1), Rocky Flats(1), Fernald(1), INEL(1)

Table C-2. Frequency of Occurrence at DOE Facilities of the Most Commonly Reported Combinations of Three Compound Classes in Soils/Sediments (Continued)

Class Combinations	Number of Waste Sites[1]	Facility Frequency of Occurrence[2]
Anions, radionuclides, PCBs	4	Hanford(1), Fernald(1), INEL(2)
Anions, chlorinated hydrocarbons, phthalates	4	Hanford(2), INEL(1), Los Alamos(1)
Anions, chlorinated hydrocarbons, ketones	4	Hanford(2), INEL(1), Los Alamos(1)
Anions, chlorinated hydrocarbons, alkyl phosphates	4	Hanford(2), INEL(1), Los Alamos(1)
Anions, phthalates, ketones	4	Hanford(2), INEL(1), Los Alamos(1)
Radionuclides, chlorinated hydrocarbons, ketones	4	Hanford(2), Rocky Flats(1), INEL(1)
Radionuclides, chlorinated hydrocarbons, pesticides	4	Fernald(3), INEL(1)
Radionuclides, PCBs, pesticides	4	Fernald(3), INEL(1)
Chlorinated hydrocarbons, phthalates, ketones	4	Hanford(2), INEL(1), Los Alamos(1)
Chlorinated hydrocarbons, PCBs, ketones	4	Hanford(1), Kansas City(1), INEL(1), Los Alamos(1)
Chlorinated hydrocarbons, PCBs, pesticides	4	Fernald(3), INEL(1)
Metals, anions, pesticides	3	Savannah River(1), Fernald(1), INEL(1)
Metals, anions, organic acids	3	Savannah River(1), Hanford(1), INEL(1)
Metals, radionuclides, ketones	3	Hanford(2), INEL(1)
Metals, radionuclides, complexing agents	3	Savannah River(1), Oak Ridge(1), INEL(1)
Metals, chlorinated hydrocarbons, organic acids	3	Hanford(1), Sandia-Albuquerque(1), INEL(1)
Metals, fuel hydrocarbons, ketones	3	Hanford(1), Sandia-Albuquerque(1), Los Alamos(1)
Metals, fuel hydrocarbons, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, fuel hydrocarbons, organic acids	3	Hanford(1), Sandia-Albuquerque(1), INEL(1)
Metals, phthalates, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Metals, PCBs, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Metals, alkyl phosphates, organic acids	3	Savannah River(1), Hanford(1), INEL(1)
Anions, radionuclides, phthalates	3	Hanford(2), INEL(1)
Anions, radionuclides, ketones	3	Hanford(2), INEL(1)
Anions, fuel hydrocarbons, PCBs	3	Fernald(1), INEL(1), Los Alamos(1)
Anions, fuel hydrocarbons, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Anions, phthalates, PCBs	3	Hanford(1), INEL(1), Los Alamos(1)
Anions, phthalates, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Anions, PCBs, ketones	3	Hanford(1), INEL(1), Los Alamos(1)
Anions, PCBs, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Anions, ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Anions, alkyl phosphates, organic acids	3	Savannah River(1), Hanford(1), INEL(1)
Radionuclides, chlorinated hydrocarbons, phthalates	3	Hanford(2), INEL(1)
Radionuclides, chlorinated hydrocarbons, alkyl phosphates	3	Hanford(2), INEL(1)
Radionuclides, fuel hydrocarbons, pesticides	3	Fernald(3)
Radionuclides, phthalates, PCBs	3	Oak Ridge(1), Hanford(1), INEL(1)
Radionuclides, phthalates, ketones	3	Hanford(2), INEL(1)
Radionuclides, alkyl phosphates, organic acids	3	Savannah River(1), Hanford(1), INEL(1)
Chlorinated hydrocarbons, fuel hydrocarbons, pesticides	3	Fernald(3)
Chlorinated hydrocarbons, fuel hydrocarbons, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Chlorinated hydrocarbons, fuel hydrocarbons, organic acids	3	Hanford(1), Sandia-Albuquerque(1), INEL(1)
Chlorinated hydrocarbons, phthalates, PCBs	3	Hanford(1), INEL(1), Los Alamos(1)
Chlorinated hydrocarbons, phthalates, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Chlorinated hydrocarbons, PCBs, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Chlorinated hydrocarbons, ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Fuel hydrocarbons, PCBs, pesticides	3	Fernald(3)
Phthalates, PCBs, ketones	3	Hanford(1), INEL(1), Los Alamos(1)
Phthalates, ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)

[1] Number of waste sites (out of 91) reporting specific class combination.

[2] Facility frequency of occurrence is the frequency at which a particular class combination appears at a particular DOE facility.

Table C-3. Frequency of Occurrence at DOE Facilities of the Most Commonly Reported Combinations of Four Compound Classes in Soils/Sediments

Class Combinations	Number of Waste Sites[1]	Facility Frequency of Occurrence[2]
Metals, anions, radionuclides, chlorinated hydrocarbons	7	Savannah River(1), Hanford(2), Rocky Flats(1), Fernald(1), INEL(2)
Metals, radionuclides, chlorinated hydrocarbons, PCBs	7	Oak Ridge(1), Hanford(1), Fernald(3), INEL(2)
Metals, anions, radionuclides, alkyl phosphates	5	Savannah River(1), Oak Ridge(1), Hanford(2), INEL(1)
Metals, anions, chlorinated hydrocarbons, fuel hydrocarbons	5	Hanford(1), Rocky Flats(1), Fernald(1), INEL(1), Los Alamos(1)
Metals, anions, chlorinated hydrocarbons, PCBs	5	Hanford(1), Fernald(1), INEL(2), Los Alamos(1)
Metals, radionuclides, chlorinated hydrocarbons, fuel	5	Oak Ridge(1), Hanford(1), Rocky Flats(1), Fernald(1), INEL(1)
Metals, chlorinated hydrocarbons, fuel hydrocarbons, PCBs	5	Oak Ridge(1), Kansas City(1), Fernald(1), INEL(1), Los Alamos(1)
Radionuclides, chlorinated hydrocarbons, fuel hydrocarbons, PCBs	5	Oak Ridge(1), Fernald(3), INEL(1)
Metals, anions, radionuclides, fuel hydrocarbons	4	Hanford(1), Rocky Flats(1), Fernald(1), INEL(1)
Metals, anions, radionuclides, PCBs	4	Hanford(1), Fernald(1), INEL(2)
Metals, anions, chlorinated hydrocarbons, phthalates	4	Hanford(2), INEL(1), Los Alamos(1)
Metals, anions, chlorinated hydrocarbons, ketones	4	Hanford(2), INEL(1), Los Alamos(1)
Metals, anions, chlorinated hydrocarbons, alkyl phosphates	4	Hanford(2), INEL(1), Los Alamos(1)
Metals, anions, phthalates, ketones	4	Hanford(2), INEL(1), Los Alamos(1)
Metals, chlorinated hydrocarbons, phthalates, ketones	4	Hanford(2), INEL(1), Los Alamos(1)
Metals, chlorinated hydrocarbons, PCBs, ketones	4	Hanford(1), Kansas City(1), INEL(1), Los Alamos(1)
Anions, radionuclides, chlorinated hydrocarbons, fuel hydrocarbons	4	Hanford(1), Rocky Flats(1), Fernald(1), INEL(1)
Anions, radionuclides, chlorinated hydrocarbons, PCBs	4	Hanford(1), Fernald(1), INEL(2)
Anions, chlorinated hydrocarbons, phthalates, ketones	4	Hanford(2), INEL(1), Los Alamos(1)
Radionuclides, chlorinated hydrocarbons, PCBs, pesticides	4	Fernald(3), INEL(1)
Metals, anions, radionuclides, phthalates	3	Hanford(2), INEL(1)
Metals, anions, radionuclides, ketones	3	Hanford(2), INEL(1)
Metals, anions, radionuclides, organic acids	3	Savannah River(1), Hanford(1), INEL(1)
Metals, anions, fuel hydrocarbons, PCBs	3	Fernald(1), INEL(1), Los Alamos(1)
Metals, anions, fuel hydrocarbons, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, anions, phthalates, PCBs	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, anions, phthalates, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Metals, anions, PCBs, ketones	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, anions, PCBs, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, anions, ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Metals, anions, alkyl phosphates, organic acids	3	Savannah River(1), Hanford(1), INEL(1)
Metals, radionuclides, chlorinated hydrocarbons, phthalates	3	Hanford(2), INEL(1)
Metals, radionuclides, chlorinated hydrocarbons, ketones	3	Hanford(2), INEL(1)
Metals, radionuclides, chlorinated hydrocarbons, alkyl phosphates	3	Hanford(2), INEL(1)
Metals, radionuclides, fuel hydrocarbons, PCBs	3	Oak Ridge(1), Fernald(1), INEL(1)
Metals, radionuclides, phthalates, PCBs	3	Oak Ridge(1), Hanford(1), INEL(1)
Metals, radionuclides, phthalates, ketones	3	Hanford(2), INEL(1)
Metals, radionuclides, alkyl phosphates, organic acids	3	Savannah River(1), Hanford(1), INEL(1)
Metals, chlorinated hydrocarbons, fuel hydrocarbons, ketones	3	Hanford(1), Sandia-Albuquerque(1), Los Alamos(1)
Metals, chlorinated hydrocarbons, fuel hydrocarbons, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, chlorinated hydrocarbons, fuel hydrocarbons, organic acids	3	Hanford(1), Sandia-Albuquerque(1), INEL(1)
Metals, chlorinated hydrocarbons, phthalates, PCBs	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, chlorinated hydrocarbons, phthalates, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Metals, chlorinated hydrocarbons, PCBs, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, chlorinated hydrocarbons, ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Metals, phthalates, PCBs, ketones	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, phthalates, ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Anions, radionuclides, chlorinated hydrocarbons, phthalates	3	Hanford(2), INEL(1)

Table C-3. Frequency of Occurrence at DOE Facilities of the Most Commonly Reported Combinations of Four Compound Classes in Soils/Sediments (Continued)

Class Combinations	Number of Waste Sites[1]	Facility Frequency of Occurrence[2]
Anions, radionuclides, chlorinated hydrocarbons, ketones	3	Hanford(2), INEL(1)
Anions, radionuclides, chlorinated hydrocarbons, alkyl phosphates	3	Hanford(2), INEL(1)
Anions, radionuclides, phthalates, ketones	3	Hanford(2), INEL(1)
Anions, radionuclides, alkyl phosphates, organic acids	3	Savannah River(1), Hanford(1), INEL(1)
Anions, chlorinated hydrocarbons, fuel hydrocarbons, PCBs	3	Fernald(1), INEL(1), Los Alamos(1)
Anions, chlorinated hydrocarbons, fuel hydrocarbons, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Anions, chlorinated hydrocarbons, phthalates, PCBs	3	Hanford(1), INEL(1), Los Alamos(1)
Anions, chlorinated hydrocarbons, phthalates, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Anions, chlorinated hydrocarbons, PCBs, ketones	3	Hanford(1), INEL(1), Los Alamos(1)
Anions, chlorinated hydrocarbons, PCBs, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Anions, chlorinated hydrocarbons, ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Anions, phthalates, PCBs, ketones	3	Hanford(1), INEL(1), Los Alamos(1)
Anions, phthalates, ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Radionuclides, chlorinated hydrocarbons, fuel hydrocarbons, pesticides	3	Fernald(3)
Radionuclides, chlorinated hydrocarbons, phthalates, ketones	3	Hanford(2), INEL(1)
Radionuclides, fuel hydrocarbons, PCBs, pesticides	3	Fernald(3)
Chlorinated hydrocarbons, fuel hydrocarbons, PCBs, pesticides	3	Fernald(3)
Chlorinated hydrocarbons, phthalates, PCBs, ketones	3	Hanford(1), INEL(1), Los Alamos(1)
Chlorinated hydrocarbons, phthalates, ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)

[1] Number of waste sites (out of 91) reporting specific class combination.

[2] Facility frequency of occurrence is the frequency at which a particular class combination appears at a particular DOE facility.

Table C-4. Frequency of Occurrence at DOE Facilities of the Most Commonly Reported Combinations of Five Compound Classes in Soils/Sediments

Class Combinations	Number of Waste Sites[1]	Facility Frequency of Occurrence[2]
Metals, anions, radionuclides, chlorinated hydrocarbons, fuel hydrocarbons	4	Hanford(1), Rocky Flats(1), Fernald(1), INEL(1)
Metals, anions, radionuclides, chlorinated hydrocarbons, PCBs	4	Hanford(1), Fernald(1), INEL(2)
Metals, anions, chlorinated hydrocarbons, phthalates, ketones	4	Hanford(2), INEL(1), Los Alamos(1)
Metals, anions, radionuclides, chlorinated hydrocarbons, phthalates	3	Hanford(2), INEL(1)
Metals, anions, radionuclides, chlorinated hydrocarbons, ketones	3	Hanford(2), INEL(1)
Metals, anions, radionuclides, chlorinated hydrocarbons, alkyl phosphates	3	Hanford(2), INEL(1)
Metals, anions, radionuclides, phthalates, ketones	3	Hanford(2), INEL(1)
Metals, anions, radionuclides, alkyl phosphates, organic acids	3	Savannah River(1), Hanford(1), INEL(1)
Metals, anions, chlorinated hydrocarbons, fuel hydrocarbons, PCBs	3	Fernald(1), INEL(1), Los Alamos(1)
Metals, anions, chlorinated hydrocarbons, fuel hydrocarbons, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, anions, chlorinated hydrocarbons, phthalates, PCBs	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, anions, chlorinated hydrocarbons, phthalates, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Metals, anions, chlorinated hydrocarbons, PCBs, ketones	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, anions, chlorinated hydrocarbons, PCBs, alkyl phosphates	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, anions, chlorinated hydrocarbons, ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Metals, anions, phthalates, PCBs, ketones	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, anions, phthalates, ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Metals, radionuclides, chlorinated hydrocarbons, fuel hydrocarbons, PCBs	3	Oak Ridge(1), Fernald(1), INEL(1)
Metals, radionuclides, chlorinated hydrocarbons, phthalates, ketones	3	Hanford(2), INEL(1)
Metals, chlorinated hydrocarbons, phthalates, PCBs, ketones	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, chlorinated hydrocarbons, phthalates, ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Metals, anions, phthalates, PCBs, ketones	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, anions, phthalates, ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Metals, radionuclides, chlorinated hydrocarbons, fuel hydrocarbons, PCBs	3	Oak Ridge(1), Fernald(1), INEL(1)
Metals, radionuclides, chlorinated hydrocarbons, phthalates, ketones	3	Hanford(2), INEL(1)
Metals, chlorinated hydrocarbons, phthalates, PCBs, ketones	3	Hanford(1), INEL(1), Los Alamos(1)
Metals, chlorinated hydrocarbons, phthalates, ketones, alkyl phosphates	3	Hanford(2), Los Alamos(1)
Anions, radionuclides, chlorinated hydrocarbons, phthalates, ketones	3	Hanford(2), INEL(1)
Anions, chlorinated hydrocarbons, phthalates, PCBs, ketones	3	Hanford(1), INEL(1), Los Alamos(1)
Anions, chlorinated hydrocarbons, phthalates, ketones, alkyl phosphates	3	Fernald(3)
Radionuclides, chlorinated hydrocarbons, fuel hydrocarbons, PCBs, pesticides	3	Fernald(3)

[1] Number of waste sites (out of 91) reporting specific class combination.

[2] Facility frequency of occurrence is the frequency at which a particular class combination appears at a particular DOE facility.

Table C-5. Frequency of Occurrence at DOE Facilities of the Most Commonly Reported Pairs of Compound Classes in Ground Waters

Class Combinations	Number of Waste Sites[1]	Facility Frequency of Occurrence[2]
Metals, chlorinated hydrocarbons	38	Savannah River(7), Oak Ridge(6), Pinellas Plant(1), Hanford(3), Portsmouth(3), Rocky Flats(3), Pantex(1), Lawrence Livermore(1), Fernald(8), INEL(3), Brookhaven(1), Argonne(1)
Metals, radionuclides	36	Savannah River(7), Oak Ridge(3), Hanford(5), Portsmouth(2), Rocky Flats(3), Pantex(2), Fernald(8), INEL(2), Brookhaven(1), Argonne(2), Nevada Test Site(1)
Metals, anions	33	Savannah River(8), Oak Ridge(3), Hanford(5), Rocky Flats(1), Pantex(2), Lawrence Livermore(1), Fernald(8), INEL(1), Brookhaven(1), Argonne(2), Nevada Test Site(1)
Anions, radionuclides	33	Savannah River(7), Oak Ridge(1), Hanford(7), Rocky Flats(1), Pantex(2), Fernald(9), INEL(2), Brookhaven(1), Argonne(2), Nevada Test Site(1)
Radionuclides, chlorinated hydrocarbons	32	Savannah River(6), Oak Ridge(3), Hanford(3), Portsmouth(1), Rocky Flats(3), Pantex(1), Fernald(8), INEL(2), Brookhaven(4), Argonne(1)
Anions, chlorinated hydrocarbons	26	Savannah River(7), Oak Ridge(2), Hanford(3), Rocky Flats(1), Pantex(1), Fernald(8), INEL(2), Brookhaven(1), Argonne(1)
Chlorinated hydrocarbons, fuel hydrocarbons	17	Oak Ridge(2), Pinellas Plant(1), Rocky Flats(1), Lawrence Livermore(1), Fernald(8), INEL(1), Brookhaven(3)
Metals, fuel hydrocarbons	16	Oak Ridge(2), Pinellas Plant(1), Rocky Flats(1), Sandia- Livermore(1), Pantex(1), Lawrence Livermore(1), Fernald(8), INEL(1)
Metals, ketones	16	Savannah River(1), Oak Ridge(5), Pinellas Plant(1), Fernald(8), INEL(1)
Radionuclides, fuel hydrocarbons	16	Oak Ridge(2), Rocky Flats(1), Pantex(1), Fernald(8), INEL(1), Brookhaven(3)
Chlorinated hydrocarbons, ketones	16	Savannah River(1), Oak Ridge(5), Pinellas Plant(1), Fernald(8), INEL(1)
Anions, fuel hydrocarbons	12	Oak Ridge(1), Rocky Flats(1), Pantex(1), Lawrence Livermore(1), Fernald(8)
Radionuclides, ketones	12	Savannah River(1), Oak Ridge(3), Fernald(8)
Anions, ketones	11	Savannah River(1), Oak Ridge(2), Fernald(8)
Fuel hydrocarbons, ketones	11	Oak Ridge(2), Pinellas Plant(1), Fernald(8)
Metals, pesticides	4	Savannah River(4)
Anions, pesticides	4	Savannah River(4)
Radionuclides, pesticides	4	Savannah River(4)
Chlorinated hydrocarbons, pesticides	4	Savannah River(4)
Metals, phthalates	3	Savannah River(1), Oak Ridge(2)
Metals, explosives	3	Pantex(2), Lawrence Livermore(1)
Anions, phthalates	3	Savannah River(1), Oak Ridge(2)
Anions, explosives	3	Pantex(2), Lawrence Livermore(1)
Chlorinated hydrocarbons, phthalates	3	Savannah River(1), Oak Ridge(2)
Phthalates, ketones	3	Savannah River(1), Oak Ridge(2)

[1] Number of waste sites (out of 91) reporting specific class combination.

[2] Facility frequency of occurrence is the frequency at which a particular class combination appears at a particular DOE facility

Table C-6. Frequency of Occurrence at DOE Facilities of the Most Commonly Reported Combinations of Three Compound Classes in Ground Waters

Class Combinations	Number of Waste Sites[1]	Facility Frequency of Occurrence[2]
Metals, anions, radionuclides	29	Savannah River(7), Oak Ridge(1), Hanford(5), Rocky Flats(1), Pantex(2), Fernald(8), INEL(1), Brookhaven(1), Argonne(2), Nevada Test Site(1)
Metals, radionuclides, chlorinated hydrocarbons	29	Savannah River(6), Oak Ridge(3), Hanford(3), Portsmouth(1), Rocky Flats(3), Pantex(1), Fernald(8), INEL(2), Brookhaven(1), Argonne(1)
Metals, anions, chlorinated hydrocarbons	25	Savannah River(7), Oak Ridge(2), Hanford(3), Rocky Flats(1), Pantex(1), Fernald(8), INEL(1), Brookhaven(1), Argonne(1)
Anions, radionuclides, chlorinated hydrocarbons	23	Savannah River(6), Oak Ridge(1), Hanford(3), Rocky Flats(1), Pantex(1), Fernald(8), INEL(1), Brookhaven(1), Argonne(1)
Metals, chlorinated hydrocarbons, ketones	16	Savannah River(1), Oak Ridge(5), Pinellas Plant(1), Fernald(8), INEL(1)
Radionuclides, chlorinated hydrocarbons, fuel hydrocarbons	15	Oak Ridge(2), Rocky Flats(1), Fernald(8), INEL(1), Brookhaven(3)
Metals, radionuclides, fuel hydrocarbons	13	Oak Ridge(2), Rocky Flats(1), Pantex(1), Fernald(8), INEL(1)
Metals, chlorinated hydrocarbons, fuel	13	Oak Ridge(2), Pinellas Plant(1), Rocky Flats(1), Fernald(8), INEL(1)
Metals, anions, fuel hydrocarbons	12	Oak Ridge(1), Rocky Flats(1), Pantex(1), Lawrence Livermore(1), Fernald(8)
Metals, radionuclides, ketones	12	Savannah River(1), Oak Ridge(3), Fernald(8)
Radionuclides, chlorinated hydrocarbons, ketones	12	Savannah River(1), Oak Ridge(3), Fernald(8)
Metals, anions, ketones	11	Savannah River(1), Oak Ridge(2), Fernald(8)
Metals, fuel hydrocarbons, ketones	11	Oak Ridge(2), Pinellas Plant(1), Fernald(8)
Anions, radionuclides, fuel hydrocarbons	11	Oak Ridge(1), Rocky Flats(1), Pantex(1), Fernald(8)
Anions, chlorinated hydrocarbons, ketones	11	Savannah River(1), Oak Ridge(2), Fernald(8)
Chlorinated hydrocarbons, fuel hydrocarbons, ketones	11	Oak Ridge(2), Pinellas Plant(1), Fernald(8)
Anions, radionuclides, ketones	10	Savannah River(1), Oak Ridge(1), Fernald(8)
Anions, chlorinated hydrocarbons, fuel hydrocarbons	10	Oak Ridge(1), Rocky Flats(1), Fernald(8)
Radionuclides, fuel hydrocarbons, ketones	10	Oak Ridge(2), Fernald(8)
Anions, fuel hydrocarbons, ketones	9	Oak Ridge(1), Fernald(8)
Metals, anions, pesticides	4	Savannah River(4)
Metals, radionuclides, pesticides	4	Savannah River(4)
Metals, chlorinated hydrocarbons, pesticides	4	Savannah River(4)
Anions, radionuclides, pesticides	4	Savannah River(4)
Anions, chlorinated hydrocarbons, pesticides	4	Savannah River(4)
Radionuclides, chlorinated hydrocarbons, pesticides	4	Savannah River(4)
Metals, anions, phthalates	3	Savannah River(1), Oak Ridge(2)
Metals, anions, explosives	3	Pantex(2), Lawrence Livermore(1)
Metals, chlorinated hydrocarbons, phthalates	3	Savannah River(1), Oak Ridge(2)
Metals, phthalates, ketones	3	Savannah River(1), Oak Ridge(2)
Anions, phthalates, ketones	3	Savannah River(1), Oak Ridge(2)
Chlorinated hydrocarbons, phthalates, ketones	3	Savannah River(1), Oak Ridge(2)

[1] Number of waste sites (out of 91) reporting specific class combination.

[2] Facility frequency of occurrence is the frequency at which a particular class combination appears at a particular DOE facility

Table C-7. Frequency of Occurrence at DOE Facilities of the Most Commonly Reported Combinations of Four Compound Classes in Ground Waters

Class Combinations	Number of Waste Sites[1]	Facility Frequency of Occurrence[2]
Metals, anions, radionuclides, chlorinated hydrocarbons	23	Savannah River(6), Oak Ridge(1), Hanford(3), Rocky Flats(1), Pantex(1), Fernald(8), INEL(1), Brookhaven(1), Argonne(1)
Metals, radionuclides, chlorinated hydrocarbons, fuel hydrocarbons	12	Oak Ridge(2), Rocky Flats(1), Fernald(8), INEL(1)
Metals, radionuclides, chlorinated hydrocarbons, ketones	12	Savannah River(1), Oak Ridge(3), Fernald(8)
Metals, anions, radionuclides, fuel hydrocarbons	11	Oak Ridge(1), Rocky Flats(1), Pantex(1), Fernald(8)
Metals, anions, chlorinated hydrocarbons, ketones	11	Savannah River(1), Oak Ridge(2), Fernald(8)
Metals, chlorinated hydrocarbons, fuel hydrocarbons, ketones	11	Oak Ridge(2), Pinellas Plant(1), Fernald(8)
Metals, anions, radionuclides, ketones	10	Savannah River(1), Oak Ridge(1), Fernald(8)
Metals, anions, chlorinated hydrocarbons, fuel hydrocarbons	10	Oak Ridge(1), Rocky Flats(1), Fernald(8)
Metals, radionuclides, fuel hydrocarbons, ketones	10	Oak Ridge(2), Fernald(8)
Anions, radionuclides, chlorinated hydrocarbons, fuel hydrocarbons	10	Oak Ridge(1), Rocky Flats(1), Fernald(8)
Anions, radionuclides, chlorinated hydrocarbons, ketones	10	Savannah River(1), Oak Ridge(1), Fernald(8)
Radionuclides, chlorinated hydrocarbons, fuel hydrocarbons, ketones	10	Oak Ridge(2), Fernald(8)
Metals, anions, fuel hydrocarbons, ketones	9	Oak Ridge(1), Fernald(8)
Anions, radionuclides, fuel hydrocarbons, ketones	9	Oak Ridge(1), Fernald(8)
Anions, chlorinated hydrocarbons, fuel hydrocarbons, ketones	9	Oak Ridge(1), Fernald(8)
Metals, anions, radionuclides, pesticides	4	Savannah River(4)
Metals, anions, chlorinated hydrocarbons,	4	Savannah River(4)
Metals, radionuclides, chlorinated hydrocarbons, pesticides	4	Savannah River(4)
Anions, radionuclides, chlorinated hydrocarbons, pesticides	4	Savannah River(4)
Metals, anions, chlorinated hydrocarbons, phthalates	3	Savannah River(1), Oak Ridge(2)
Metals, anions, phthalates, ketones	3	Savannah River(1), Oak Ridge(2)
Metals, chlorinated hydrocarbons, phthalates, ketones	3	Savannah River(1), Oak Ridge(2)
Anions, chlorinated hydrocarbons, phthalates, ketones	3	Savannah River(1), Oak Ridge(2)

[1] Number of waste sites (out of 91) reporting specific class combination.

[2] Facility frequency of occurrence is the frequency at which a particular class combination appears at a particular DOE facility.

Table C-8. Frequency of Occurrence at DOE Facilities of the Most Commonly Reported Combinations of Five Compound Classes in Ground Waters

Class Combinations	Number of Waste Sites[1]	Facility Frequency of Occurrence[2]
Metals, anions, radionuclides, chlorinated hydrocarbons, fuel hydrocarbons	10	Oak Ridge(1), Rocky Flats(1), Fernald(8)
Metals, anions, radionuclides, chlorinated hydrocarbons, ketones	10	Savannah River(1), Oak Ridge(1), Fernald(8)
Metals, radionuclides, chlorinated hydrocarbons, fuel hydrocarbons, ketones	10	Oak Ridge(2), Fernald(8)
Anions, radionuclides, chlorinated hydrocarbons, fuel hydrocarbons, ketones	9	Oak Ridge(1), Fernald(8)
Metals, anions, radionuclides, fuel hydrocarbons, ketones	9	Oak Ridge(1), Fernald(8)
Metals, anions, chlorinated hydrocarbons, fuel hydrocarbons, ketones	9	Oak Ridge(1), Fernald(8)
Metals, anions, radionuclides, chlorinated hydrocarbons, pesticides	4	Savannah River(4)
Metals, anions, chlorinated hydrocarbons, phthalates, ketones	3	Savannah River(1), Oak Ridge(2)

[1] Number of waste sites (out of 91) reporting specific class combination.

[2] Facility frequency of occurrence is the frequency at which a particular class combination appears at a particular DOE facility.

Appendix D

Specific Chemicals Identified

The table in this appendix is a tabulation of the specific inorganic and organic chemicals identified and chemical measurements made in ground waters and soils/sediments on DOE lands.

Table D-1. Chemicals Quantified or Chemical Measurements Made in Ground Waters and Soils/Sediments at DOE Facilities

Class/Constituent	Ground Water	Soils/Sediments
Chlorinated Hydrocarbons		
Dichloromethane	X	X
Chloroform	X	X
Carbon tetrachloride	X	X
Freon	X	X
1,1-Dichloroethane	X	X
1,2-Dichloroethane	X	X
1,1,1-Trichloroethane	X	X
1,1,2-Trichloroethane	X	-
1,1,1,2-Tetrachloroethane	X	-
1,1,2,2-Tetrachloroethane	X	X
Vinyl chloride	X	X
1,1-Dichloroethylene	X	X
1,2-Dichloroethylene	X	X
Trichloroethylene	X	X
Tetrachloroethylene	X	X
Chlorobenzene	X	X
1,2-Dichloropropane	X	-
1,3-Dichloropropane	X	-
1,2-Dichlorobenzene	X	-
2-Chloronaphthalene	-	X
Fuel Hydrocarbons		
Pentane	X	-
Hexane	-	X
Cyclohexane	X	X
Total hydrocarbons	X	X
Aliphatic hydrocarbons	X	X
Benzene	X	X
Toluene	X	X
Xylenes	X	X
BTX	X	-
BTEX	X	X
Ethylbenzene	X	X
Naphthalene	X	X
2-Methylnaphthalene	-	X
Phenanthrene	-	X
Anthracene	-	X
Acenaphthalene	-	X
Fluoranthene	-	X
Pyrene	-	X
Benzo(a)pyrene	-	X
Chrysene	X	X
Benzo(a)anthracene	X	X
Benzo(b)fluoranthene	-	X
Benzo(g,h,i)perylene	-	X
Benzo(k)fluoranthene	-	X
Indeno(1,2,3,c,d)pyrene	-	X
Plasticizers		
Bis(2-ethylhexyl)phthalate	X	X
Di-n-octylphthalate	X	X
Di-n-butylphthalate	X	X
Butylbenzylphthalate	X	X
Diethylphthalate	X	X
Polychlorinated Biphenyls		
Total PCB	X	X
Arochlor 1016	X	X
Arochlor 1242	X	X
Arochlor 1248	-	X
Arochlor 1254	X	X
Arochlor 1260	X	X
Ketones		
Methyl ethyl ketone	X	X
Methyl isobutyl ketone	X	X
Trimethylbicycloheptanone	X	-
Triethylbicycloheptanone	X	-
Acetone	X	X
2-Pentanone	-	X
2-Hexanone	-	X
Pesticides		
Heptachlor epoxide	X	-
Endosulfan 1	X	X
Endosulfan 2	-	X
Chlordane	X	X
Lindane	X	-
Methoxychlor	X	-
Toxaphene	X	-
2,4-Dichlorophenoxyacetic acid (2,4-D)	X	-
Fenthion	X	-
Endrin	-	X
Aldrin	X	X
Benzenehexachloride	X	X
Heptachlor	X	-
Dicamba	-	X
4,4'-DDT	X	X
Ethyl parathion	-	X
Methyl parathion	-	X
Malathion	-	X
Heptachlor	-	X
Dieldrin	-	X
Explosives		
RDX	X	X
HMX	X	X
Trinitrotoluene	-	X
PETN	X	X
Phenols		
2,4,5-Trichlorophenol	X	-
2,4-Dinitrophenol	X	-
2-Methylphenol	X	X
P-Chloro-m-cresol	-	X
2,4-Dimethylphenol	-	X
Phenol	-	X
Anions		
Fluoride	X	X
Nitrate	X	X
Cyanide	X	X

Table D-1. Chemicals Quantified or Chemical Measurements Made in Ground Waters and Soils/Sediments at DOE Facilities (Continued)

Class/Constituent	Ground Water	Soils/Sediments
Metals		
Chromium	X	X
Lead	X	X
Mercury	X	X
Arsenic	X	X
Barium	X	X
Cadmium	X	X
Zinc	X	X
Nickel	X	X
Copper	X	X
Radionuclides		
Uranium (234,235,238)	X	X
Tritium	X	X
Strontium-90	X	X
Plutonium (238,239,240)	X	X
Cesium-137	X	X
Technetium-99	X	X
Thorium (228,230,232)	-	X
Cobalt-60	X	X
Iodine-129	X	-

Class/Constituent	Ground Water	Soils/Sediments
Miscellaneous Organics		
N-Nitrosodiphenylamine	X	-
Triethylsilanol	X	-
Trimethylsilanol	X	-
Acrylonitrile	X	-
Bromoform	X	-
Benzoic acid	X	-
Diacetone alcohol	X	-
3,3'-Dichlorobenzidine	X	-
Vinyl acetate	X	-
Acetonitrile	-	X
Isopropyl alcohol	X	X
2-Propylfuran	X	-
Tetrahydrofuran	X	X
Butanol	X	X
Carbon disulfide	X	X
4-Chlorophenyl-phenylether	-	X
Ethanol	-	X
2-Methyl-2-propanol	-	X
Dioxane	-	X

Example of Site-Specific Data

Introduction

This appendix uses the Hanford Site as an example to demonstrate the kinds of chemical processes used at DOE facilities. It describes (1) several of the major chemical processes used at Hanford for production and extraction of nuclear materials and (2) historical disposal inventories of terrestrial waste sites associated with specific chemical processing areas. The discussion shows—

- The origin of many of the chemical contaminants on DOE lands and how these chemical agents were used in the production of nuclear materials.
- The relationship between chemical processing activities and organic substances reportedly disposed of to the ground.

Although this example focuses on the Hanford Site, data exist to perform comparable assessments for Oak Ridge National Laboratory, Savannah River Plant, and other DOE facilities.

Background

In February 1943, the Hanford Site, in south central Washington State, was designated by the War Department as a site to be used for the production of plutonium to be used in the construction of the first atomic bombs. To perform this function and others added later, the site's 558 mi^2 (1,450 km^2) of semiarid terrain were divided into three operational areas comprising (1) reactors for making plutonium (100 Areas), (2) facilities for separating plutonium from the irradiated reactor fuel (200 East and West Areas), and (3) facilities for process development and fabrication of reactor fuel (300 Area) (Figure E-1).

After fabrication by such processes as coextrusion (in which enriched uranium was encased in aluminum or zirconium alloy), the fuel was transported to the 100 Areas, where it was placed in a reactor. In early years, irradiated fuel (uranium-238 with trace amounts of plutonium-239) was removed from the reactor, transported to the 200 East Area (B-Plant), and subjected to a process that used bismuth phosphate to separate the plutonium from uranium and other fission products. Beginning in 1951, the bismuth phosphate process was replaced by the REDOX process, and that process, in turn, was replaced by the Plutonium Uranium Extraction (PUREX) process in 1956. The PUREX process is still used in fuels processing at Hanford. Other processes were used in the recovery of valuable radioactive elements. For example, at Z-Plant (in the 200 West Area), a process called "recouplex" was used to recover purified plutonium nitrate solutions from plutonium scrap materials. By replacing certain organic solvent components, americium could be recovered in the same process. The specifics of these processes are discussed below.

Fuel Fabrication and Separations Process Development (300 Area)

Since 1943, activities in the 300 Area have included the fabrication of reactor fuel and the pilot-scale evaluation of separations processes before their full-scale application in the 200 Area processing plants. For over four decades, liquid wastes (specifically, chemically and radiologically contaminated waste waters) associated with these activities were discharged to ponds, trenches, and cribs located within the area, by means of an intricate system of sewer lines linking facilities to the waste disposal areas.

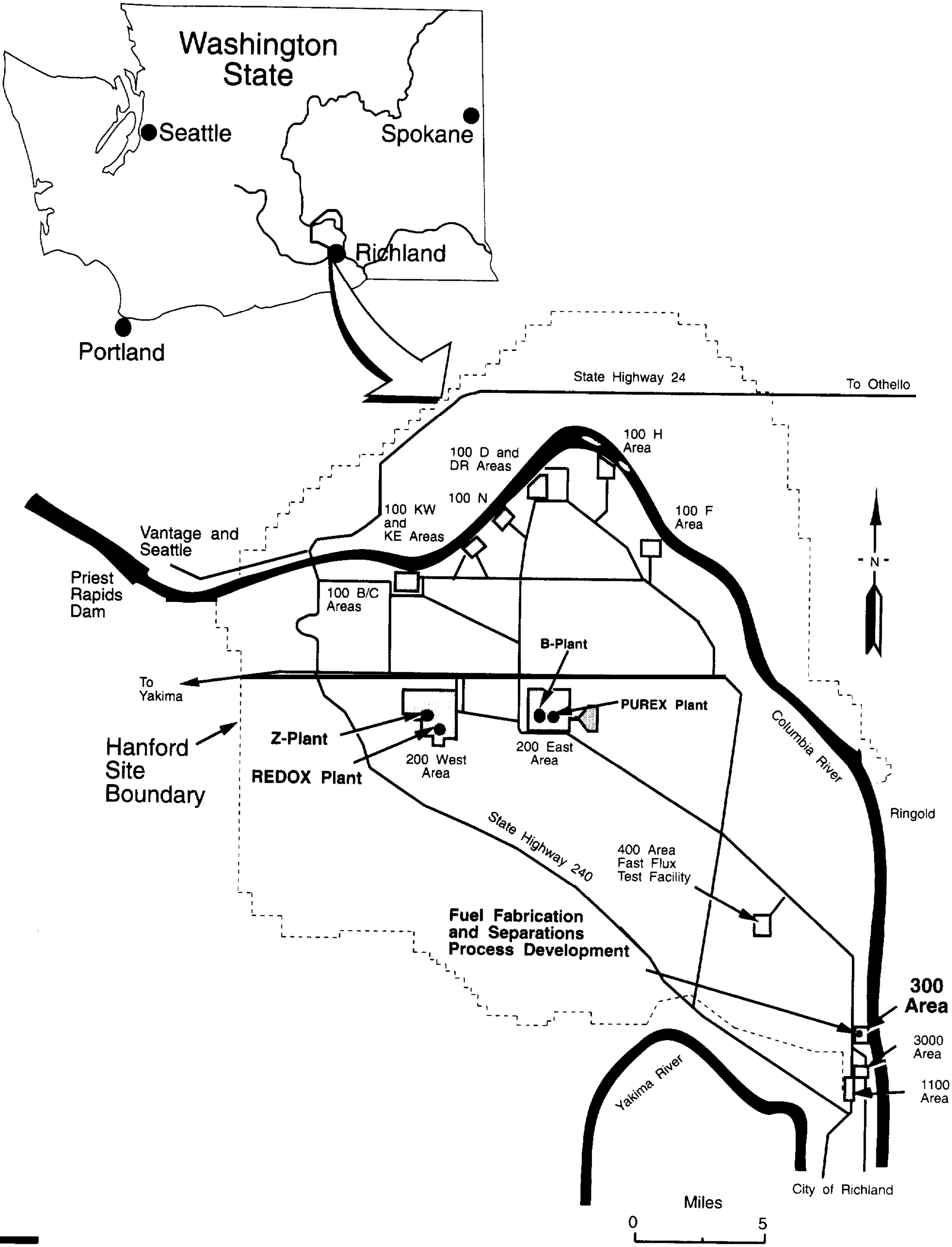

Figure E-1. Location of Fuel Fabrication and Processing Areas at Hanford

Fuel fabrication consisted of a coextrusion process and treatment of pellets to form completed fuel elements. In one version of the process, primary materials (e.g., zirconium and uranium-silicon) were protected with a copper jacket, and the jacket was lubricated prior to extrusion. Following extrusion into pellets, the lubricants were removed with organic solvents (e.g., trichloroethylene (TCE) and perchloroethylene (PCE)), and the copper jacket was removed by dissolution in nitric acid. Next, chemical milling was performed using copper sulfate, nitric acid, and sulfuric acid. Then, a zirconium end cap was brazed onto the ends of the pellets, and beryllium formed the completed fuel element. Completed fuel elements were heat treated, etched with solutions containing oxalic acid (for instance) to remove scale, and steam-autoclaved to test for perforations. Fuel elements occasionally ruptured during this activity, requiring that the autoclave be decontaminated with solutions containing ammonium citrate and disodium dihydrogen ethylenediaminetetraacetate dihydrate (EDTA). The solvents that were routinely used in decreasing (TCE and PCE) and drying (methanol) were stored in aboveground tanks and piped to various buildings.

A pilot plant built in the 300 Area in 1944 and operated until the middle of 1954 was used for the development of the bismuth phosphate, REDOX, and PUREX processes. Nitric acid solutions containing uranyl nitrate and small amounts of thorium nitrate (to simulate plutonium) were routinely processed, using such solvents as methyl isobutyl ketone (hexone).

Fuel Processing

The 200 Areas, located near the middle of the Hanford Site, were dedicated to chemical separations and waste management activities, including processing of irradiated fuel and waste storage.

Bismuth Phosphate Process (B-Plant, 200 East Area) The bismuth-phosphate process separated plutonium from uranium and fission products by precipitating the plutonium. The process involved (1) removal of the aluminum jacket (by dissolution in sodium hydroxide-sodium nitrate solution), (2) dissolution of the fuel element in nitric acid, (3) uranium complexation (by addition of sulfuric acid), (4) adjustment of the plutonium oxidation state using sodium nitrite, and (5) addition of bismuth phosphate to the solution to precipitate a solid cake containing the plutonium. The plutonium precipitate was further purified through a series of dissolution/precipitation reactions using selected oxidizing (sodium bismuthate and sodium dichromate) and reducing (sodium nitrite and oxalic acid) agents. The purified cake was then subjected to other treatments (transfer to a lanthanum fluoride carrier, subsequent solubilization, ammonium sulfate reduction, peroxide precipitation, and dissolution) and final concentration as a plutonium nitrate solution.

Recouplex Process (Z-Plant, 200 West Area) The recouplex process was used at the Z-Plant from 1955 to 1962 to recover plutonium from scrap materials and to produce a purified plutonium nitrate solution. The plutonium scrap was dissolved in a solution of nitric and hydrofluoric acids and subsequently extracted with a mixture of tributylphosphate and carbon tetrachloride to recover purified plutonium nitrate. Aluminum nitrate was added to the aqueous solution to provide extraction selectivity (for plutonium) and eliminate interference from fluoride ions during extraction. Americium was recovered in the same process by replacing the tributylphosphate with dibutylbutylphosphonate.

REDOX Process (REDOX Plant, 200 West Area) The REDOX process was used to separate uranium and plutonium from fission products and from each other. Cladding was removed from fuel elements using a solution of sodium hydroxide and sodium nitrate. The declad fuel elements were dissolved in nitric acid, and sodium dichromate was added to oxidize the plutonium to a state suitable for extraction by organic solvent. Aluminum nitrate was also added as a salting agent to facilitate uranium and plutonium extraction by the organic solvent (methyl isobutyl ketone). A second extraction, using an aqueous solution that contained a reducing agent, separated the uranium from the plutonium (which was driven to aqueous phase). Each liquid stream was processed further to produce concentrated products (e.g., uranylnitratehexahydrate and plutonium nitrate).

PUREX Process (PUREX Plant, 200 East Area) In the PUREX process, uranium, plutonium, and neptunium were separated from other fission products through a series of steps involving decladding of the fuel element, dissolution of uranium metal, solvent extraction, and ion exchange. A solution of ammonium nitrate/ammonium fluoride was used to remove the zirconium cladding from fuel elements. The declad fuel elements were dissolved in nitric acid and subjected to extraction using a 30 percent solution of tributylphosphate in normal paraffin hydrocarbon (kerosene). Subsequent extraction, partitioning, recycling, backcycling, and ion exchange steps resulted in individual liquid streams that were concentrated in plutonium nitrate, uranylnitratehexahydrate, and neptunium.

Assessment

Throughout the more than 40 years of Hanford Site operations, fuel fabrication, fuel process development, and processing facilities have generated large quantities of waste effluents that were disposed of to the ground in the 200 and 300 Areas. Effluent volumes have been substantial. For example, during their time in service (1949-1974 and 1943-1975, respectively), the 300 Area North and South Process Ponds received a combined volume of 30 billion liters of liquid effluent consisting of low-level and organic wastes.

Table E-1 describes the types and estimated quantities of organic chemicals that were disposed of at selected waste sites associated with the specific processing activities. The table documents the disposal of thousands of metric tons of chemicals used as (1) extractants (e.g., paraffinic hydrocarbons, carbon tetrachloride, methyl isobutyl ketone, alkyl phosphates), (2) degreasers (e.g., trichloroethylene and tetrachloroethylene), and (3) purification and decontamination agents (e.g., oxalate, citrate, and EDTA). The complexity of some of these wastes was increased by the codisposal of "fab oil" (a mixture of 50 percent carbon tetrachloride and 50 percent lard oil that was used as a cutting oil during the machining of plutonium).

Some of the compounds listed in Table E- I (e.g., chlorinated hydrocarbons and fuel hydrocarbons) have been selectively measured (or at least looked for) in soils/sediments and ground water at the Hanford waste sites (and others across the DOE complex) based on the need to satisfy regulatory compliance issues associated with continued operation or restoration of these waste sites. In contrast, however, actual subsurface concentrations of other chemical compound classes (e.g., chelating agents, organic acids, and alkyl phosphates) and their associated degradation products remain virtually unknown, despite historical records indicating that large quantities of these materials have been disposed of to the ground at Hanford (and perhaps at other major facilities in the DOE complex). The absence of such data for chelating agents. organic acid complexing agents, and alkyl phosphates may be the result of several factors including the following: (1) they are unregulated chemicals and are not routinely measured as part of environmental compliance programs at DOE facilities, and (2) analytical sampling and measurement methodologies may be inadequate to accurately measure, monitor, or even detect these constituents in the environment.

Table E-1. Chemical Processing Agents Reportedly Disposed of in Various Hanford Waste Sites

Process	Waste Site	Chemical (quantity in kg)
Fabrication/Process Development, Bismuth-Phosphate, REDOX, PUREX Processes	300 Area: North/South Process Ponds	Citric acid salts, EDTA salts, oxalic acid salts, methyl isobutyl ketone, trichloroethylene (200,000), carbon tetrachloride, tetrachloroethylene
	North Crib (316-14)	Methyl isobutyl ketone (3,000)
Fuel Processing, PUREX Process	200 East Area: 216-A-2 Crib	Tributylphosphate (70,000), paraffin hydrocarbons (120,000)
	216-A-7 Crib	Tributylphosphate (100,000), paraffin hydrocarbons (180,000)
	216-A-24 Crib	Butylphosphates (90,000), paraffin hydrocarbons (30,000)
Fuel Processing, Bismuth-Phosphate Process	200 East Area: 216-B-5 Reverse Well	Oxalate (12,000)
	216-B-7A/7B Cribs	Oxalate (60,000)
	216-B-8 Crib	Oxalate (6,000)
Fuel Processing, Recouplex Process	200 West Area: 216-Z-1 Tile Field	80 vol% carbon tetrachloride, 20 vol% tributylphosphate (4,400 gal/yr for 5 years); 70 vol% carbon tetrachloride, 30 vol% dibutylbutylphosphonate (6,600 gal/yr for 5 years)[1]
	216-Z-9 Crib	15 to 25% tributylphosphate in carbon tetrachloride, dibutylbutylphosphonate, trace amounts of monobutyl phosphate (109,000); 50% carbon tetrachloride, 50% lard oil (54,000)[2]
	216-Z-18 Crib	Tributylphosphate (22,000), dibutylbutylphosphonate (15,000), carbon tetrachloride (260,000)
Fuel Processing, REDOX Process	200 West Area: 216-S-13 Crib	Methyl isobutyl ketone (10,000)

[1] The 5-year period was from 1964 to 1969.

[2] The quantities in parentheses represent the quantities of organics, as these mixtures, estimated to have been released to the crib.