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Compilation of Data to Estimate Groundwater Migration Potential for Constituents in Active Liquid Discharges at the Hanford Site

L. L. Ames
R. J. Serne

March 1991

Prepared for the U.S. Department of Energy
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Pacific Northwest Laboratory
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EXECUTIVE SUMMARY

A preliminary characterization of the constituents present in the 33 liquid waste streams at the U.S. Department of Energy's Hanford Site has been completed by Westinghouse Hanford Company. In addition, Westinghouse Hanford has summarized the soil characteristics based on drill logs collected at each site that receives these liquid wastes. Literature searches were conducted and available Hanford-specific data were tabulated and reviewed. General literature on organic chemicals present in the liquid waste streams was also reviewed. Specifically, values for water solubility, soil adsorption, sediment organic carbon adsorption properties, octanol-water partition coefficients ($K_{O/W}$), Henry's Law constants (a measure of volatility), and biodegradation half-lives were gleaned from the literature to allow estimates of migration potential. Using all of this information, Pacific Northwest Laboratory has developed a best estimate of the transport characteristics (water solubility and soil adsorption properties) for those radionuclides and inorganic and organic chemicals identified in the various waste streams.

We assume that the potential for transport is qualified through the four geochemical parameters: solubility, distribution coefficient, persistence (radiogenic or biochemical half-life), and volatility. Summary tables of these parameters are presented for more than 50 inorganic and radioactive species and more than 50 organic compounds identified in the liquid waste streams. Brief descriptions of the chemical characteristics of Hanford sediments, solubility, and adsorption processes, and of how geochemical parameters are used to estimate migration in groundwater-sediment environments are also presented. Groundwater monitoring data are tabulated for wells neighboring the facilities that receive the liquid wastes.

The radioactive and organic constituents measured in groundwaters can be used to infer actual migration potentials for comparison with the literature assessments. In general the comparison is good. Compounds that appear to be mobile include methylene chloride, chloroform, bis(2-ethylhexyl) phthalate, acetone, methyl ethyl ketone, tetrachloroethylene, ^{129}I , ^{60}Co , ^{106}Ru , ^{99}Tc , ^3H , ^{137}Cs , and ^{90}Sr . Bis(2-ethylhexyl) phthalate, ^{137}Cs , and ^{90}Sr are not expected (based on their adsorption properties) to be mobile, but all of the

other species identified are expected to be mobile. The report recommends data collection activity to gather important data on the solubility, adsorption, and degradation properties of the potentially mobile species identified.

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1.0 INTRODUCTION

Operating facilities at the Hanford Site in Washington State have historically discharged large quantities of liquid effluent, the bulk of which did not routinely contain radioactive materials, into the sediments. Because the radionuclide contents of the waste streams were generally low, this technique of disposal was chosen after consideration of the sediment column's cation exchange capacity characteristics, unsaturated sediment column depth, and groundwater migration rates.

The U.S. Department of Energy, Richland Operations Office (DOE-RL) established a policy in 1984 to eliminate discharges of contaminated liquid to the sediment column and to meet all applicable federal and state environmental regulations. A plan and schedule were prepared in response to a request by Congress for discontinuation of the disposal of contaminated solutions into the sediment column.

At the request of the Washington State Department of Ecology (Ecology) and the U.S. Environmental Protection Agency (EPA), DOE-RL has initiated a study by its contractors, Westinghouse Hanford Company and Pacific Northwest Laboratory (PNL),^(a) of the characteristics of liquid discharges at the Hanford Site. This report addresses in some detail the 33 waste streams identified in the Waste Stream Characterization Report (Westinghouse Hanford 1989) to provide a best estimate of the waste stream constituents' potential for migration. In this report, the potential for transport is assumed to be quantified by three geochemical parameters: water solubility, adsorption distribution coefficient, and persistence (radiogenic or biochemical half-life). The 33 waste streams and their respective disposal units are listed in Table 1. Seven of the waste streams go to the same facility (216-B-3 pond system), and three go to double-shell tanks for interim storage.

(a) PNL is operated for DOE by Battelle Memorial Institute.

TABLE 1. The 33 Liquid Effluent Streams and the Facilities Receiving the Streams (Westinghouse Hanford 1989)

<u>Effluent Stream</u>	<u>Receiving (Disposal) Facility^(a)</u>
B Plant process condensate	Double-shell tanks ^(b)
PUREX Plant ammonia scrubber condensate	Double-shell tanks ^(c)
241-AY, 241-AZ steam condensate	Double-shell tanks ^(d)
N Reactor effluent	1325-N crib
PUREX Plant process condensate	216-A-45 crib
UO ₂ Plant process condensate	216-U-17 crib
Plutonium Finishing Plant wastewater	216-Z-20 crib
PUREX Plant chemical sewer	216-A-29 ditch/216-B-3 pond
B Plant chemical sewer	216-B-83 trench
222-S Laboratory wastewater	216-S-26 crib
2101-M Laboratory wastewater	2101-M pond ^(e)
209-E Laboratory wastewater	216-C-7 crib
T Plant wastewater	216-T-4-2 ditch
300 Area process wastewater	300 Area process trenches ^(e)
103-D Filter backflush wastewater	100-D ponds ^(e)
B Plant steam condensate	216-B-55 crib
PUREX Plant steam condensate	216-A-30/216-A-37 cribs
S Plant wastewater	216-S-10 ditch/pond
242-A Evaporator steam condensate	216-B-3 pond system ^(e)
242-A Evaporator process condensate	216-A-37-1 crib ^(f)
2724-W Laundry wastewater	216-W-LWC crib
103-N Demineralized wastewater	1324-N/NA pond ^(e)
UO ₂ Plant wastewater	216-Y-14 ditch
B Plant cooling water	216-B-3 pond system ^(e)
PUREX Plant cooling water	216-B-3 pond system ^(e)
T Plant laboratory wastewater	216-T-1 ditch
241-A Tank Farm cooling water	216-B-3 pond system ^(e)
242-A Evaporator cooling water	216-B-3 pond system ^(e)
242-S Evaporator steam condensate	216-U-14 ditch
244-AR Vault cooling water	216-B-3 pond system ^(e)
284-E Powerplant cooling water	216-B-3 pond system ^(e)
284-W Powerplant cooling water	200-W Powerhouse pond
400 Area secondary cooling water ^(g)	400 Area pond

(a) Disposition as of September 1989.

(b) Discharged to 216-B-82 crib until January 1988. Currently discharged to double-shell tanks; will be rerouted to 216-B-82.

(c) Discharged to 216-A-36-B crib unit September 1987. Currently discharged to double-shell tanks.

(d) Discharged to 216-A-8 crib until 1983. Currently discharged to double-shell tanks. Resumption of discharge to 216-A-8 is pending review by Westinghouse Hanford and approval by DOE-RL.

(e) Resource Conservation and Recovery Act of 1976 (RCRA) disposal unit.

(f) Current discharge has been suspended; studies are under way to identify a future disposal site.

(g) 400 Area secondary cooling water is not related to Fast Flux Test Facility reactor heat removal.

2.0 DESCRIPTION OF WASTE STREAMS

The waste streams contain dissolved inorganics, organics, and radionuclides, as well as suspended solids. Because the chemical composition of the waste streams (e.g., the pH and types and amounts of dissolved salts) influences the solubility and adsorption properties of radionuclides and regulated chemicals, a discussion of the overall chemical nature of the waste streams is provided here. Each of these constituents will be discussed for the 33 streams for which data are available. The waste stream samples used for chemical analyses were collected over short time intervals and therefore may not be representative of overall chemical compositions for the life of the waste stream. The same can be said for the stream volumes given in this report, because the waste stream volumes were taken over a short time interval and the streams often fluctuate widely in volume.

2.1 CONSTITUENTS

2.1.1 Inorganics

A total of 33 inorganic constituents make up the bulk of the inorganic materials (not including radionuclides) that have been measured in the waste streams. These are listed in Table 2 in terms of analytical reporting frequency, N. Uranium, which is classifiable as either a radionuclide or a heavy metal, was the most frequently reported analyte, followed by sodium, calcium, and potassium. Magnesium and zinc are also commonly reported in these chemical analyses.

Average inorganic chemical analyses have been published for each waste stream (Westinghouse Hanford 1989). The averaged analyses were used to determine total waste stream inorganic content, by converting the average cation concentration to molarities and summing them. This treatment assumes that anions are present to maintain an electrostatic balance, but it is not a material-balancing procedure. Using the inorganic cation analysis averages presented by Westinghouse Hanford (1989) often conceals the considerable range in the individual analyses making up the average. For example, the analytical sodium content of B Plant chemical sewage varies from 4 to 6,000 mg/L for

TABLE 2. Inorganic Analyte Reporting Frequency (N) for the Waste Stream Analyses (Westinghouse Hanford 1989)

<u>Analyte</u>	<u>N</u>	<u>Analyte</u>	<u>N</u>
Uranium	314	Mercury	97
Sodium	310	Silicon	74
Calcium	307	Lead	61
Potassium	300	Nickel	43
Zinc	285	Cadmium	39
Magnesium	281	Chromium	38
Sulfate	277	Vanadium	33
Barium	265	Phosphate	24
Chloride	250	Sulfide	16
Iron	227	Beryllium	5
Fluoride	178	Silver	4
Manganese	171	Lithium	2
Copper	155	Arsenic	1
Nitrate	146	Antimony	1
Strontium	136	Tin	1
Aluminum	128	Titanium	1
Ammonium	124		

individual analyses. It is doubtful that the sampling period was long enough or the number of individual analyses large enough to obtain a representative sample average.

Of more interest to determining environmental fate is the total waste stream content of inorganics, as shown in Table 3. For comparison, the analyte contents of Hanford groundwater and Columbia River waters range from 7×10^{-3} to 1×10^{-3} M. Most of the waste streams are more dilute than these natural waters. The wastewaters from power plants were among the highest in total dissolved inorganics. Only three of the waste streams show average field pH values less than pH 6.0, and even these three have pH values at or above 5.2. The overall inorganic analyte discharge rates (kg/mo) are given in Table 4. The amounts of Ca, Mg, SO_4 , HCO_3 , K, and NH_4 discharged each month exceed or approach 5,000 kg, and NO_3 exceeds five times that amount. There are several known inorganic carcinogens and/or toxic substances in this list, including beryllium, cadmium, lead, silver, and mercury. The allowable limits for these constituents have been given by Ecology (1987). If these toxic metals were homogeneously distributed in the water discharged each month, concentrations would be below the maximum permissible limits and in the range 0.01 to 3 $\mu\text{g/L}$, depending on the metal. The chemical analyses do not, however, indicate how these metals are distributed or their forms in the wastes.

2.1.2 Organics

There are 51 organic constituents that were identified at least twice in analyses of the 33 waste streams. These are listed with their frequencies in Table 5. These 51 organic constituents are classified by structure group in Appendix A. Along with the structure, the data pertaining to soil sorption, solubility, and volatility are given for most of the organic constituents. Chloroform was the most prevalent organic analyte, even though it is not used in any of the chemical processes at the Hanford Site (Jungfleisch 1988). The chlorination of natural waters has been shown to commonly produce chloroform as well as other halogenated hydrocarbons (Dowty et al. 1975; Rook 1977; Larson and Rockwell 1979; Norwood et al. 1980). Chloroform and the phthalates

TABLE 3. Waste Stream Inorganic Analyte Content and Mean Field pH Based on Reported Data (Westinghouse Hanford 1989)

Waste Stream	Total Inorganics, M	Mean Field pH
N Reactor effluent	2.98×10^{-4}	7.8
163-N Demineralizer wastewater	1.27×10^{-2}	6.1
183-D Filter backflush wastewater	6.09×10^{-3}	6.3
PUREX Plant chemical sewer	5.74×10^{-3}	6.2
PUREX Plant process condensate	2.39×10^{-3}	6.6
PUREX Plant ammonia scrubber condensate	2.05×10^{-2}	9.3
PUREX Plant stream condensate	6.20×10^{-4}	6.1
PUREX Plant cooling water	8.29×10^{-4}	6.7
B Plant chemical sewer	1.07×10^{-1}	7.4
B Plant process condensate	1.57×10^{-4}	8.2
B Plant steam condensate	2.70×10^{-5}	6.3
B Plant cooling water	7.71×10^{-4}	6.8
Plutonium Finishing Plant wastewater	1.05×10^{-3}	6.4
S Plant wastewater	7.40×10^{-4}	6.6
T Plant headend wastewater	3.68×10^{-4}	6.8
T Plant wastewater	7.11×10^{-4}	6.3
UO ₃ Plant process condensate	1.58×10^{-1}	5.8
UO ₃ /U Plants wastewater	7.39×10^{-4}	6.6
241-A Tank Farm cooling water	8.65×10^{-4}	6.4
241-AY, 241-AZ Tank Farms steam condensate	3.99×10^{-5}	5.2
242-A Evaporator process condensate	2.09×10^{-2}	10.4
242-A Evaporator steam condensate	4.15×10^{-4}	6.1
242-A Evaporator cooling water	7.76×10^{-4}	6.2
242-S Evaporator steam condensate	7.71×10^{-4}	5.7
244-AR Vault cooling water	7.80×10^{-4}	6.8
209-E Laboratory reflector water	8.01×10^{-4}	7.3
222-S Laboratory wastewater	7.27×10^{-4}	6.3
2101-M Laboratory wastewater	5.71×10^{-4}	6.2
2724-W Laundry wastewater	6.55×10^{-3}	9.1
284-E Powerplant wastewater	5.43×10^{-1}	8.3
284-W Powerplant wastewater	1.52	8.2
300 Area process wastewater	8.93×10^{-4}	6.0
400 Area secondary cooling water	6.74×10^{-3}	8.0

TABLE 4. Discharge Rate of Principal Inorganic Analytes
(Jungfleisch 1988)

<u>Inorganic Analyte</u>	<u>Discharge Rate, kg/mo</u>
Aluminum sulfate	10,866
Ammonium nitrate	281.2
Ammonium bicarbonate	5,896.8
Ammonium hydroxide	4.128
Barium sulfate	140.6
Beryllium sulfate	95.26
Cadmium sulfate	0.313
Calcium nitrate	185,976
Calcium bicarbonate	15,422
Calcium sulfate	19,051
Sodium chromate	1.225
Copper sulfate	331.13
Ferrous sulfate	2,948.4
Lead sulfate	21.773
Magnesium nitrate	68,040
Magnesium bicarbonate	5,443.2
Manganese sulfate	226.8
Mercury sulfate	0.077
Nickel sulfate	0.907
Potassium sulfate	6,804.0
Silver sulfate	5.897
Sodium bicarbonate	4,399.9
Strontium chloride	3.992
Uranyl nitrate	11.34
Vanadyl sulfate	3.72
Zinc sulfate	263.09
Sodium chloride	5,896.8
Sodium cyanide	0.0953
Sodium fluoride	412.78
Sodium nitrate	771.12
Sodium phosphate monobasic	362.88
Sodium phosphate dibasic	1,088.6
Sodium bisulfide	385.56
Sodium sulfate	14,061

TABLE 5. Analytical Frequency (N) for the Organic Analytes
(Westinghouse Hanford 1989)

Organic Analyte	N	Organic Analyte	N
Chloroform	153	3,5-dimethylpyridine	3
Acetone	97	Ethyl alcohol	3
Butyl alcohol	44	Heptadecane	3
Tributyl phosphate	39	Hexadecane	3
Methyl ethyl ketone	35	Hexadecanoic acid	3
Tridecane	31	Methyl formate	3
2-butoxyethanol	30	Acetophenone	2
Tetradecane	30	Benzaldehyde	2
Tetrahydrofuran	26	Butoxydiglycol	2
Butoxyglycol	21	Butylbenzyl phthalate	2
Methyl-n-butyl ketone	19	Decane	2
Butyraldehyde	17	Di-n-butyl phthalate	2
Bis (2-ethylhexyl) phthalate	16	Dichlorofluoromethane	2
Benzyl alcohol	13	Dimethoxymethane	2
2-propanol	12	Dimethylnitrosoamine	2
MIBK (hexone)	11	Di-n-octyl phthalate	2
Dodecane	9	Methoxydiglycol	2
Methylene chloride	9	Methoxytriglycol	2
Methyl n-propyl ketone	8	2-methylnonane	2
Butyl nitrate	7	2-methyl-5-propylnonane	2
Methyl nitrate	6	Morpholine	2
Pentadecane	6	Pelargic acid	2
Phenol	6	Phenanthrene	2
N-methoxymethanamine	5	Tetrachloroethylene	2
Ethoxytriethylene glycol	4	Undecane	2
Benzoic acid	3		

are of concern because they are carcinogens (Ecology 1987). Table 6 lists those compounds designated as acutely and moderately toxic by Ecology that were identified in the 33 active waste streams.

The waste streams containing the highest concentrations of organic analytes are listed in Table 7. The PUREX Process Condensate stream contains the highest concentration of organics.

Discharge rates for several organic constituents within the 33 waste streams are shown in Table 8. Tributyl phosphate and aliphatic hydrocarbons were present in the largest quantities, and tetrachloroethylene and chloroform were also high in ranking.

In addition to the organic analyte content of the 33 waste streams that is listed in Table 5, there is a considerable volume of data on organic compounds found in groundwaters taken from wells associated with the waste stream disposal sites. For example, Table 9 gives the analytical data on three 200 West Area wellwater samples. A large amount of wellwater sample analytical data were reported by Westinghouse Hanford (1989) as being associated with the ground disposal of the 33 waste streams. These data show that little degradation or sediment sorption is occurring for many of the organic constituents of the waste. Many of the organics in effluent streams were used to extract uranium and plutonium from spent fuel. The origins, uses, and degradation sequences of the uranium and plutonium extractants, the solvents, and their degradation products are discussed in detail by Burr (1958), Lane (1960, 1963), Dennis and West (1961), Blake et al. (1963), Huggard and Warner (1963), Gaumann et al. (1972), and Nowak (1971).

Several characteristics of the organic compounds found in the waste streams relating to migration are given in detail, with references, in Appendix A.

TABLE 6. Classifications of Some Hazardous Chemicals Found in the 33 Waste Streams (Ecology 1987; Jungfleisch 1988)

<u>Persistent Substance</u>
Chloroform
Methylene chloride
Pentachlorophenol
<u>Positive Carcinogen</u>
Beryllium sulfate
Cadmium sulfate
Lead sulfate
Bis(2-ethylhexyl) phthalate
Chloroform
<u>Ignitable Substance</u>
Sodium bisulfide
Acetone
Benzyl alcohol
2-butoxyethanol
Butyl alcohol
Dodecane
Isopropyl alcohol (2-propanol)
Phenol
Pyridine
Tetradecane
Tetrahydrofuran
<u>Reactive Substance</u>
Sodium cyanide
Sodium bisulfide
<u>Toxic Contaminant</u>
Barium
Cadmium
Chromium
Lead
Mercury
Silver

TABLE 7. Waste Streams Containing the Largest Contents of Organic Analytes (Westinghouse Hanford 1989)

<u>Waste Stream</u>	<u>Total Organic Contents, ppb</u>
PUREX Plant process condensate	240,945
242-A Evaporator process condensate	24,757
2724-W Laundry wastewater	8,962
UO ₃ Plant process condensate	2,465
2101-M Laboratory wastewater	737
UO ₃ /U Plants wastewater	510
B Plant process condensate	485
Plutonium Finishing Plant wastewater	421
B Plant chemical sewer	195
241-AY, 241-AZ Tank Farms steam condensate	99

2.1.3 Radionuclides

The radioactivity within the 33 waste streams is wide-ranging, as seen in Table 10. The radionuclide occurrence frequency (N) is shown for the samples collected. The fission and activation products ⁹⁰Sr, ¹³⁷Cs, and ²³⁹Pu are the most prevalent, as might be expected. Most of the radioactivity is concentrated in four waste streams, as shown in Table 11. Although the N Reactor effluent (105-N cooling water and fuel basin water) contained more than half of the total radioactivity in the 33 waste streams, this waste stream no longer exists in the same volume because the N Reactor is not in operation, but rather in a cold-standby status (Millikin 1989).

2.2 WASTE STREAM VOLUME ESTIMATES

A best estimate of the volumes of the 33 waste streams is given in Table 12. The disposal sites for 163-N demineralized wastewater, the PUREX steam condensate, and the T Plant headend wastewater are listed by Westinghouse Hanford (1989) as being currently inactive. Therefore, the values in Table 12 for these streams are no longer valid.

TABLE 8. Daily Discharge of Organic Analytes Based on Analyses
and Effluent Volumes of the 33 Waste Streams
(Westinghouse Hanford 1989)

<u>Organic Analyte</u>	<u>Daily Discharge Amount, g</u>
Tributyl phosphate	13,977.750
Tridecane	8,676.711
Tetradecane	7,683.627
Dodecane	2,794.086
Pentadecane	303.900
Tetrachloroethylene	284.070
Chloroform	273.045
Bis(2-ethylhexyl) phthalate	159.174
Undecane	103.380
2-butoxyethanol	81.693
Butyl alcohol	69.693
Acetone	57.636
Hexadecane	48.494
Methyl nitrite	43.577
Dimethoxymethane	41.934
Heptadecane	38.466
Octadecane	33.420
Decane	33.359
Methyl formate	28.197
Phenol	24.870
N-methoxymethanamine	23.271
Di-n-butyl phthalate	22.630
Benzyl alcohol	16.071
Methylene chloride	15.427
Di-n-octyl phthalate	14.370
Benzoic acid	13.646
Methyl ethyl ketone	11.126
Butylbenzyl phthalate	9.895
2-methyl-5-propylnonane	9.615
Pelargic acid	4.688

TABLE 9. Organic Analytes Reported in Three 200 West Area Wellwater Samples

Organic Analyte	Concentration, ppb		
	Well 699-38-70	Well 699-35-78	Well 699-49-79
<u>Volatile Compounds</u>			
Carbon tetrachloride	5.95	--	--
Chloroform	13.56	0.33	81.90
Dichloromethane	2.94	1.15	0.29
Trichloroethylene	0.90	--	--
Cyclohexane	0.71	--	--
Methylcyclohexane	12.91	--	20.48
Toluene	9.51	--	--
2-butoxyethanol	11.33	--	--
2-ethyl-1-hexanol	2.56	--	--
<u>Solvent Extractable Compounds</u>			
Tri-n-butylphosphate (TBP)	3	--	--
Di-n-octyladipate	--	590	--
Bis(2-ethylhexyl) phthalate	2	--	2
Di-n-octylphthalate	--	8	--
Phthalates, mixed	--	140	10
<u>Chelating Agents</u>			
Ethylenediaminetetraacetic acid (EDTA)	≤0.1	--	≤0.1

TABLE 10. Frequency (N) of Radionuclides in the 33
Waste Streams (Westinghouse Hanford 1989)

<u>Radionuclide</u>	<u>N</u>	<u>Radionuclide</u>	<u>N</u>
Gross β	1,745	^{134}Xe	64
^{137}Cs	1,006	^{133}I	61
^{239}Pu	941	^{135}Xe	60
^{90}Sr	900	^{135}I	59
^3H	803	^{24}Na	53
Gross α	717	^{155}Eu	51
^{60}Co	509	^{85}Kr	46
^{54}Mn	464	^{88}Kr	41
^{144}Ce	321	^{56}Mn	40
Total U	279	^{138}Cs	40
^{95}Nb	254	^{239}Np	40
^{103}Ru	254	^{91}Sr	34
^{238}Pu	243	^{154}Eu	31
^{59}Fe	214	^{113}Sn	30
^{95}Zr	200	^{125}Sb	28
^{140}La	190	^{153}Sm	27
^{141}Ce	175	^{129}I	24
^{131}I	155	^{65}Zn	24
^{134}Cs	146	^{87}Kr	24
^{241}Pu	137	^{125}Sb	22
^{32}P	136	^{97}Zr	16
^{58}Co	130	^{234}U	13
^{99}Mo	130	^{235}U	13
^{89}Sr	121	^{238}U	13
^{140}Ba	118	$^{110\text{m}}\text{Ag}$	10
^{106}Ru	117	^{99}Tc	5
^{147}Pm	114	^{122}Sb	3
^{51}Cr	87	^{236}U	2
^{241}Am	84	^{41}Ar	1
^{132}I	80	Mixed fission products	1

TABLE 11. Waste Streams with the Bulk of the Total
Radioactivity in the 33 Waste Streams

<u>Waste Stream</u>	<u>Total Activity, Ci/yr</u>	<u>Percent of Total Activity</u>
N Reactor effluent (1976 - 1988)	2,400	54.00
PUREX Plant process condensate	1,500	35.00
242-A Evaporator cooling water	280	6.30
242-A Evaporator process condensate	<u>150</u>	<u>3.50</u>
Total	4,330	98.80

TABLE 12. Waste Stream Volume Estimates (from Stordeur and Flyckt 1988)

Effluent Stream	Volume, (a) millions of L/yr	Percent of Total Flow
PUREX Plant cooling water	7,800.00	33.39
242-A Evaporator cooling water	5,300.00	22.69
B Plant cooling water	2,800.00	11.99
300 Area process wastewater	1,900.00 (b)	8.13
241-A Tank Farm cooling water	880.00	3.73
PUREX Plant chemical sewer	840.00	3.60
N Reactor effluent (c)	760.00	3.25
163-N Demineralizer wastewater (c)	600.00	2.57
PUREX Plant steam condensate	590.00 (d)	2.53
B Plant chemical sewer	350.00	1.50
UO ₃ /U Plants wastewater	340.00	1.46
Plutonium Finishing Plant wastewater	200.00	0.86
S Plant wastewater	200.00	0.86
284-E Powerhouse cooling water	180.00 (b)	0.77
244-AR Vault cooling water	120.00	0.51
284-W Powerhouse cooling water	110.00 (b)	0.47
T Plant wastewater	72.00 (b)	0.31
2724-W Laundry wastewater	61.00	0.27
PUREX Plant process condensate	51.00	0.22
400 Area secondary cooling water	49.00 (b)	0.21
242-A Evaporator steam condensate	45.00	0.20
222-S Laboratory wastewater	34.00	0.15
PUREX Plant ammonia scrubber condensate	28.00	0.12
242-A Evaporator process condensate	25.00	0.11
242-S Evaporator steam condensate	14.00	0.06
B Plant steam condensate	4.20	0.02
B Plant process condensate	3.90 (d)	0.02
2101-M Laboratory wastewater	3.80 (b)	0.02
UO ₃ Plant process condensate	0.64	0.00
AY/AZ Tank Farm steam condensate	0.23 (e)	0.00
209-E Laboratory reflector water	NA (f)	
T Plant laboratory (or headend) wastewater	NA	
183-D Filter backflush wastewater	NA	
Total	23,336.18	100.00

(a) 1987 flow data (except as noted).

(b) Estimated.

(c) These have decreased as a result of the placement of N Reactor into cold-standby status.

(d) 1986 flow data used.

(e) 1985 flow data used.

(f) NA = Not available, minor contribution to total.

3.0 CHARACTERISTICS OF HANFORD SEDIMENTS

Cation exchange capacity (CEC) is one of the more important soil characteristics associated with determining the fate of constituents when liquid waste is disposed into sediments. The CEC values for Hanford Site sediments were given by McHenry (1957), Routson et al. (1981), and Delegard and Barney (1983) for the 200 Areas (process areas) and vicinity and by Bensen et al. (1963) for the 100 Areas (reactors). These CEC values are not necessarily comparable because the results are a function of how the CEC is measured, including the cation used to saturate the exchange sites and the one used to replace the adsorbed cation. More recent CEC particle size and carbon data for 200 Area (separations areas) and 100 Area (reactors) sediments are given in Table 13. The typical 200 Area sediment is high in sand content, with an average CEC of 4.3 meq/100 g and an average organic carbon (OC) content of slightly less than 0.10 wt%. The 100 Area sediments also have very low values for OC content. Total carbon, in the case of the 100 Area sediments, was determined by microcombustion and infrared analysis. Particle size analysis for the 200 Area soils was conducted using the technique of Gee and Bauder (1986), and total carbon was determined by dry combustion with the coulometric method of Huffman (1977). Inorganic carbon was determined by the same coulometric method after the samples had been digested for 10 min in 3 N HCl at 80°C to release all inorganic carbon. Both the total and the inorganic carbon procedures were calibrated with reagent-grade CaCO_3 . Organic carbon was obtained as the difference, if any, between the total carbon and the inorganic carbon.

The organic carbon content of the soil/sediment is important because neutral hydrophobic organic compounds (compounds having a water solubility of less than a few parts per million) have been shown to adsorb preferentially onto the organic carbon fraction of the soil (Lambert et al. 1965; Briggs 1973). Lambert et al. suggested that the role of organic matter in the sediment was similar to that of an organic solvent in solvent extraction and that the partitioning of a neutral organic compound between sediment organic matter and water should correlate well with its partitioning between water and an immiscible solvent. Briggs (1973) developed a regression equation relating

TABLE 13. Recent Sediment Data That Include Organic Carbon Values

Well Number	Depth, ft	Cation Exchange Capacity, meq/100 g	Wt%					
			TC(a)	IC(b)	OC(c)	Sand	Silt	Clay
299-E28-26	39-40	5.1	0.10	0.04	0.06	61.59	16.15	22.26
299-E28-26	129-130	4.2	0.39	0.18	0.21	93.82	4.40	1.78
299-E28-26	129-130	4.4	0.16	0.16	0.00	90.63	6.06	3.31
299-E28-26	294-295	1.6	0.04	0.04	0.00	85.66	11.00	3.34
299-E28-26	319-320	2.6	0.02	0.01	0.01	91.17	7.48	1.35
299-E33-30	39-40	3.6	0.13	0.11	0.02	70.37	20.33	9.31
299-E33-30	139-140	2.5	0.15	0.10	0.05	--	--	--
299-E34-2	49-50	4.7	0.22	0.11	0.11	63.63	26.37	10.00
299-E34-2	145-150	2.0	0.14	0.18	0.00	88.36	6.45	5.09
299-E34-2	230	4.2	0.09	0.03	0.06	66.45	14.65	18.89
299-E34-3	49-50	2.2	0.11	0.07	0.04	74.68	19.99	5.33
299-E34-3	119-120	3.5	0.26	0.14	0.12	93.79	4.83	1.38
299-E34-3	120	2.4	0.78	0.13	0.65	93.46	4.46	2.08
299-E34-3	164-165	2.9	0.13	0.08	0.05	68.87	27.29	3.85
299-E34-3	210	2.9	0.03	0.04	0.00	74.29	16.96	8.76
299-W7-2	64-65	6.0	0.48	0.73	0.00	--	--	--
299-W7-2	94-95	2.3	0.13	0.13	0.00	88.28	9.32	2.40
299-W7-2	155	2.2	0.04	0.01	0.03	--	--	--
299-W7-2	220	3.6	0.15	0.15	0.00	78.92	16.51	4.58
299-W7-3	450	3.2	0.02	0.01	0.01	87.24	9.25	3.52
299-W7-5	10	6.9	0.32	0.20	0.12	--	--	--
299-W10-13	45	2.9	0.27	0.19	0.08	--	--	--
299-W10-13	115	4.1	0.28	0.26	0.02	--	--	--
299-W10-13	160	1.5	0.42	0.04	0.38	--	--	--
299-W10-13	160	1.8	0.07	0.04	0.03	--	--	--
299-W10-13	200	3.2	0.03	0.01	0.02	73.67	12.80	13.53
299-W10-13	240	6.2	0.01	0.00	0.01	78.38	11.00	10.63
299-W10-14	440	6.2	0.05	0.03	0.02	--	--	--
299-W15-16	40	9.0	0.24	0.14	0.10	--	--	--
299-W15-16	110	5.3	0.17	0.17	0.00	74.30	12.10	13.60
299-W15-16	149-150	8.5	2.75	2.58	0.18	--	--	--
299-W15-16	225	4.0	0.02	0.10	0.01	--	--	--
299-W15-17	425	6.1	1.07	0.16	0.91	--	--	--
299-W15-17	425	4.9	0.13	0.10	0.03	--	--	--
299-W18-21	40	5.3	0.17	0.18	0.00	--	--	--
299-W18-21	40	5.9	0.67	0.16	0.51	--	--	--
299-W18-21	94-95	3.3	0.25	0.28	0.00	--	--	--
299-W18-21	139-140	5.3	0.48	0.44	0.04	--	--	--
299-W18-21	210	8.1	0.02	0.00	0.02	--	--	--
299-W18-22	429-431	6.2	0.09	0.05	0.04	73.43	15.73	10.85

(a) TC = total carbon, TC = IC + OC.

(b) IC = inorganic carbon.

(c) OC = organic carbon.

soil/sediment sorption of phenyl urea herbicides to their octanol-water partition coefficient, $K_{O/W}$. Karickhoff et al. (1979) then used this concept to determine sorption isotherms for 10 hydrophobic organic compounds on natural sediments.

The adsorption data for all of the organic compounds fit well, over a broad range of water phase concentrations, to linear isotherms where $X = K_p C$. The variable X is the concentration of sorbate (ppb) on the sediment relative to the sediment's dry weight, C is the equilibrium solution sorbate concentration (ppb), and K_p is the partition coefficient (unitless). When adsorption depends on only organic carbon, $K_{OC} = K_p / f_{OC}$. The f_{OC} is the fractional mass of organic carbon in the sediment, and K_{OC} is a normalized partition coefficient. When the $\log K_{O/W}$ (octanol-water partition coefficient) is plotted versus the $\log K_{OC}$ or $\log S$ (water solubility expressed as a mole fraction), relationships such as $\log K_{OC} = 1.00 \log K_{O/W} - 0.21$ and $\log K_{OC} = -0.54 \log S + 0.44$ were obtained. The covariation of K_{OC} and $K_{O/W}$ were linear, but K_{OC} varies nonlinearly with S .

These relationships would be very useful as they make it possible for the hydrophobic organic compound distribution coefficients to be easily computed from available data, except for one circumstance. As can be seen from Table 12, Hanford sediments are relatively low in organic carbon content, averaging slightly less than 0.1 wt%. Hanford sediments often contain no organic carbon at all. According to Means et al. (1982), the reliability of predictive equations is impaired for substrates with very low carbon contents, such as the Hanford sediments. Means et al. found that correlations between K_{OC} and K_p were erratic for sediments that contain less than 1.0 wt% organic carbon content, as do Hanford sediments. Hence, application of generic hydrophobic organics-water-sediment relationships to Hanford sediments cannot be justified, except as a means of roughly estimating Hanford sediment reactions with organic analytes.

Hydrophilic compounds, by definition, prefer an aqueous environment and minimal sediment sorption can be expected. Some organic compounds can dissociate, such as the benzoic or hexadecanoic acids reported in Table 5. These ionized compounds are theoretically able to adsorb on the sediment as an exchangeable cation or anion under the appropriate conditions. However,

benzoic acid is not known to sorb on sediments (see Appendix A) and little is known about the sorption properties of the other dissociating compounds shown in Table 5.

4.0 SEDIMENT INTERACTIONS

Transport of solutes (including contaminants) in the subsurface is controlled by advection, hydrodynamic dispersion, molecular diffusion, and geochemical interaction. Advection and hydrodynamic dispersion refer to movement of solute at a rate dependent on the various water pathways and velocities. Molecular diffusion refers to the gradual mixing of molecules of two or more substances as a result of random motion and/or a chemical concentration gradient. Diffusion flux spreads solute via the concentration gradient (i.e., according to Fick's law). Diffusion is a dominant transport mechanism when advection is insignificant but is usually negligible when water is being advected in response to various forces. Variability in the advection process gives rise to hydrodynamic dispersion. Hydrodynamic dispersion is a result of variability in travel paths, that is, velocities, taken by the advected solute. Geochemical interactions cover all reactions that are driven by chemical and biochemical forces.

Once the liquid wastes contact the vadose zone sediments, they can chemically interact with the soils and sediments. The major geochemical processes affecting transport include dissolution/precipitation, adsorption/desorption, filtration of colloids and small suspended particles, diffusion into micropores within mineral grains, and volatilization and eventual escape to the atmosphere. Dissolution/precipitation and adsorption/desorption are considered the most important for the inorganic wastes present in the 33 active waste streams at the Hanford Site. However, when assessing the organics in the waste streams, volatilization should also be considered. Furthermore, for the disposal of low-level radioactive waste (LLW) at the Hanford Site, precipitation is likely to be significant only for cases where pH and/or redox changes occur when waste streams contact the sediments. In most active liquid discharge situations at the Hanford Site, we speculate that adsorption processes are the key to inorganic contaminant migration. The knowledge base for the environmental fate of organics identified in the wastes is meager, and we cannot offer an opinion on what specific process dominates their fate.

Adsorption reactions have been acknowledged to be the most important contaminant retardation process in far-field transport analyses conducted for hazardous waste-disposal options. Adsorption processes are known to increase the travel times for some contaminants by 10^3 to 10^6 times relative to the groundwater. Such long travel times allow nuclides to decay to lower concentrations and less hazardous nuclides before they reach the accessible environment (i.e., the biosphere). Furthermore, some adsorption processes are effectively irreversible and permanently prevent contaminants from reaching the groundwater, thus preventing their release to the biosphere.

4.1 CONSTANT DISTRIBUTION COEFFICIENT

To predict the effects of retardation using mathematical codes, adsorption processes must be described in quantitative terms. An empirical parameter, the distribution coefficient (often called R_d or K_d), is readily measured by laboratory experimentation and allows such a quantitative estimate of migration and retardation. Knowledge of the R_d and of either media bulk density and porosity (for porous flow) or media fracture surface area, aperture width, and matrix diffusion attributes (for fracture flow) allows calculation of the retardation factor, R or R_f . The retardation factor is defined as $R = \frac{V_w}{V_n}$, where V_w is the velocity of water through a control volume and V_n is the velocity of the contaminant.

For one-dimensional advection-dispersion flow with chemical reaction, the transport equation can be written as

$$\frac{\partial C_i}{\partial t} = \frac{D_x \frac{\partial^2 C_i}{\partial x^2} - V_x \frac{\partial C_i}{\partial x}}{R_i} \quad (1)$$

where C_i = concentration of a particular radioactive species i in solution (mass/length³)

D_x = dispersion coefficient of species i (length²/time)

V_x = pore velocity of groundwater (length/time)

R_i = retardation factor for species i .

(For simplicity, radioactive decay has been left out.)

The retardation factor is a function of all of the contaminant retardation mechanisms: 1) chemical precipitation/dissolution of bulk solid phases, 2) chemical substitution of one element for another in a solid phase, 3) exchange of a stable isotope of an element with a radioactive isotope in solution, 4) physical filtration of colloids, 5) cation and anion exchange, and 6) adsorption (Muller et al. 1983), plus for organic compounds, 7) microbial and other degradation. Typically, all these mechanisms are melded into a single empirical distribution coefficient that implicitly assumes that the reactions go to equilibrium and are reversible and that the chemical environment along a solute flow path does not vary over either space or time. The limitations associated with these assumptions are well known to investigators, but the current paucity of Hanford Site-specific geochemical data precludes a more rigorous conceptual model at this time. Even though geochemical processes may be irreversible or at least directionally dependent (e.g., adsorption and de-sorption may be represented by different model parameters), the assumption of reversibility and use of single-valued model parameters are standard with the justification that the approach builds conservatism into the analysis.

In the constant R_d model, the distribution of the contaminant of interest between the solid adsorbent and solution is assumed to be a constant value. There is no explicit accommodation of dependence on characteristics of the sediments, groundwater, or contaminant concentration. Typically, an R_d value for a given contaminant is determined in the laboratory using sediment from the study area and actual or simulated groundwater to which a radionuclide tracer is added. Then

$$R_d = \frac{\text{amount of radionuclide adsorbed on solid per gram}}{\text{amount of radionuclide in solution per milliliter}} \quad (2)$$

The mass or activity of the tracer must be sufficient to facilitate good counting statistics. The solids and liquids are often equilibrated by contacting the solid with several aliquots of the liquid before adding the radiotracer, to attempt to approach the condition expected in the field.

Several standardized laboratory techniques are commonly used to determine this ratio (Serne and Relyea 1983; ASTM 1984).

Most of the laboratory experiments performed to measure distribution coefficients do not systematically investigate the effect of various important parameters and do not attempt to identify the processes causing the adsorption that is observed. Because it is an empirical measurement, the R_d value does not necessarily denote an equilibrium value or require some of the other assumptions inherent in the use of the more rigorous term K_d . The term R_d will be used to refer to the observed distribution ratio for the nuclide between the solid and solution. The term K_d will be reserved for true equilibrium reactions that show reversibility and that do not yield a distribution ratio that is dependent on the tracer concentration in solution.

It is customary with the constant R_d model to measure the total concentration or radioactivity of the tracer and thus to treat the tracer as being one species. This assumption is not an inherent requirement, but it is generally applied for convenience. If the tracer is known to distribute among several species and the distribution can be measured or predicted, separate R_d values can and should be calculated for each species.

This conceptual model, which depends on experimental determination of the distribution coefficient R_d , is quite simple, but it is also limited in that it does not address sensitivity to changing conditions. If the groundwater properties (e.g., pH, dissolved solids content) change, a new value for R_d must be obtained.

The constant R_d model is mathematically very simple and readily incorporated into transport models and codes via the retardation factor term. That is, for porous flow

$$R = 1 + \frac{\rho_b}{\phi \epsilon} R_d \quad (3)$$

or

$$R = 1 + \frac{1 - \phi \epsilon}{\phi \epsilon} \rho_p R_d \quad (4)$$

where R = the retardation factor

ρ_b = porous media bulk density (mass/length³)

Φ_e = effective porosity at saturation of media

R_d = distribution coefficient

ρ_p = particle density (mass/length³).

For the constant R_d model, the retardation factor (R) is a constant for each layer of geologic media (each layer is assumed to have a constant bulk density and saturated effective porosity). Therefore, this transport equation does not require knowledge of any other parameters, such as pH or surface area, and it is easily solved to determine the solution concentration as a function of time and for any given point. However, the use of the constant R_d conceptualization in the retardation factor has caused criticism because few natural groundwater pathways are spatially or geochemically homogeneous enough for the retardation factor of a species to remain constant.

4.2 INTRODUCTION TO ESTIMATING ADSORPTION CONSTANTS

The purpose of this subsection is to document any available Hanford Site-specific data that provide actual R_d values for identified contaminants. Because the database is small and the constant R_d adsorption model is simplistic, we do not discuss the adsorption potential of each contaminant from each waste stream separately.

As mentioned above, the adsorption tendencies of contaminants are influenced by characteristics of the waste stream, sediments, and contaminants. Vadose zone sediments at the Hanford Site do not show large ranges for such characteristics as organic carbon content, CEC, soil paste pH, and so on. Thus we do not gain much understanding of contaminant adsorption by attempting detailed differentiation (i.e., categorization) of Hanford sediments. On the other hand, the effects of solution characteristics (e.g., pH, Eh, dissolved solids, dissolved organic content) on inorganic contaminant adsorption are better understood and the ranges of solution characteristics of Hanford waste streams can be quite large. Therefore, all available waste stream data have been categorized into generic types based on five independent parameters (Figure 1).

		HIGH VOLUME (>2.0% of total)				LOW VOLUME (>2.0% of total)			
		HIGH DISSOLVED SOLIDS (>10 ⁻² M)		LOW DISSOLVED SOLIDS (<10 ⁻² M)		HIGH DISSOLVED SOLIDS		LOW DISSOLVED SOLIDS	
		HIGH ORGANICS (>2,000 ppb)	LOW ORGANICS (<2,000 ppb)	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
LOW ACIDITY (Neutral to Basic pH; pH>6.0)	LOW ACTIVITY	A.6	A.9, A.30, A.31		A.14, A.16, A.19, A.22, A.25, A.32		A.2	A.29	A.3, A.4, A.7, A.8, A.10, A.11, A.12, A.13, A.15, A.18, A.26, A.27, A.28, A.33
	HIGH ACTIVITY				A.23	A.21		A.5	A.1
HIGH ACIDITY (pH <6.0)	LOW ACTIVITY (<1% of total)				A.24	A.17			A.20
	HIGH ACTIVITY (>1% of total)								

FIGURE 1. Classification of Waste Streams Based on Five Key Parameters of Acidity, Radioactivity, Organic Content, Dissolved Solids Content, and Waste Stream Volume. The definitions for the parameters are given in parentheses under each heading. The waste stream identifications (A.1, etc.) are listed in Table 14.

TABLE 14. Waste Stream Identification

Designation	Waste Stream
A.1	N Reactor effluent
A.2	163-N Demineralizer wastewater
A.3	183-D Filter backflush wastewater
A.4	PUREX Plant chemical sewer
A.5	PUREX Plant process condensate
A.6	PUREX Plant ammonia scrubber condensate
A.7	PUREX Plant steam condensate
A.8	PUREX Plant cooling water
A.9	B Plant chemical sewer
A.10	B Plant process condensate
A.11	B Plant steam condensate
A.12	B Plant cooling water
A.13	Plutonium Finishing Plant wastewater
A.14	S Plant wastewater
A.15	T Plant headend wastewater
A.16	T Plant wastewater
A.17	UO ₃ Plant process condensate
A.18	UO ₃ /U Plants wastewater
A.19	241-A Tank Farm cooling water
A.20	241-AY, 241-AZ Tank Farms steam condensate
A.21	242-A Evaporator process condensate
A.22	242-A Evaporator steam condensate
A.23	242-A Evaporator cooling water
A.24	242-S Evaporator steam condensate
A.25	244-AR Vault cooling water
A.26	209-E Laboratory reflector water
A.27	222-S Laboratory wastewater
A.28	2101-M Laboratory wastewater
A.29	2724-W Laundry wastewater
A.30	284-E Powerplant wastewater
A.31	284-W Powerplant wastewater
A.32	300 Area process wastewater
A.33	400 Area secondary cooling water

A volume quantity of more than 2% of the total waste stream flow was arbitrarily chosen as the high-volume category. This choice put nine of the 33 waste streams into the high-volume category. These nine streams contained 92% of the total waste stream volumes (Table 12). It should be kept in mind, however, that these volume data are from 1988 and may not be accurate for present waste stream flows.

The dissolved solids content of 10^{-2} M was chosen to define the high category because natural groundwater at Hanford contains dissolved solids ranging from 1×10^{-3} to 7×10^{-3} M. Migration of many cations through sediments in pore waters would tend to be accelerated by contact with high-ionic-strength solutions. Hence, streams showing dissolved solids contents higher than 10^{-2} M would tend to accelerate ion migration.

The pH parameter was used to define a neutral-to-basic category ($\text{pH} > 6.0$) and an acidic ($\text{pH} < 6.0$) category, with acidity being known to adversely affect the sorption of many cationic radionuclides (McHenry 1954, 1957, 1958), such as ^{90}Sr and ^{137}Cs , as well as the transuranics. Therefore, acidic streams, of which there are only three, would be higher-priority candidates for treatment or cessation than the 30 neutral-to-alkaline streams.

Four of the waste streams included 98.8% of the radioactivity being subjected to ground disposal. One of the four high-activity streams, N Reactor effluent (A.1), is no longer produced. The high-activity category was defined to include any streams having more than 1% of the total waste stream radioactivity. It is assumed that the higher radionuclide concentrations tend to enhance radionuclide migration.

The organic contents of the waste streams are generally low, ranging from about 100 to 241,000 ppb. There are only four streams with organic contents above 2,000 ppb (Table 7), and only 10 of the 33 streams have measurable organic contents at all. Therefore, the dividing line between categories was placed at an organic content of 2,000 ppb. Waste streams having organic contents above 2,000 ppb are considered to be high in organics, although the presence of these organics may or may not be detrimental to radionuclide sorption on sediments. Very little work has been done to date on the effects of organics on radionuclide sorption on Hanford soils.

Table 14 lists the 33 waste streams and their designations (A.1 to A.33). Figure 1 shows each waste stream as a member of one of the 32 categories based on the data obtained from Westinghouse Hanford (1989). In general, migration potential and resultant hazard from a waste stream increase with increasing volume, dissolved solids, organics, radionuclide activity, and acidity. Conversely, waste streams with low values for volume, dissolved solids, activity, and organics and a high value for pH are not likely to promote migration of contaminants.

Most of the active waste streams identified in Table 14 are in the categories that do not promote migration. Waste streams A.3, A.4, A.7, A.8, A.10 to A.13, A.15, A.18, A.26 to A.28, and A.33 have low values for all five parameters (note that low acidity = high pH). Waste streams A.14, A.16, A.19, A.22, A.25, and A.32 are low in all parameters but discharge volume. These "low-value" waste streams represent chemical sewerage, steam and process condensates, cooling waters, and miscellaneous laboratory wastewaters.

Three waste streams have three high values and two low values for the five parameters. These three streams may warrant closer scrutiny than all of the others because of their higher potential for contaminant migration. The three waste streams are the PUREX ammonia scrubber condensate, which has high volume, high dissolved solids content, and high organic content; UO₃ Plant process condensate, which has high dissolved solids, high organics, and acid pH; and 242-A evaporator steam condensate, which has high dissolved solids, high organics, and high radionuclide content.

4.3 DISTRIBUTION COEFFICIENTS FOR INORGANICS AND RADIONUCLIDES

Figures 2 through 16 provide estimates of distribution coefficient (R_d) values for selected inorganic and radionuclide constituents found in the 33 active waste streams. R_d values are presented for each of eight waste types based on the waste streams' pH, total dissolved solids content, and organic content (see Figure 1 to determine which waste streams belong in each category).

The R_d figures provide estimates for each waste stream category for a typical Hanford sediment. To obtain accurate R_d values requires testing of

	HIGH DISSOLVED SOLIDS		LOW DISSOLVED SOLIDS	
	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
NEUTRAL TO BASIC	3-15 (5)	7-70 (7.5)	15-70 (15)	15-200 (20)
ACID	0.1-5 (1.5)	0.5-15 (3.5)	3-15 (7.5)	7-15 (10)

FIGURE 2. R_d Estimates (mL/g) for Beryllium, Calcium, and Magnesium. The numbers in parentheses are conservative R_d ranges above them. See Figure 1 for parameter definitions.

	HIGH DISSOLVED SOLIDS		LOW DISSOLVED SOLIDS	
	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
NEUTRAL TO BASIC	5-20 (7) Rhodes (1956) Routson et. al (1981)	10-100 (10) Routson et. al (1981)	20-100 (20)	20-200 (25) Rhodes (1956) McHenry (1958) Routson et. al (1981)
ACID	0.1-5 (2) Knoll (1969)	0.5-20 (5) Hawkins and Short (1965)	5-15 (10)	50-20 (5) Rhodes (1957a)

FIGURE 3. R_d Estimates (mL/g) for Strontium and Barium. The numbers in parentheses are conservative R_d averages estimated from the R_d ranges above them. See Figure 1 for parameter definitions.

	HIGH DISSOLVED SOLIDS		LOW DISSOLVED SOLIDS	
	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
NEUTRAL TO BASIC	0-30 (1)	0-30 (2)	1-30 (2)	1-30 (4) Buel et al. (1988)
ACID	0-10 (0)	0-10 (0)	0-10 (0)	0-10 (1)

FIGURE 4. R_d Estimates (mL/g) for Lithium, Potassium, Sodium, and Ammonium. The numbers in parentheses are conservative R_d ranges above them. See Figure 1 for parameter definitions.

	HIGH DISSOLVED SOLIDS		LOW DISSOLVED SOLIDS	
	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
NEUTRAL TO BASIC	0.1-10 (3) Haney (1967) Barney (1978)	5-20 (10) Routson et al. (1981)	0.1-10 (3) Wilding and Rhodes (1963)	10-3000 (50) Routson et al. (1981)
ACID	0 Haney (1957) Rhodes and Nelson (1957)	0.2-20 (5)	0	0.2-20 (5)

FIGURE 5. R_d Estimates (mL/g) for Cobalt, Iron, and Manganese. The numbers in parentheses are conservative R_d ranges above them. See Figure 1 for parameter definitions.

	HIGH DISSOLVED SOLIDS		LOW DISSOLVED SOLIDS	
	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
NEUTRAL TO BASIC	0-100 (10)	0-200 (30)	0-200 (10)	100-200 (30)
ACID	0-10 (2)	5-50 (6)	0-40 (2)	10-100 (10)

FIGURE 6. R_d Estimates (mL/g) for Lead, Zinc, Cadmium, Copper, Nickel, Silver, and Mercury. The numbers in parentheses are conservative R_d ranges above them. See Figure 1 for parameter definitions.

	HIGH DISSOLVED SOLIDS		LOW DISSOLVED SOLIDS	
	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
NEUTRAL TO BASIC	0-2 (0)	0-5 (0) Haney (1967) Ames and Rai (1978)	0-2 (0)	0-40 (0)
ACID	0-5 (0)	2-20 (2)	0-5 (0)	2-40 (2)

FIGURE 7. R_d Estimates (mL/g) for Antimony, Molybdenum, and Sulfide. The numbers in parentheses are conservative R_d ranges above them. See Figure 1 for parameter definitions.

	HIGH DISSOLVED SOLIDS		LOW DISSOLVED SOLIDS	
	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
NEUTRAL TO BASIC	0-30 (10) Prout (1959)	20-500 (20)	2-20 (10)	10-1,000 (40) Rhodes (1957a)
ACID	0-10 (5) Prout (1959)	10-500 (10)	2-20 (5)	10-1,000 (20) Rhodes (1957a)

FIGURE 8. R_d Estimates (mL/g) for Zirconium, Niobium, and Tin. The numbers in parentheses are conservative R_d ranges above them. See Figure 1 for parameter definitions.

	HIGH DISSOLVED SOLIDS		LOW DISSOLVED SOLIDS	
	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
NEUTRAL TO BASIC	0	0 Brown and Haney (1964) Brown (1967)	0	0 Haney (1964) Wildung et al. (1975) Routson et al. (1976)
ACID	0	0	0	0

FIGURE 9. R_d Estimates (mL/g) for Chromium(VI), Tritium, Technetium, Chloride, Fluoride, Iodine, Sulfate, Nitrate, Xenon, Krypton, and Argon. The numbers in parentheses are conservative R_d ranges above them. See Figure 1 for parameter definitions.

	HIGH DISSOLVED SOLIDS		LOW DISSOLVED SOLIDS	
	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
NEUTRAL TO BASIC	3-300 (10) Barney (1978)	3-300 (10) Rhodes and Nelson (1957) Hajek and Ames (1968) Routson et al. (1981)	50-3,000 (50) Barney (1978)	50-3,000 (50) Rhodes and Nelson (1957) Hajek and Ames (1968) Routson et al. (1981)
ACID	5-50 (5) Knoll (1969)	5-50 (5) McHenry (1954) Rhodes and Nelson (1957)	10-100 (30)	10-100 (30) McHenry (1954) Rhodes and Nelson (1957)

FIGURE 10. R_d Estimates (mL/g) for Cesium. The numbers in parentheses are conservative R_d ranges above them. See Figure 1 for parameter definitions.

	HIGH DISSOLVED SOLIDS		LOW DISSOLVED SOLIDS	
	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
NEUTRAL TO BASIC	0-10 (2)	10-200 (100) Benson (1960) Hajek (1966)	0-20 (5)	100-500 (200) Benson (1960) Routson et al. (1976) Sheppard et al. (1976)
ACID	0-2 (0) Knoll (1969)	10-40 (20) Rhodes (1957a) Hajek and Knoll (1966)	0-10 (2)	50-200 (100) Rhodes (1957a) Routson et al. (1976)

FIGURE 11. R_d Estimates (mL/g) for Chromium(III), Rare Earths (Ce, La, Eu, Pm), Americium, and Curium. The numbers in parentheses are conservative R_d ranges above them. See Figure 1 for parameter definitions.

	HIGH DISSOLVED SOLIDS		LOW DISSOLVED SOLIDS	
	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
NEUTRAL TO BASIC	0.2-20 (10)	20-200 (50) Rhodes (1957b)	0.2-20 (10)	100-2,000 (25) Rhodes (1957b) Emery and Garland (1974) Emery et al. (1974)
ACID	0.1-1.0 (0.5) Benson (1960) Knoll (1969)	1-20 (5) Hajek and Knoll (1966)	0.1-10 (2)	20-200 (20) Rhodes (1957b)

FIGURE 12. R_d Estimates (mL/g) for Plutonium. The numbers in parentheses are conservative R_d ranges above them. See Figure 1 for parameter definitions.

	HIGH DISSOLVED SOLIDS		LOW DISSOLVED SOLIDS	
	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
NEUTRAL TO BASIC	0.2-20 (1)	0.2-200 (0.5) Routson et al. (1976)	0.2-20 (1)	2-2,000 (2) Benson (1961) Routson et al. (1976) Sheppard et al. (1976)
ACID	0.1-1.0 (0.5)	2-20 (10)	0.1-10 (0.5)	20-200 (20)

FIGURE 13. R_d Estimates (mL/g) for Neptunium and Uranium. The numbers in parentheses are conservative R_d ranges above them. See Figure 1 for parameter definitions.

	HIGH DISSOLVED SOLIDS		LOW DISSOLVED SOLIDS	
	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
NEUTRAL TO BASIC	1-1,000 (10)	5-2,000 (20)	10-1,000 (20)	10-2,000 (20)
ACID	3-1,000 (3)	5-2,000 (5)	10-1,000 (20)	10-2,000 (20)

FIGURE 14. R_d Estimates (mL/g) for Aluminum, Silicon, and Titanium. The numbers in parentheses are conservative R_d ranges above them. See Figure 1 for parameter definitions.

	HIGH DISSOLVED SOLIDS		LOW DISSOLVED SOLIDS	
	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
NEUTRAL TO BASIC	10-300 (20)	30-300 (50)	50-3,000 (50)	50-3,000 (50)
ACID	5-500 (15)	5-500 (20)	10-500 (20)	10-1,000 (30)

FIGURE 15. R_d Estimates (mL/g) for Phosphate and Vanadium. The numbers in parentheses are conservative R_d ranges above them. See Figure 1 for parameter definitions.

	HIGH DISSOLVED SOLIDS ^(a)		LOW DISSOLVED SOLIDS	
	HIGH ORGANICS	LOW ORGANICS	HIGH ORGANICS	LOW ORGANICS
NEUTRAL TO BASIC	0-30 (0) Raymond (1964, 1965)	0-500 (2) Ames and Rai (1978) Barney (1978)	2-20 (5) Wilding and Rhodes (1963)	10-1,000 (20) Rhodes (1957a)
ACID	0-10 (2)	1-500 (50)	2-1,000 (20)	10-1,000 (40) Rhodes (1957a)

(a) Presence of high nitrates and/or nitrites lowers ruthenium adsorption tendencies; other salts are not important.

FIGURE 16. R_d Estimates (mL/g) for Ruthenium. The numbers in parentheses are conservative R_d ranges above them. See Figure 1 for parameter definitions.

site-specific sediments and the specific waste stream of interest. However, the R_d values in the figures provide a conservative estimate that can be used for scoping performance assessment calculations and an estimate of the range in values. If data on a Hanford sediment and liquid waste similar to one of the 33 active discharges are available, the specific reference is cited. Where no citations are given, we relied on experience and general knowledge of contaminant-sediment interactions to develop the estimates (e.g., Coughtrey et al. 1983-1984; Ames and Rai 1978; Serne and Wood 1990).

4.4 SOLUBILITY OF INORGANIC AND RADIONUCLIDE CONSTITUENTS

Solubility (dissolution-precipitation) reactions are often important in controlling the fate of inorganic contaminants that have been disposed of to sediments. Certain constituents are very insoluble with the slightly alkaline pH and alkaline earth-rich pore waters present in Hanford sediments. Generally oxide, hydroxide, carbonate, and phosphate minerals of certain metallic elements can be expected to control solution concentrations at low values. Some common solubility controls include Al and Si oxides; Pb and Ca carbonates or phosphates; Ti, Cr, Mn, Fe, Zr, lanthanum, and actinide oxides and hydroxides; and Ba sulfate. Krupka (in Evans et al. 1988b) has discussed solubility calculations for Hanford groundwaters and suggested that many of the elements listed above could be controlled by these minerals under existing conditions in the upper unconfined aquifer. Rai and Serne (1978), Lindsay (1979), Stumm and Morgan (1981), Drever (1982), and Nordstrom and Munoz (1985) have all presented generic discussions of solubility controls in soils and sediments and presented methods to aid researchers in performing such calculations for site-specific conditions. It should be pointed out that a solubility limit is not a constant value in a chemically dynamic system. That is, the solubility limit (e.g., on Pu, Sr, Cd, or Pb) is determined by the product of the thermodynamic activities of species that constitute the solid. If the system chemistry changes, then the individual species activities will likely change. For example, if the controlling solid for plutonium is the hydrous oxide $\text{Pu}(\text{OH})_4$, the solubility product is $[\text{Pu}][\text{OH}]^4 = K_{\text{sp}}$, where brackets indicate activities. The value of K_{sp} is fixed, but the values of $[\text{Pu}]$ and $[\text{OH}]$ can vary. In fact, if the pH decreases 1 unit (meaning that

[OH] decreases by 10), then for K_{sp} to remain constant, [Pu] must increase by 10^4 , with all else held constant. A true solubility model must consider the total system and does not reduce to a fixed value for the concentration of a constituent under all conditions. Numerous constant-concentration (i.e., empirical solubility) models are used in performance assessment activities; such models assume a controlling solid and fix the chemistry of all constituents to derive a fixed value for the concentration of specific contaminants. However, the value obtained is only valid for the specific conditions assumed.

Solubility-controlled release models assume that a known solid is present, or rapidly forms, and controls the solution concentration of the constituents being released. Solubility models are thermodynamic equilibrium models and do not consider kinetics (i.e., the time required for the solid to dissolve or completely precipitate). When identification of the probable controlling solid is difficult or when kinetic constraints are suspected, empirical solubility experiments are often performed to gather data that can be used to generate an empirical solubility release model (a model with mathematical similarity to solubility but no identified thermodynamically acceptable controlling solid).

Currently, two commonly used performance assessment codes, TRANSS and the Multimedia Environmental Pollutant Assessment System (MEPAS), can accommodate only the constant solubility release model. The geochemical code MINTEQA (Felmy et al. 1984; Peterson et al. 1987) is the current detailed solubility model and code used at PNL. Less detailed, constant-concentration-limit models have been generated from empirical studies (Delegard and Gallagher 1983; Delegard et al. 1984).

The active waste streams identified by Westinghouse Hanford (1989) generally have near-neutral to slightly alkaline pH and low to moderate total dissolved solids contents. On contact between the waste stream and the Hanford sediments, we do not expect any dramatic changes in pH or redox state, two variables that can cause significant dissolution/precipitation reactions. Thus, it is not likely that most contaminants within the liquid waste streams,

aside from very insoluble constituents (e.g., Al, Fe, Mn, Am, Pu, PO_4), will be controlled by solubility processes.

Another way of looking at the waste streams' fate is that the measurements of the chemical composition available reflect precipitation reactions that have already occurred within the process facilities. That is, highly insoluble constituents are not found in the liquid effluents discharged to Hanford sediments because they have already been removed before reaching the disposal crib. The active waste effluents contain soluble constituents that, in general, will remain soluble in the sediment pore waters.

Qualitative solubility rankings for important inorganic contaminants in Hanford waste streams are provided by Serne and Wood (1990, Appendix A). For convenience, a similar table for the major inorganic and radionuclide constituents identified in active waste streams is provided here (Table 15).

At present, we recommend that preliminary performance assessments assume that solubility effects are incorporated into the R_d value used to calculate retardation factors. Therefore, no additional computing provisions other than the R_d values presented in Figures 2 through 16 must be made to predict the fate of contaminants.

The organic carbon content of most active waste streams does not appear to be significant and probably would not influence the fate of the identified hazardous inorganics and radionuclides. Only five waste streams contain more than 2 ppm organics (see Figure 1). The organic content of only streams A.5 and A.21 have concentrations of known complexers (e.g., tributylphosphate) that reach the parts per million range. Thus, if more detailed and mechanistic modeling of contaminant migration were required, the available thermodynamic data, codes (i.e., MINTEQ), and waste stream analyses could be used to determine plausible solubility controls for most inorganic and radionuclide constituents in at least 31 of the 33 waste streams. MINTEQ currently contains thermodynamic data for the following components of interest to active disposal of liquid waste: Li, B, C, NO_2^- , NO_3^- , NH_4^+ , F, Na, Mg, Al, Si, PO_4^{3-} , S^{2-} , SO_4^{2-} , Cl, K, Ca, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Se, Br, Rb, Sr, Mo, Ag, Cd, Sb, I, Sc, Ba, Hg, Tl, Pb, Ra, U, Am, and Pu(III), Pu(IV), Pu(V), and Pu(VI). Currently absent from the MINTEQ database are

TABLE 15. Qualitative Estimate of Mineral Solubility of Hanford Sediment in Pore Water

Constituent	High Organic Carbon Solution (>2,000 ppb)	Low Organic Carbon Solution (<2,000 ppb)	Limiting Solid
H	VS (a)	VS	--
Li	VS	VS	--
Be	Unknown	Unknown	--
NH ₄ ⁺	VS	VS	--
NO ₃ ⁻	VS	VS	--
F	MS (b)	MS	CaF ₂
Na	VS	VS	--
Mg	MS	MS	Carbonates
Al	LS (c)	LS	Oxides
Si	MS	MS	Oxides
P	MS	LS	Ca phosphates
SO ₄ ²⁻	VS	MS	CaSO ₄ ·2H ₂ O
S	MS	MS	Metal sulfides
Cl	VS	VS	--
Ar	MS	MS	--
K	VS	VS	--
Ca	MS	MS	Carbonates, phosphates
Ti	LS	LS	Oxides
V	MS	MS	--
Cr (VI)	VS	VS	--
Cr (III)	LS	LS	Mixed Fe(OH) ₃
Mn	MS	LS	Oxides, hydroxides
Fe	MS	LS	Oxides, hydroxides
Co	MS	MS	Hydroxides
Cu	MS	MS	Hydroxides, carbonates
Zn	MS	MS	Hydroxides, carbonates
As	VS	VS	--
Kr	MS	MS	--
Sr	MS	MS	Carbonates
Zr	MS	LS	Hydroxides, oxides
Nb	MS	LS	Hydroxides, oxides
Mo	VS	MS	--
Tc	VS	VS	--
Ru	Unknown	Unknown	--
Ag	MS	LS	Chlorides
Cd	MS	MS	Carbonates
Sn	MS	LS	Hydroxides, oxides
Sb	VS	VS	--
I	MS	MS	--
Xe	MS	MS	--
Cs	VS	VS	--
Ba	LS	LS	Sulfate
Lanthanides	MS	LS	Hydroxides, phosphates
Hg	Unknown	Unknown	--
Pb	MS	LS	Carbonate-hydroxide mix
U	MS	MS	Phosphate, oxide, alkaline earth uranate
Np	MS	MS	Hydroxides
Pu	MS	LS	Hydroxides
Am	MS	LS	Hydroxides, phosphates

- (a) VS = Very soluble; common controlling solids in Hanford sediments/waste stream environments (pH between 5.5 and 10.5) would allow more than 1,000 mg/L in solution.
- (b) MS = Moderately soluble; common controlling solids in Hanford sediments/waste stream environments (pH between 5.5 and 10.5) would allow no more than 25 mg/L in solution.
- (c) LS = Low solubility; common controlling solids in Hanford sediments/waste stream environments (pH between 5.5 and 10.5) would allow less than 1 mg/L in solution.

thermodynamic data for Be, Ti, Zr, Nb, Sn, Tc, Ru, lanthanides, Np, and Cm. Detailed solubility calculations for these neglected components would require an effort to collect data from the literature, critically review the information, and enter the reviewed data into the appropriate data files. Depending on complexity and data quantity, the cost of performing such activities would be between \$20,000 and \$30,000 for each element.

4.5 CHEMICAL/RADIOLOGICAL HALF-LIVES

Inorganic contaminants found in the active waste streams do not degrade biotically or convert into other constituents and can therefore be considered to remain present forever. Certain nutrients (N- and P-containing compounds), such as NH_4^+ , NO_2^- , NO_3^- , and PO_4^{3-} , can be transformed by microbiological reactions, but we will not consider such reactions here. Microbiological activity is not currently considered to be significant in Hanford vadose zone sediments. Nitrate plumes from past and current disposal practices are extensive in the Hanford Site's upper unconfined aquifer (see, for example, Evans et al. 1988a, 1988b, 1989). From this fact we infer that biological degradation of nitrate is not significant and that it is probably not significant for other inorganic nutrients.

All of the radionuclides identified in the 33 active waste streams decay to other elements with a characteristic half-life, as presented in Table 16. For probable scenarios of concern (e.g., liquid disposal to the vadose sediments, percolation to the water table, and subsequent transport in the upper unconfined aquifer to a future domestic drinking water well or the Columbia River), nonreacting nuclides with half-lives longer than 100 years can be considered stable. That is, how long it takes for water to reach the well or river after disposal to the vadose zone sediments is likely to vary between tens of days to many tens of years (e.g., DOE 1987; USGS 1987; Buelt et al. 1988). Mobile contaminants that do not significantly interact with the sediments would reach the well or river in about the same lengths of time as the water. Conversely, contaminants that do interact significantly with the sediments will travel at reduced rates, as quantified by the retardation

TABLE 16. Half-Life for Radionuclides Identified in Active Waste Streams

Isotope	Half-Life, yr	Isotope	Half-Life, yr
^3H	12.3	^{125}Sb	2.7
^{24}Na	1.7×10^{-3}	^{129}I	$1.7 \times 10^{+7}$
^{32}P	3.9×10^{-2}	^{131}I	2.2×10^{-2}
^{41}Ar	2.1×10^{-4}	^{132}I	2.6×10^{-4}
^{51}Cr	7.6×10^{-2}	^{133}I	2.3×10^{-3}
^{54}Mn	8.3×10^{-1}	^{135}I	7.6×10^{-4}
^{56}Mn	2.9×10^{-4}	^{135}Xe	1.0×10^{-3}
^{59}Fe	1.2×10^{-1}	^{134}Cs	2.0
^{58}Co	2.0×10^{-1}	^{137}Cs	30.0
^{60}Co	5.3	^{138}Cs	6.1×10^{-5}
^{65}Zn	6.7×10^{-1}	^{140}La	4.6×10^{-3}
^{85}Kr	10.8	^{140}Ba	3.5×10^{-2}
^{87}Kr	1.4×10^{-4}	^{141}Ce	8.9×10^{-2}
^{88}Kr	3.2×10^{-4}	^{144}Ce	7.8×10^{-1}
^{89}Sr	1.4×10^{-1}	^{147}Pm	2.6
^{90}Sr	27.7	^{153}Sm	5.3×10^{-3}
^{91}Sr	1.1×10^{-3}	^{154}Eu	16
^{95}Zr	1.8×10^{-1}	^{155}Eu	1.8
^{97}Zr	1.9×10^{-3}	^{234}U	$2.5 \times 10^{+5}$
^{95}Nb	9.6×10^{-2}	^{235}U	$7.1 \times 10^{+8}$
^{99}Mo	7.6×10^{-3}	^{236}U	$2.4 \times 10^{+7}$
^{99}Tc	$2.1 \times 10^{+5}$	^{238}U	$4.5 \times 10^{+9}$
^{103}Ru	1.1×10^{-1}	^{239}Np	6.4×10^{-3}
^{106}Ru	1.0	^{238}Pu	86.4
$^{110\text{m}}\text{Ag}$	7.0×10^{-1}	^{239}Pu	$2.4 \times 10^{+4}$
^{113}Sn	3.0×10^{-1}	^{241}Pu	13.2
^{122}Sb	7.7×10^{-3}	^{244}Am	1.2×10^{-3}
^{124}Sb	1.7×10^{-1}		

factor [see Equation (3)]. In such cases, even radionuclides with half-lives as long as thousands of years may in fact decay before reaching the well or river. Performance assessment codes will explicitly consider the decay during transportation of nuclides if one supplies the retardation factor, radionuclide half-life, and water travel time.

Table 16 lists all of the radionuclides identified in the 33 active waste streams. The list is extensive but only a small portion of the radionuclides have half-lives longer than 3 months, an arbitrarily chosen cut-off time for environmental concern for typical Hanford active discharges. Table 17 lists those radionuclides from Table 15 that have half-lives longer than 3 months. The uranium isotopes, ^{129}I , and ^{99}Tc have half-lives longer than 100,000 years and for most scenarios germane to active liquid discharges at the Hanford Site, these isotopes will not decay significantly prior to reaching the accessible environment.

TABLE 17. Radionuclides with Half-Lives Long Enough for Environmental Concern

<u>Isotope</u>	<u>Half-Life, yr</u>	<u>Isotope</u>	<u>Half-Life, yr</u>
^{238}U	4.5×10^9	^{60}Co	5.3
^{235}U	7.1×10^8	^{125}Sb	2.7
^{236}U	2.4×10^7	^{147}Pm	2.6
^{129}I	1.7×10^7	^{134}Cs	2.0
^{234}U	2.5×10^5	^{155}Eu	1.8
^{99}Tc	2.1×10^5	^{106}Ru	1.0
^{238}Pu	86.4	^{54}Mn	0.8
^{137}Cs	30	^{144}Ce	0.8
^{90}Sr	27.7	^{62}Zn	0.7
^{154}Eu	16	$^{110\text{m}}\text{Ag}$	0.7
^{241}Pu	13.2	^{113}Sn	0.3
^{85}Kr	10.8		

4.6 DISTRIBUTION COEFFICIENTS FOR ORGANICS

The processes affecting migration rates of both organic and inorganic compounds are listed in Table 18. The transformation processes in Table 18 can be graded relative to the properties of a compound, and field data for environmental factors yield a good indication of the compound's persistence in the sediment/water column. Volatilization is an important exchange process that occurs between a compound being dissolved in solution that is vaporized in the atmosphere. Organic compounds with high vapor pressures and low water solubilities are most susceptible to volatilization (for example, aliphatic hydrocarbons, monocyclic aromatics, and some nitrogen-substituted compounds). The magnitude of the Henry's law constant is used as an indicator of compound volatility because it accounts for compound water solubility and vapor pressure. However, quantitative measurement of compound volatility also must take into account wind velocity, water turbulence, and temperature.

Photolysis is another transformation process that depends on both compound properties and environmental conditions. The degree of photolysis is dependent on the amount of light (energy) a chemical can absorb and the efficiency with which it uses that energy, as well as sunlight intensity, cloud cover, time of day, season, latitude, ozone layer thickness, and water turbidity.

The migration behavior of organic compounds in the environment is primarily a result of the interaction between the physical and chemical properties of the compound and the sorbent. The effect of these properties in the water and sediment column may be subject to changes in such variables as pH, Eh, dissolved organics and inorganics, temperature, and water hydrodynamics. The transformation processes shown in Table 18 are quantified using the parameters shown in Table 19. From knowledge of the values for each parameter, one can rank the importance of the various processes, as shown in Table 20. For some groups, such as halogenated aliphatic hydrocarbons, a single process dominates transformation and fate in most environments. The fates of many organic compounds are more complex and depend on competing processes that vary in importance depending on compound properties and

TABLE 18. Physical and Chemical Processes Used to Assess the Distribution and Fate of Organic Compounds (Witkowski et al. 1987)

Process	Definition and Controlling Variables
Volatilization	Evaporative loss of a chemical. Depends on vapor pressure and water solubility of the chemical and on environmental variables such as wind, water turbulence, and temperature. Potentially important for compounds with high vapor pressures, low solubilities, and high activity coefficients.
Sorption	General term encompassing surface attraction (adsorption) and partition (solubilization). Depends on the hydrophilic and lipophilic properties of the chemical and the composition of the sorbent. Indicative parameters are solubility, octanol-water partition coefficient, and sorbent organic carbon content.
Photolysis	Nonmetabolic degradation requiring light energy: chemical undergoes either a direct transformation reaction from the absorbed energy or an indirect change from a reaction (e.g., oxidation) with an excited chemical species or free radical. Depends on the chemical's absorption spectrum coefficient in the ultraviolet to visible range, as well as the sunlight intensity distribution for a given time of day, season, latitude, depth in water, and ozone thickness. Also depends on the chemical's reaction quantum yield.
Chemical oxidation	Breaking down of the chemical bonds in organic compounds through a chemical reaction with photochemically derived oxidants (single oxygen or free radicals). Depends on the number and types of possible reactive sites and on the presence of oxidants. Rate constants either measured directly or estimated from structure-activity relations.
Hydrolysis	Reaction of a chemical with water, hydrogen, or hydroxide ion, commonly resulting in the introduction of a hydroxyl group in exchange for the removal of another functional group. Depends on the presence and number of hydrolyzable functional groups at neutral pH plus the catalytic effect of the addition of acids and bases at other pHs.
Bioaccumulation	Uptake and retention of chemicals in the water column by aquatic organisms through intake from water or diet. Depends on the nature of the chemical (i.e., if lipophilic) and the organism's fat content and metabolic and depuration rates.
Biotransformation and biodegradation	Enzyme-catalyzed transformation of chemicals as a source of energy, carbon, and nutrients. Depends on the refractory and toxic nature of the chemical and on the presence of an acclimated microbial population and a host of environmental factors, including pH, temperature, dissolved oxygen, available nutrients, and cometabolites.

TABLE 19. Physicochemical Parameters Used in Evaluation of Transport Properties of Organic Compounds (Witkowski et al. 1987)

Characteristics	Definitions
Water solubility	Indicative of chemical's hydrophobic/hydrophilic nature, the limiting load in water, and its potential behavior in solution. Units: mass per volume.
Vapor pressure	The partial pressure of vapor that is in equilibrium with a substance in its impure state at a specified temperature. Relative or qualitative measure of the volatility of the chemical in its pure state. Units: mass/length ² time ² (e.g., pascal, atm).
Henry's law constant	Relative equilibrium concentration of a compound in air and water at standard temperature and pressure. Ratio of the vapor pressure divided by the chemical's water solubility; indicative of the compound's volatility. Units: atm ³ /mol.
Reaeration rate ratio	Ratio of the first-order rate constant for loss of a chemical from aqueous, solution divided by the rate constant for oxygen uptake by the same solution. Unitless. Estimate of the volatility of compounds with Henry's law constants >3,500 torr per molar for which the volatilization rate constant is limited by diffusion through the liquid-phase boundary layer.
Partition coefficient (K)	Equilibrium distribution of a compound solubilized between two immiscible solvents. Unitless (see soil/sediment partition coefficient below).
Octanol-water partition coefficient (K _{ow})	Equilibrium distribution of a compound between water and n-octanol. Indicative characteristic of the bioconcentration potential of compounds. Unitless.
Soil/sediment partition coefficient (K _p)	Equilibrium distribution of a compound between water and a sediment/soil substrate. Mass of chemical per mass of sediment divided by the dissolved mass of chemical in solution per mass of solution. Unitless.
Soil/sediment organic carbon partition constant (K _{oc})	Soil/sediment partition coefficient divided by the soil/sediment percent organic carbon content. This normalizes the partition coefficient to a soil/sediment substrate that is 100% organic carbon, permitting comparison of partition coefficients between substrates of differing carbon content. Unitless.
Absorption spectrum coefficient	Quantity of light absorbed by the chemical at a particular wavelength in the ultraviolet-visible range of the electromagnetic spectrum.
Reaction quantum yield	Efficiency of light utilization by a chemical. Ratio of the number of moles of the chemical transformed to the quantity (flux) of light adsorbed. Unitless.
Photolysis rate constant	First-order rate constant for direct photolysis. Units: reciprocal time.
Oxidation rate constant	Sum of the rate constants for each individual type of reactive site in the compound. Units: reciprocal time.
Hydrolysis rate constant	First-order rate constant at pH of 7 and the second-order rate constants for acid- and base-promoted hydrolysis. Units: reciprocal time.
Bioconcentration factor	Concentration of a chemical in tissue on a dry-weight basis divided by the concentration in water. Also the ratio of the uptake to depuration rates for a compound in a given organism. Unitless.
Biotransformation rate	Second-order rate constant dependent on the chemical concentration and the microbial biomass. Units: reciprocal time.

TABLE 20. Environmental Processes Affecting the Organic Compounds Identified in the 33 Waste Streams (Witkowski et al. 1987)

Chemical Group	Primary Mechanism	Secondary Mechanism	Comments
Halogenated aliphatic hydrocarbons	Volatilization		Compounds with more than five chlorine atoms are sorptive. Have a potential for bioaccumulation.
Halogenated ethers Aliphatic	Hydrolysis	Volatilization and photo-oxidation in atmosphere	Some persistence due to high solubility. Also persistence potential due to lipophilicity.
Aromatic	Sorption	Bioaccumulation and biodegradation	
Monocyclic aromatics	Volatilization	Atmospheric oxidation/photolysis	Volatilization/sorption are competing reactions with environmental conditions determining which dominates. Some persistence from high solubility.
	Sorption and bioaccumulation	Slow biodegradation (especially nitrogen compounds)	
Phenols	Photolysis	(near air-water surface)	No accumulation/persistence except for nitrophenols, which sorb readily to clays.
	Biodegradation	(near water sediment if sufficient microbes)	
Monocyclic aromatics and phenols with five or more chlorines	Sorption and bioaccumulation		Chlorine content dominates compound behavior.
Phthalate esters	Sorption	Bioaccumulation, biotransformation, and biodegradation	Biologically reactive in metabolic processes. Because of sorption, transport depends on hydrogeologic conditions.
Polynuclear aromatic hydrocarbons	Sorption, bioaccumulation, and biodegradation	Photolysis (for compounds with low ring numbers)	Bioaccumulation short-term because readily metabolized. Sorption increases and biodegradation decreases with increasing number of benzene rings.
Nitrogen compounds Aliphatic	Photolysis		Mainly hydrospheric photolysis due to high solubility but also atmospheric.
Aromatic	Sorption	Biodegradation	

prevailing environmental conditions. For example, monocyclic aromatics are susceptible to either volatilization followed by atmospheric photolysis or sorption followed by bioaccumulation. In this example, the transformation processes that control compound persistence vary with environmental factors, such as wind speed, temperature, and availability of particulates in the water column for sorption.

The presence of solvents other than water can alter an organic compound's water solubility. Hence, the presence of cosolutes must be considered when attempting to predict the transport of organic contaminants through the subsurface. In general, sediment contaminated with low-water-solubility organics tend to bind other organics to the organic carbon fraction of the sediment. However, if existing sorbed organics are contacted by other low-water-solubility (i.e., hydrophobic) organics (cosolvents), the sorbed organics may be mobilized in the cosolvents.

Data on transformation of organic compounds (e.g., biological degradation) in water and sediments are available in many cases but are not very useful in predicting contaminant fate at the Hanford Site because of the numerous uncertainties derived from the influences of many environmental factors on transformation or degradation rates. These environmental factors include the presence, number, and species of organisms in the sediments, sediment pH, sediment type, moisture content, and temperature of the environment. Degradation rates or organic compound half-lives tend to be specific for a given environment and often cover a wide range of values for a single organic. Because the bulk of the half-lives given in the literature lack applicability to the Hanford Site, the values listed in Appendix A should not be given much credence because none were obtained in environments specific to the Hanford Site. Rather, the half-life information should be considered as qualitative guidance.

The soil/sediment partition coefficient, K_p , is defined as the ratio of adsorbed organic chemical per unit weight of the sediment to the weight of the aqueous solute per the same unit weight of solution. K_p is unitless. The K_{oc} , or partition constant, used to compare organic compound sorption of soils

or sediments with varying organic content is defined as

$$K_{OC} = \frac{K_p}{f_{OC}} \text{ or } \frac{(100)(K_p)}{\% f_{OC}} \quad (5)$$

where f_{OC} is the fractional mass of organic carbon in the soil or sediment. In fact, R_d values for organics are equivalent to $(K_{OC} \cdot f_{OC})/\rho_b$ where f_{OC} = fractional weight of naturally occurring organic carbon in the sediment (0.001 for typical Hanford sediments) and ρ_b is the sediment bulk density (1.5 ± 0.3 g/cm³ for most Hanford sediments). Organic compounds that bind strongly to organic carbon have characteristically low water solubilities. Likewise, organic compounds with little tendency to sorb onto organic carbon have high water solubilities. Organics that do sorb onto organic materials, if they are present in an aquifer, are retarded in their movement in respect to the groundwater.

If the K_{OC} of a compound is known, the unitless retardation factor (R) can be calculated using Equation (3). The R_d in Equation (3) is related to K_{OC} by the equation

$$K_{OC} = \frac{R_d \rho_b}{f_{OC}} \quad (6)$$

For many compounds (Farmer 1976), a linear relationship between the amount sorbed (C_s) and the concentration of the compound in the equilibrium solution (C_w) has been demonstrated: $C_s = K_p \cdot C_w$, where K_p is the linear partition coefficient. It is equivalent to a Freundlich constant (R_d) when $1/n$ equals unity: $C_s = R_d \cdot C_w^{1/n}$.

The $K_{O/W}$ of an organic solute is the n-octanol/water partition coefficient and defined as the equilibrium ratio of the solute concentration in the water-saturated n-octanol phase to the solute concentration in the n-octanol-saturated water phase. $K_{O/W}$ values are unitless. For ionizable organic compounds (acids, amines, and phenols), $K_{O/W}$ values are a function of pH. If a $K_{O/W}$ value is reported for an ionizable compound, the pH also should be reported (see Means et al. 1982). For sorption based on organic carbon (K_{OC}), Karickhoff et al. (1979) reported a significant correlation between the

adsorption of several aromatic hydrocarbons and the partitioning of the aromatic hydrocarbons between octanol and water ($K_{O/W}$)

$$\log K_{OC} = 1.00 \log K_{O/W} - 0.21 \quad (R^2 = 1.00) \quad (7)$$

where R^2 is the least-squares linear regression coefficient of determination. Linear least-squares fitting of the $K_{O/W}$ and K_{OC} data from a series of polycyclic aromatics and chlorinated hydrocarbons ranging in water solubility from 1 ppb to 1,000 ppm gave the equation $K_{OC} = 0.63 K_{O/W}$ ($R^2 = 0.96$). Other similar regression equations found in the literature and used to estimate K_{OC} values where none were available are listed in Table 21. Unfortunately, as Means et al. (1982) point out, these relationships are applicable only to hydrophobic, nonionizable organic compounds and to sediments containing more than 1 wt% organic carbon content. As can be seen from the organic carbon contents listed in Table 11, Hanford sediments are very low in organic carbon, generally containing less than 0.10 wt%. Hence these $K_{O/W}$ and K_{OC} relationships are not applicable to Hanford conditions except as a tool for very roughly estimating one when the other is known.

The Henry's law constant, sometimes referred to as the air-water partition coefficient, is defined as the ratio of the partial pressure of a compound in air to the concentration of the compound in water under equilibrium conditions. If the vapor pressure and water solubility of a compound are known, the Henry's law constant can be calculated at 1 atm (760 mm Hg) as

$$H = \frac{(P)(S)}{(760)(FW)} \quad (8)$$

where H = Henry's law constant ($\text{atm} \cdot \text{m}^3/\text{mol}$)

P = vapor pressure of the compound (mm Hg at 25°C)

S = water solubility (g/L)

FW = formula weight of the compound (g/mol).

TABLE 21. Regression Equations Useful for Estimation of Partition Coefficients (K_{OC} ; Witkowski et al. 1987)

Regression equation(a)	Number of Compounds	R ² (b)	Units for Solubility	Compound Groups	References
$\log K_{O/w} = -0.747 \log S + 0.730$	156	0.874	Moles per liter	Low-molecular-weight organics	Hansch et al. (1968)
$\log K_{O/w} = -0.670 \log S + 5.00$	33	0.970	Micromoles per liter	Pesticides and polychlorinated biphenyls	Chiou et al. (1977)
$\log K_{om} = -0.557 \log S + 4.040$	15	0.988	Micromoles per liter	Pesticides and hydrocarbons	Chiou et al. (1979)
$\log K_{OC} = -0.54 \log S + 0.44$	10	0.940	Mole fraction	Chlorinated hydrocarbons	Karickhoff et al. (1979)
$\log K_{OC} = -0.686 \log S + 4.273$	22	0.933	Micrograms per liter	PAHs	Means et al. (1980b)
$\log K_{OC} = -0.594 \log S + 0.197$	5	0.945	Mole fraction	PAHs	Karickhoff (1981)
$\log K_{OC} = -0.83 \log S + 0.93 - 0.01(MP-25)^{(c)}$	47	0.93	Mole fraction	Chlorinated hydrocarbons	Karickhoff (1984)
$\log K_{OC} = 1.00 \log K_{O/w} - 0.21$	10	1.00	NA ^(d)	Chlorinated hydrocarbons	Karickhoff et al. (1979)
$\log K_{OC} = 1.00 \log K_{O/w} - 0.317$	22	0.98	NA	PAHs	Means et al. (1980b)
$\log K_{OC} = 0.72 \log K_{O/w} - 0.49$	13	0.95	NA	Substituted hydrocarbons	Schwarzenbach and Westall (1981)
$\log K_{OC} = 0.9370 \log K_{O/w} - 0.006$	9	0.95	NA	Herbicides	Brown and Flagg (1981)
$\log K_{OC} = 0.989 \log K_{O/w} - 0.346$	5	0.997	NA	PAHs	Karickhoff (1981)
$\log K_{OC} = 1.029 \log K_{O/w} - 0.18$	13	0.91	NA	Pesticides	Karickhoff (1984)

(a) S = water solubility of the organic solute.

$K_{O/w}$ = octanol-water partition coefficient. Unitless.

K_{OC} = measured partition coefficient/organic carbon content of soil or sediment sample. Unitless. Organic matter, depending on composition, contains about 58% organic carbon (Hamaker and Thompson 1972) and consequently $K_{OC} = 1.72 K_{om}$.

K_{om} = measured partition coefficient/organic matter content of soil or sediment sample. Unitless.

(b) The linear regression coefficient of determination.

(c) The last term in this equation compensates for melting-point effects that occur in the phase transition of organic compounds that are initially solids.

(d) NA = Not applicable.

According to Lyman et al. (1982), if H is less than 10^{-7} atm•m³/mol, the substance has low volatility. If H is greater than 10^{-7} but less than 10^{-5} atm•m³/mol, the substance will volatilize slowly. Volatilization becomes an important transfer mechanism when H is between 10^{-5} and 10^{-3} atm•m³/mol. When H is larger than 10^{-3} atm•m³/mol, volatilization becomes a principal transfer mechanism. Estimating the Henry's law constant for many compounds assumes that the gas phase obeys the ideal gas law and that the aqueous solution acts as an ideal dilute solution. Neither of these assumptions always holds. In addition, the solubility and vapor pressure data used in Equation (8) are generally obtained from the pure substances. Many of the contaminants are not derived from pure substances, and vapor pressure and solubility data are often obtained without regard to standard states and temperatures. Therefore, many of the Henry's law constants given in Appendix A are actually only crude estimates.

The data presented in Appendix A on adsorption parameters, Henry's law constants, water solubilities, and degradation rates for the organic chemicals were mainly obtained from two computer databases. The two databases are the Soil Transport and Fate Database available from Utah State University's Department of Civil and Environmental Engineering (Sims et al. 1988) and Syracuse Research Corporation's Environmental Fate Data Base (EFDB), as described by Howard et al. (1986).

Appendix A presents Freundlich adsorption constants for some organic substances. Like the half-life data, these are closely tied to the conditions under which they were obtained (e.g., soil type, temperature, solution composition). These constants are listed when available, but the conditions under which they were obtained must be examined before their applicability to Hanford conditions can be judged.

Little, if any, data were available for several of the organic compounds in Appendix A. In fact, for a few compounds, we could not even identify a Chemical Abstracts Service Registry Number (CAS No.). The available data describing physical properties were included when no specific adsorption and solubility data are presented for a given constituent. When no values are

present, the reader may assume that we were unable to find any information in the literature.

In Tables 22 and 23, we summarize the adsorption, water solubility, volatilization (Henry's law constants), and degradation tendencies from Appendix A for those organic compounds identified in Table 5. When no data were found in the literature, we have estimated qualitatively whether the compound would exhibit high, medium, or low adsorption, water solubility, volatility, or degradation rates in Hanford sediments containing a solution representative of the 33 active waste streams. The qualitative rankings for all the organics identified in Table 5 are shown in Table 23. This table will allow scoping performance assessment activities to evaluate those compounds that have greater mobility.

Based on the organic data (especially K_{OC} values) given in Appendix A, R_d values were estimated for the most prevalent organic analytes, assuming a 0.1 wt% content of organic carbon for Hanford sediment and a bulk density of 1.5 g/cm^3 . The results are shown in Table 22. The R_d data are given only to show trends. As mentioned previously, R_d values computed from K_{OC} values for soils containing less than 1.0 wt% organic carbon are speculative.

TABLE 22. Available Physicochemical Data for the Organic Compounds Listed in Table 5. An R_d was determined assuming an f_{OC} of 0.1 wt% carbon. The relationship utilized for determination of an R_d value was $(K_{OC})(f_{OC})/\rho_b = R_d$. For details and references, see Appendix A.

Organic Compound	Water Solubility at 25°C	Henry's Law Constant, atm·m ³ /mol at 25°C	$K_{O/W}$	K_{OC}	Estimated R_d , mL/g ^(a)	Dissociation Constants, Acids and Bases
Tributylphosphate	280 mg/L	1.9×10^{-2}	1×10^3	6×10^3	4	
Tridecane	1×10^{-3} mg/L	NA ^(b)	4.5×10^6	2.8×10^6	2.0×10^3	
Tetradecane	0.3 to 7×10^{-3} mg/L	0.3 to 1.2	1.6×10^7	1.01×10^7	6.7×10^3	
Dodecane	3 to 8×10^{-3} mg/L	7.5 ± 2.5	1.0×10^6	6.3×10^5	4.0×10^2	
Pentadecane	7×10^{-5} mg/L	NA	5.2×10^7	3.28×10^7	2.0×10^4	
Tetrachloroethylene	200 mg/L	1.84×10^2	400 to 2,500	238 to 1,600	0.1 to 1	
Chloroform	7.95 g/L	3.67×10^{-3}	93	45	0.03	
Bis(2-ethylhexyl) phthalate	0.40 mg/L	1.47×10^{-5}	4,170 to 12,800	87,000	58	
Undecane	1 to 4×10^{-2} mg/L	1.8 ± 0.8	0.4 to 5.5×10^6	2.5×10^5 to 3.5×10^6	200 to 2,000	
2-butoxyethanol	45 g/L	2.8×10^{-7}	6.76	67	0.05	
Butyl alcohol	74 g/L	8.81×10^{-6}	NA	72	0.05	
Acetone	Miscible	3.88×10^{-5}	0.575	18	0.07	
Hexadecane	0.02 to 6.3×10^{-3} mg/L	0.3 to 2.3×10^{-1}	1.8×10^8	1.13×10^8	6×10^4	
Methyl nitrate ^(c)						
Dimethoxymethane ^(d)						
Heptadecane	6×10^{-6} mg/L	NA	0.6 to 2.1×10^9	3.8×10^8 to 1.3×10^9	2.6 to 7×10^5	
Octadecane	2 to 6×10^{-3} mg/L	NA	6.17×10^8	3.9×10^8	2.6×10^5	
Decane	2 to 5×10^{-2} mg/L	7 ± 3	1.0×10^5	6.3×10^4	40	
Methyl formate ^(e)	170 g/L	9.12×10^{-3}				
Phenol	82.8 g/L	3.33×10^{-7}	28.84	38.8	0.02	10
N-methoxymethanamine ^(f)						
Di-n-butylphthalate	11.2 mg/L	2.8×10^{-7}	758 to 52,490	170,000	110	
Benzyl alcohol	40 g/L	NA	12.30	95.5	0.06	
Methylene chloride	13.7 g/L	2.19×10^{-3}	17.38	28	0.02	
Di-n-octylphthalate	3.0 mg/L	4.45×10^{-7}	7.4×10^9	3.6×10^9	2×10^6	
Benzoic acid	3.4 g/L	0.287×10^{-5}	74.13	182	0.006	4.205
Methyl ethyl ketone	223 g/L	5.59×10^{-5}	1.07	5.2	0.003	
Butylbenzyl phthalate	2.69 mg/L	1.26×10^{-6}	81,280	17,000	11	

TABLE 22. (cont'd)

Organic Compound	Water Solubility at 25°C	Henry's Law Constant, atm·m ³ /mol at 25°C	K _{o/w}	K _{oc}	Estimated R _d , mL/g ^(a)	Dissociation Constants, Acids and Bases
2-methyl-5-propylnonane ^(f)						
Pelargic acid ^(g)						
Tetrahydrofuran	Miscible	NA	2.88	Low	Very low	
Butoxyglycol	Miscible	2.08×10^{-7}	6.76	67	0.045	
Methyl n-butyl ketone	17.5 g/L	1.1×10^{-5}	23.99	15	0.01	
Butyraldehyde	71 g/L	1.15×10^{-4}	7.586	9.4	0.006	
2-propanol	Miscible	7.89×10^{-6}	1.122	25	0.016	
MIBK (hexone)	19 g/L	4.2×10^{-5}	15.48	19	0.013	
Methyl n-propyl ketone	43 g/L	6.36×10^{-5}	8.129	Low	Very low	
Butylnitrate	Low	NA	High	Medium	Low	
Ethoxytriethylene glycol	High	Low	Low	Low	Low	
3,5-dimethylpyridine	9.5% (W/W)	Medium	NA	Medium	Low	
Ethyl alcohol	Miscible	1.2×10^{-5}	0.49	0.30	0.002	
Hexadecanoic acid	Insoluble	NA	High	High	Medium	
Acetophenone	6.13 g/L	1.07×10^{-5}	38-48	23-45	0.015-0.03	
Benzaldehyde	3 g/L	Medium	30.2	Medium	Low	
Butoxydiglycol	Miscible	Low	Low	Low	Very low	
Dichlorofluoromethane	Low	High	NA	NA	Low	
Dimethylnitrosamine	Miscible	2.63×10^{-7}	0.269	12	0.01	
Methoxydiglycol	Miscible	Low	Low	Low	Very low	
Methoxytriglycol	Miscible	Low	Low	Low	Very low	
2-methylnonane	0.074 mg/L	NA	82,000	High	High	
Morpholine	Miscible	1.44×10^{-7}	0.138	Very low	Very low	
Phenanthrene	1.15 mg/L	2.28×10^{-5}	28,840	230,000	150	

(a) Assumed $f_{oc} = 0.1$ wt% OC and $\rho_b = 1.5$ g/cm³.

(b) NA = Not available.

(c) Slightly water soluble; explosive vapor at room temperature; density = 1.2075 (air = 1); melting point = 82.3°C; boiling point (explosive) = 64.6°C.

(d) Moderately water soluble, colorless gas; flammable; density = 1.617 (air = 1); one volume of water dissolves 37 volumes of gas; flash point = -41°C.

(e) Colorless, flammable liquid; flash point, closed cup = -19°C; density at 15°C = 0.987.

(f) Compound not found in literature.

(g) Compound not found in literature; probably pelargonic acid, for which no environmental characterization data are available.

TABLE 23. Qualitative Ranking of Geochemical Attributes of the Organic Compounds Listed in Table 5.

Organic Compound	Comment	Qualitative Estimate of			
		Solubility ^(a)	Volatility ^(b)	Sorption ^(c)	Degradation
Tributylphosphate	Readily degrades, $t_{1/2} = 6$ days in river water	Medium	High	Medium	Medium
Tridecane	Sorbed on sediment clays and organic carbon	Low	High	High	Medium
Tetradecane	Sorbed on sediment clays and organic carbon	Low	High	High	Medium
Dodecane	Sorbed on sediment clays and organic carbon	Low	High	High	High
Pentadecane	Sorbed on sediment clays and organic carbon	Low	High	High	Medium
Tetrachloroethylene	Little sorption	Medium	High	Low	Low
Chloroform	Little sorption	High	Medium	Low	Low
Bis(2-ethylhexyl) phthalate	Sorbed on sediment clays and organic carbon	Medium	Low	High	Medium
Undecane	Sorbed on sediment clays and organic carbon	Low	High	High	Medium
2-butoxyethanol	Little sorption	High	Low	Low	Medium
Butyl alcohol	Little sorption	High	Low	Low	Medium
Acetone	Little sorption	High	Low	Low	High
Hexadecane	Sorbed on sediment clays and organic carbon	Low	High	High	Medium
Methyl nitrate	No literature available	Medium	High	Low	Low
Dimethoxymethane	No literature available	Medium	High	Low	Low
Heptadecane	Sorbed on sediment clays and organic carbon	Low	High	High	Medium
Octadecane	Sorbed on sediment clays and organic carbon	Low	High	High	Medium
Decane	Sorbed on sediment clays and organic carbon	Low	High	Medium	Medium
Methyl formate	No literature available	High	High	Low	Low
Phenol	Sorption a function of pH	High	Low	Low	Medium
N-methoxymethanamine	No compound with this structure in literature	--(d)	--	--	--
Di-n-butylphthalate	Sorbed on sediment clays and organic carbon	Medium	Low	High	Medium
Benzyl alcohol	Little sorption	High	Low	Low	Medium
Methylene chloride	Little sorption	High	Medium	Low	Medium
Di-n-octylphthalate	Sorbed on sediment organic carbon	Medium	Low	High	Medium
Benzoic acid	Sorption a function of pH	High	Low	Low	Low
Methylethyl ketone	Little sorption	High	Low	Low	High
Butylbenzyl phthalate	Sorbed on sediment organic carbon	Medium	Low	Medium	High
2-methyl-5-propylnonane	No compound with this structure in literature	--	--	--	--
Pelargic acid	No literature available	--	--	--	--

TABLE 23. (cont'd)

Organic Compound	Comment	Qualitative estimate of			
		Solubility	Volatility	Sorption	Degradation
Tetrahydrofuran	Little sorption	High	High	Low	Low
Butoxyglycol	Little sorption on organic carbon; some clay sorption	High	Low	Low	Medium
Methyl n-butyl ketone	Little sorption	High	Medium	Low	Low
Butyraldehyde	Little sorption	High	Medium	Low	Medium
2-propanol	Little sorption	High	Medium	Low	Low
MIBK (hexone)	Little sorption	High	Medium	Low	Medium
Methyl n-propyl ketone	Little sorption	High	Medium	Low	Medium
Butylnitrate	Little sorption	High	Medium	Low	Low
Ethoxytriethylene glycol	Little sorption on organic carbon; some clay sorption	High	Low	Low	Medium
3,5-dimethylpyridine	Little sorption; odor of pyridine and peppermint	High	Medium	Low	Low
Ethyl alcohol	Little sorption	High	Medium	Low	High
Hexadecanoic acid	Sorption a function of pH; ordinarily a solid	Low	Low	High	Low
Acetophenone	Little sorption	High	Medium	Low	High
Benzaldehyde	Little sorption	High	Medium	Low	Medium
Butoxydiglycol	Little sorption on organic carbon; some clay sorption	High	Low	Low	Medium
Dichlorofluoromethane	Little sorption	High	Medium	Low	Medium
Dimethylnitrosamine	Little sorption	High	Low	Low	Medium
Methoxydiglycol	Little sorption on organic carbon; some clay sorption	High	Low	Low	Medium
Methoxytriglycol	Little sorption on organic carbon; some clay sorption	High	Low	Low	Medium
2-methylnonane	Good sorption	Low	High	High	Medium
Morpholine	Little sorption	High	Low	Low	Medium
Phenanthrene	Good sorption	Medium	Low	High	Medium

(a) Solubility: High > g/L; g/L $\geq$ Medium $\geq$ mg/L; Low < mg/L

(b) Volatility: High > 5×10^{-2} atm•m³/mol; $5 \times 10^{-2} \geq$ Medium $\geq 1 \times 10^{-4}$ atm•m³/mol; Low < 1×10^{-4} atm•m³/mol.

(c) Sorption: High $R_d > 50$ mL/g; $50 \text{ mL/g} \geq$ Medium ≥ 2 mL/g; Low < 2 mL/g

(d) -- = No basis to make an estimate.

5.0 FUTURE WORK

Regulations dealing with waste disposal require risk, health, and performance assessment analyses before licensing or remedial cleanup of disposal sites. These assessment analyses must predict the transport of radionuclides/contaminants from the waste source to a receptor via pathways that are considered credible. The groundwater pathway is generally most significant when long-term effects are considered. Geochemical reactions between contaminants and the groundwater pathway and hydrologic characteristics largely control release and transport to the accessible environment or receptor. Consequently, data that quantify these geochemical reactions are required to adequately complete a risk/health/performance assessment.

Sites at Hanford that contain contaminated soil include injection wells, covered French drains, cribs (covered drain fields), trenches, and ponds. Currently, the contaminants within inactive disposal sites with contaminated soil exist as precipitated radionuclides and/or hazardous constituents that are bound in the soil column after discharged waste solutions have drained. The types of liquid wastes that were or are currently being disposed of at the Hanford Site range from very-low-ionic-strength cooling waters and condensates to high-salt process wastes, with pH values ranging from less than 1 to more than 12. As mentioned in Section 2.0, the pH of the 33 active waste streams ranges between 5 and 10.5. Many of the alkaline waste streams disposed of in the past contained suspended particles of insoluble compounds. Some waste streams contained significant concentrations of organic solvents and complexing agents. Geochemical conditions (ambient water chemistry, soil exchange capacity, and soil buffering capacities) in the soil may vary widely as a function of discharge fluid chemistry and spatial proximity to the source of discharge.

Conceptual leaching models for contaminated soils have not been well established. It appears that two conceptual models, desorption and solubility, will be needed, depending on the contaminant of interest. To characterize and predict release and transport of radionuclides and/or

hazardous constituents, solubility and sorption values specific to these various environments are needed. The quantity and quality of available experimental and theoretical data vary with the environments. The best, most complete database is the one that corresponds to the moderately alkaline, low-ionic-strength, organic-free groundwater contacting sandy soil, an environment that is in fact typical of much of the Hanford Site's vadose zone and unconfined aquifer. Although the amount of actual data in the database (radionuclide sorption and solubility measurements using Hanford soil and groundwater) is moderate, sufficient experimental work has been reported in the literature that a plausible range of sorption and solubility values can be estimated for many radionuclides and inorganic contaminants. The database needed to quantify, with technical defensibility, specific solubility or sorption values for radionuclides and/or hazardous constituents is generally inadequate, and current transport modeling predictions should be considered as initial, rough estimates. The problem of inadequacy is compounded by the lack of specific data that quantify concentrations of radionuclides, hazardous constituents, and organic and inorganic complexants at existing contaminated soil sites.

To generate a useful database despite the lack of site-specific information, a list of potential conditions and important chemical constituents has been identified from records and past site-specific investigations (Serne and Wood 1990). It is recommended that a series of sorption and empirical solubility tests be run on the basis of the information available on inactive waste streams from Serne and Wood (1990) and the information on active waste streams from Westinghouse Hanford (1989). Hanford Site soils should be used in these tests to provide ranges of sorption and solubility values for use in transport modeling. Because of the current lack of information, emphasis must be placed on organic constituent interactions with Hanford sediments. Actual data that describe the effects of partial saturation on radionuclide or contaminant transport in Hanford soils are very sparse and more must be obtained. The primary tests to be completed include 1) batch sorption/desorption tests to develop distribution coefficients or empirical solubility values and to identify areas requiring further study, and 2) flow-through column tests to quantify retardation factors under the

combined influences of hydrologic flow and chemical/reactivity so that sorption/desorption hysteresis and effects of unsaturated moisture contents, if any, can be determined. The parameters other than the chemical components that should be varied in the test matrix include soil types, moisture content, and flow characteristics (e.g., advection flow rates and diffusion fluxes as a function of moisture content).

The sorption/desorption of an organic group, such as the alkanes or phthalates, should be experimentally examined as a function of several mixed waste compositions. Emphasis should be placed on sorption/desorption systems involving methylene chloride, chloroform, bis(2-ethyhexyl) phthalate, acetone, methyl ethyl ketone, and tetrachloroethylene, which have been recently identified as leaking through the soil column into groundwater monitoring wells adjacent to wastewater disposal sites (Appendix B). Accompanying radionuclides that are also commonly detected as leaking through the soil column into the groundwater with these organics include ^3H , ^{60}Co , ^{90}Sr , ^{99}Tc , ^{106}Ru , ^{129}I , and ^{137}Cs . In many Hanford waste streams, the Co, I, Ru, and Tc are usually anionic or partially anionic and can therefore be expected to sorb poorly on the soil column (i.e., to be mobile). Tritium is present as water and would also be expected to be mobile. However, Cs and Sr are normally present as cations and hence could be expected to sorb readily on the soil column. The fact that ^{90}Sr and ^{137}Cs are commonly found in groundwaters adjacent to wastewater disposal sites suggests that there may be unknown reactions between these radionuclides and the organics in mixed wastes, such as complexing, that have resulted in the leakage of radionuclides that are ordinarily adsorbed strongly. It is suggested that ^{85}Sr and ^{134}Cs or ^{137}Cs , as gamma-emitting isotopes, be added as tracers during selected experiments with the mixed-waste column studies proposed above. The two radionuclides can be counted together to reduce the total number of experiments required to understand the mixed-waste system.

Furthermore, some biodegradation studies (in batch reactors) of the organics and of others in Table 5 that have low adsorption and high water solubility potential should be performed under Hanford-specific conditions. Initial studies should be performed on Hanford sediments and active waste

streams that have been acclimated to optimize growth of native microbes. Particular attention should be paid to the effects of moisture content on the rates of microbial degradation.

These initial batch equilibration and column tests would be used to furnish data for models to describe the process of contaminant sorption/desorption/migration through actual Hanford sediments. This data collection scheme emphasizes laboratory testing based on empiricism; in the tests the expected environment is simulated, and geochemical and microbial reactions are measured through standard adsorption, solubility, and degradation tests. The data collection effort should rely on feedback from performance analyses (Serne and Wood 1990, pp. 1.4-1.6) to ascertain when adequate data have been collected. The data collection scheme proposed is estimated to take 3 person-years effort per year for a total duration of 4 years.

In the constant R_d model, the distribution of the contaminant of interest between the solid adsorbent and solution is assumed to be a constant value. There is no explicit accommodation of dependence on characteristics of the sediment, groundwater, or contaminant concentration. Possible retardation mechanisms include 1) chemical precipitation of bulk solid phases, 2) chemical substitution of one element for another in a solid phase, 3) exchange of a stable isotope of an element with a radioactive isotope in solution, 4) physical filtration of colloids, 5) cation and anion exchange, 6) chemisorption, and 7) physical adsorption. All these mechanisms are melded into the empirical distribution coefficient. The limitations associated with this approach are well known to investigators, but the paucity of Hanford Site-specific geochemical data precludes a more rigorous conceptual retardation model at this time. The constant R_d model is mathematically very simple and can be readily incorporated into transport models and codes.

A second practical conceptual model for adsorption is the parametric R_d model. Numerous statistical strategies have been used to develop empirical relationships that describe R_d as a function of other variables, such as the amount and types of minerals present in the sediment, amounts and types of dissolved species in the groundwater, pH, and Eh. Parametric R_d relationships delineate apparent effects of key variables but do not conclusively identify

controlling processes. These statistical approaches have been demonstrated to yield accurate predictions for conditions within the range of conditions studied. When the parametric R_d retardation model is used, the performance assessment code must keep track of the current values of all of the independent variables that determine the value of R_d . Because of the added complexity of solving the transport equation, explicit use of the parametric R_d model has been rare. On the other hand, the parametric R_d approach can be used to objectively develop a suite of time- or space-dependent constant R_d values to be used in a given performance assessment analysis. This modified approach is recommended for near-future Hanford performance assessment activities. To pursue the parametric R_d approach, the same types of batch and column tests are required but more thorough characterization of the sediments and solutions is necessary. The projected cost for the more detailed characterization would be increased by a factor of 1.5 to 2.

As the data are collected, it would be beneficial to explore the efficacy of more detailed mechanistic studies to elucidate the controlling solubility, adsorption, microbiological, and physical (e.g., volatilization) reactions that determine the fate of the contaminants. Knowledge of the controlling reactions/processes is required to lend credibility to the predictions made using performance, risk, or health assessment computer codes. The costs of performing such mechanistic tests cannot be determined at this time. Again, feedback from performance assessment activities (e.g., sensitivity studies, identification of key contaminants from consequence or health effects modeling) should be used to focus and prioritize the mechanistic tests to be performed.

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APPENDIX A

ENVIRONMENTAL FATE OF ORGANIC ANALYTES
REPORTED IN THE 33 WASTE STREAMS

APPENDIX A

ENVIRONMENTAL FATE OF ORGANIC ANALYTES REPORTED IN THE 33 WASTE STREAMS

Classes of organic analytes found in the 33 waste streams are organized by functional groups. Classes of organics in the 33 waste streams (see Table 5 in main text) include alkanes, alcohols, organic acids, amines, polyhydric alcohols or glycols, ethers, phthalic acid- and carboxylic acid-esters, nitro compounds, caustic aromatics, ketones, aldehydes, halides and polynuclear aromatic hydrocarbons. The above structures are illustrated in Table A.1. In addition to the structural group involved, this appendix also lists other physical and chemical properties of the identified analytes, organized by class. Properties such as the Freundlich 1/N and retardation factor where available, octanol-water partition coefficients ($K_{O/W}$), and soil organic carbon adsorption coefficients (K_{OC}), water solubility, and Henry's law constant used to predict volatility are also provided (sources are identified in the reference list at the back of the appendix). Explanations of these terms are given in Section 4.6 of this report. The Chemical Abstracts Service Registry Number (CAS No.) is given under each analyte when available. Hazardous categories for many of the organic analytes given in this appendix are given by Jungfleisch (1988).

TABLE A.1. Classification of Organic Analytes According to Functional Groups

Analyte Class	Functional Group	Example	
		Formula	Name
Alkane		$\text{H}_3\text{CCH}_2\text{CH}_2\text{CH}_3$	n-butane
Alcohol		H_3COH	methanol
Ether		H_3COCH_3	dimethyl ether
Ester		HCOOCH_3	methylformate (carboxylic acid ester)
		$\text{C}_{16}\text{H}_{22}\text{O}_4$	n-butylphthalate (phthalic acid ester)
Aldehyde		$\text{H}_3\text{CCH}_2\text{CHO}$	propionaldehyde
Ketone			2-butanone
Carboxylic Acid			acetic acid
Amine	$-\text{NH}_2$	CH_3NH_2	methyl amine
Halide	F, Cl, Br or I	H_3CF	methyl fluoride
Nitro Compound			2-nitropropane
Polyhydric Alcohol	Two or more hydroxyl groups that may be substituted		ethylene glycol
Polynuclear Aromatic Hydrocarbon	Benzene rings with common ortho positions		naphthalene
Phenols	Coal tar derivatives based on benzene		phenol
Phosphate	PO_4		tributylphosphate

A.2 ALKANES

Decane

CAS No. 124-18-5

Synonyms: n-decane

Melting Point: -30°C (Buckingham 1982, V2:1459)

Boiling Point: 174°C (Buckingham 1982, V2:1459)

Density: 0.73 g/cm^3 liquid at environmental temperatures
(Buckingham 1982, V2:1459)

Vapor Pressure: 0.175 KPa ($1.75 \times 10^{-3} \text{ atm}$) (MacKay and Shiu 1981)

Solubility: 0.0254 mg/L (MacKay et al. 1981; MacKay and Shiu 1981)
 0.052 mg/L (MacKay and Shiu 1981; Coates et al. 1985)

Henry's Law Constant: $0.3 \text{ atm}\cdot\text{m}^3/\text{mol}$ (Wakeham et al. 1986)
 $5 \text{ to } 1.08 \times 10^4 \text{ atm}\cdot\text{m}^3/\text{mol}$ (MacKay and Shiu 1981)
recommended value $7 \pm 3 \text{ atm}\cdot\text{m}^3/\text{mol}$

$K_{\text{O/W}}$: 1.02×10^5 (Coates et al. 1985)
 1.66×10^6 (Hawker and Connell 1989)

Dodecane

CAS No. 112-40-3

Freezing Point: -12°C (Buckingham 1982, V2:2 389-90)
 -9.6°C (MacKay and Shiu 1981)

Boiling Point: 214.5°C (Buckingham 1982, V2:2 389-90)
 216.3°C (MacKay and Shiu 1981)

Vapor Pressure: $1.57 \times 10^{-2}\text{kPa}$ ($1.57 \times 10^{-4}\text{ atm}$) (MacKay and Shiu 1981)
at 25°C

Solubility: 0.0034 mg/L (MacKay and Shiu 1981);
 0.0037 mg/L (MacKay and Shiu 1981; Sutton and Calder 1974)
 0.0084 mg/L (MacKay and Shiu 1981; Coates et al. 1985)

Henry's Law Constant: $3.17\text{ to }7.86\text{ atm}\cdot\text{m}^3/\text{mol}$ (MacKay and Shiu 1981)
recommended value $7.5 \pm 2.5\text{ atm}\cdot\text{m}^3/\text{mol}$

$K_{\text{O/W}}$: 1.26×10^6 (Coates et al. 1985)
 10^6 (Wakeham et al. 1983)

Degradation Rate: $t_{1/2} \sim 5$ days in soil slurry when dodecane conc 3.3 mg/L
(Haines and Alexander 1974)

$t_{1/2} \sim 10\text{-}15$ days in sediment/seawater (Nazata and
Kondo 1977)

Tridecane

CAS No. 629-50-5

Freezing Point: -5.5°C (Buckingham 1982, V5:5463)

Boiling Point: 234°C (Buckingham 1982, V5:5463)

Density: 0.7564 g/cm^3 ; liquid at environmental temperatures
(Buckingham 1982, V5:5162)

Solubility: 0.00104 mg/L (Coates et al. 1985)

$K_{\text{O/W}}$: 4.47×10^6 (Coates et al. 1985)

Tetradecane

CAS No. 629-59-4

Melting Point: 5.9°C (Buckingham 1982, V5:5162; MacKay and Shiu 1981)

Boiling Point: 253.7°C (Buckingham 1982, V5:5162; MacKay and Shiu 1981)

Density: 0.7628 g/cm³ liquid at environmental temperatures
(Buckingham 1982, V5:5162)

Vapor Pressure: 1.24 to 1.27 x 10⁻³ kPa; liquid at environmental temperatures
(Buckingham 1982, V5:5162)

Solubility: 0.0022 mg/L (MacKay and Shiu 1981; Sutton and Calder 1974)
0.0077 mg/L (MacKay and Shiu 1981; Sutton and Calder 1974)
0.00028 mg/L (Coates et al. 1985)
0.00033 mg/L (Coates et al. 1985)

Henry's Law Constant: 3.47 x 10⁻¹ to 1.1 x 10⁻⁰ atm•m³/mol (MacKay and Shiu 1981)

K_{O/w}: 1.58 x 10⁷ (MacKay and Shiu 1981)

Pentadecane

CAS No. 629-62-9

Melting Point: 10°C (Buckingham 1982, V4:4513)

Boiling Point: 270°C (Buckingham 1982, V4:4513)

Density: 0.7685 g/cm³; could be liquid or solid at environmental temperatures

Solubility: 0.000076 mg/L (Coates et al. 1985)

K_{o/w}: 5.25 x 10⁷ (Coates et al. 1985)

Hexadecane

CAS No. 544-76-3

Synonym: n-hexadecane
cetane

Melting Point: 18.2°C (Buckingham 1982, V3:2895; MacKay and Shiu 1981)

Boiling Point: 287°C (Buckingham 1982, V3:2895; MacKay and Shiu 1981)

Density: 0.7733; liquid at environmental temperatures
(Buckingham 1982, V3:3895)

Vapor Pressure: 8.98×10^{-5} to 9.17×10^{-4} kPa (MacKay and Shiu 1981)
(8.98×10^{-7} to 9.17×10^{-6} atm)

Solubility: 6.3×10^{-3} mg/L (MacKay and Shiu 1981; Coates et al. 1985)
 9.0×10^{-4} mg/L (MacKay and Shiu 1981; Sutton and Calder 1974)
 2.1×10^{-5} mg/L (Coates et al. 1985)

Henry's Law Constant: 3.24×10^{-2} to 2.26×10^{-1} atm•mol (MacKay and Shiu 1981)

K_{oc} : 47 to 387 (Nathwani and Phillips 1977)

$K_{o/w}$: 1.78×10^8 (Nathwani and Phillips 1977)

Adsorption: 56% of a 100-μg/L solution in seawater adsorbed onto bentonite clay
(Meyer and Quinn 1973)
<1% of a 100-μg/L solution in seawater adsorbed onto marine sediments
that contained <1% organic carbon (Meyer and Quinn 1973)

	<u>Silty Clay</u>	<u>Sandy Loam</u>	<u>Silt Loam</u>
pH	5.4	5.1	4.3
Org Content %	9.4	5.8	0.6
Sand %	6.7	72.7	43.7
Silt %	47.9	23.7	48.9
Clay %	45.4	3.6	7.4

Spiked hexadecane 1-100 ppm into Alberta crude oil, batch test 1,000 g soil/L
of liquid

Freundlich K	36.4	4.37	0.271
Freundlich 1/n	0.68	1.21	1.10
K_{oc}	38.7	75.3	46.7

only 60-80% of adsorbed hexadecane desorbed off soils into water (Nathwani
and Phillips 1977)

Heptadecane

CAS No. 629-78-7

Melting Point: 22°C (Buckingham 1982, V3:2852)

Boiling Point: 303°C (Buckingham 1982, V3:2852)

Density: 0.7780 g/cm³; solid at most environmental temperatures
(Buckingham 1982, V3:2852)

K_{o/w}: 3.16 x 10⁸ (Wakeham et al. 1983)

6.17 x 10⁸ (Coates et al. 1985)

Solubility: 6 x 10⁻⁶ mg/L (Coates et al. 1985)

2-methylnonane

CAS No. 871-83-0

Synonym: isodecane

Melting Point: -74.7°C (Buckingham 1982, V4:3958)

Boiling Point: 166.8°C (Buckingham 1982, V4:3958)

Density: 0.7281 g/cm^3 ; liquid at environmental temperatures
(Buckingham 1982, V4:3958)

Solubility: 0.074 mg/L (calculated, not measured) (Coates et al. 1985)

$K_{\text{O/W}}$: 8.2×10^4 (calculated, not measured) (Coates et al. 1985)

Undecane

CAS No. 1120-21-4

Freezing Point: -25.6°C (Buckingham 1982, V5:5661)

Boiling Point: 196°C (Buckingham 1982, V5:5661)

Density: 0.7402 g/cm^3 ; liquid at environmental temperatures
(Buckingham 1982, V5:5661)

Vapor Pressure: $5.22 \times 10^{-2}\text{ kPa}$ ($5.22 \times 10^{-4}\text{ atm}$) (MacKay and Shiu 1981)

Solubility: 0.044 mg/L (MacKay and Shiu 1981)
 0.014 mg/L (Coates et al. 1985)

Henry's Law Constant: $1.85\text{ atm}\cdot\text{m}^3/\text{mol}$ recommended value $1.855 \pm 0.76\text{ atm}\cdot\text{m}^3/\text{mol}$
(MacKay and Shiu 1981)

$K_{\text{o/w}}$: 3.80×10^5 (Coates et al. 1985)
 5.50×10^6 (Hawker and Connell 1989)

Octadecane

CAS NO. 593-45-3

Melting Point: 28°C; a solid at temperatures below 82°F (Buckingham 1982, V4:4351)

Boiling Point: 305 - 307°C (Buckingham 1982, V4:4351)

Water Solubility: 2×10^{-3} to 6×10^{-3} mg/L (Coates et al. 1985)

Henry's Law Constant: very low (Sutton and Calder 1974)

$K_{O/W}$: 2.09×10^9 (Coates et al. 1985)

K_{OC} : 1.29×10^9 (Computed using $K_{OC} = 1.00 \log K_{O/W} - 0.21$)

2-methyl-5-propylnonane

CAS No. = unknown

Compound not found in the literature

A.2 ALCOHOLS

C-OH

Ethyl Alcohol

C_2H_5OH

CAS No. 64-17-5

Synonym: ethanol

$K_{O/W}$: 0.49 (Strengge and Peterson 1989)
0.49 (Hansch and Leo 1985)

Water Solubility: 280 g/L (Strengge and Peterson 1989), miscible
(Riddick et al. 1986)

K_{OC} : 0.30 (Strengge and Peterson 1989)
16 (Syracuse Research Corp. 1988)

Henry's Law Constant: $1.2 \times 10^{-5} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Strengge and Peterson 1989)
 $5.20 \times 10^{-6} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Snider and Dawson 1985)

Vapor Pressure: 59 mm Hg (Strengge and Peterson 1989)

Degradation Rate: $t_{1/2} < 1$ day in river water (Apoteker and Thevenot 1983)
degrades rapidly < 1 day in silty clay loam
(Griebel and Owens 1972)

Butyl Alcohol

CAS No. 71-36-3

Synonyms: n-butyl alcohol
1-butanol

$K_{\text{O/W}}$: 1.224 (Hansch and Leo 1985)
5.6 (Streng and Peterson 1989)
0.88 (Verschuere 1983)

Core Sorption: Freundlich $1/N=1.16$ at 65°C , 500 to 50,000 mg 1-butanol/L;
Freundlich $1/N=1.11$ at 93°C , 500 to 50,000 mg 1-butanol/L,
all on a cleaned core of Cottage Grove sandstone
(Donaldson et al. 1975)

Montmorillonite Sorption: see Stul et al. (1979)

Water Solubility: 74 g/L at 25°C (calculated) (Merck Index 1976)
63.2 g/L at 25°C (Tewari et al. 1982)
79 g/L (Streng and Peterson 1989)

K_{OC} : 72 (calculated) (Syracuse Research Corp. 1988)
4.7 (Streng and Peterson 1989)

Henry's Law Constant: $8.81 \times 10^{-6} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Buttery et al. 1969)
 $4.8 \times 10^{-6} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Streng and Peterson 1989)

Degradation Rate: $t_{1/2} \sim 6$ days in seawater when 3-10 mg/L butyl alcohol-laden
wastewater mixed (Price et al. 1974)

$t_{1/2} \sim 4$ days in freshwater when 3 mg/L added (Hammerton 1955)

$t_{1/2} = 52$ days in soil (Streng and Peterson 1989)

2-Butoxyethanol

CAS No. 111-76-2

Synonyms: ethylene glycol mono-n-butyl ether
butyl cellosolve

$K_{\text{O/W}}$: 6.761 (Hansch and Leo 1985)

Henry's Law Constant: $2.08 \times 10^{-7} \text{ atm}\cdot\text{m}^3/\text{mol}$
(Syracuse Research Corp. recommended)

Water Solubility: miscible (Riddick et al. 1986); 4.5 g/L at 25°C
(Dorigan et al. 1976)

K_{OC} : 67 (calculated) (Syracuse Research Corp. 1988)

2-Propanol

CAS No. 6763-0

Synonyms: isopropyl alcohol
isopropanol
secondary propyl alcohol

$K_{O/W}$: 1.122 (Hansch and Leo 1985)

Water Solubility: miscible (Riddick et al. 1986)

K_{OC} : 25 (calculated) (Syracuse Research Corp. 1988)

Henry's Law Constant: $7.89 \times 10^{-6} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Snider and Dawson 1985)

Degradation Rate: in seawater that has isopropanol (3-10 mg/L)-laden
wastewater added, $t_{1/2} \approx 12$ days (Price et al. 1974)

Benzyl Alcohol

CAS No. 100-51-6

Synonyms: benzenemethanol
phenylmethanol
 α -hydroxytoluene

$K_{O/W}$: 12.30 (Hansch and Leo 1981)

Soil Sorption: Eastern Australian Red-Brown Earth, 1.09% organic carbon,
pH 8.0, 10 mg benzyl alcohol/L in influent solution;
Freundlich adsorption of 0.17 mg/g (Briggs 1981)

Water Solubility: 40 g/L at 25°C (Ringk and Theimer 1978)

A.3 ETHERS

C-O-C

Dimethoxymethane

CAS No. 109-87-5

Synonyms: formaldehyde dimethyl acetal
          methylal
          formal

Melting Point: 105°C (Buckingham 1982, V2:2048)

Boiling Point: 42°C (Buckingham 1982, V2:2048)

Tetrahydrofuran

CAS No. 109-99-9

Synonyms: diethylene oxide
tetramethylene oxide
oxolane

$K_{O/w}$: 2.88 (Hansch and Leo 1979)

Water Solubility: miscible (Dunlop 1966)

Melting Point: -65°C (Grasselli and Ritchey 1975, III:f386)

Boiling Point: 67°C (Grasselli and Ritchey 1975, III:f386)

Density: 0.889 at 20°C (Grasselli and Ritchey 1975, III:f386)

A.4 ESTERS

carboxylic acid esters

phthalic acid esters

Methyl Formate

HCOOCH_3

CAS No. 107-31-3

Synonyms: formic acid methyl ester

Freezing Point: -99°C (Buckingham 1982, V4:3858)

Boiling Point: 31.5°C (Buckingham 1982, V4:3858)

Very flammable; flash point at $\sim 19^{\circ}\text{C}$ (Buckingham 1982, V4:3858)

Density: 0.974 at 20°C (Grasselli and Ritchey 1975, III:f297)

Water Solubility: very soluble (Grasselli and Ritchey 1975, III:f297)

Di-n-Butyl Phthalate

CAS No. 84-74-2

Synonyms: n-butyl phthalate
elacol
DBP
1,2-benzenedicarboxylic acid dibutyl ester
phthalic acid dibutyl ester

$K_{O/W}$: 52,490 (Hansch and Leo 1985)
40,000 (Streng and Peterson 1989)

Soil Sorption: Natural seawater with 19 to 3,930 μg dibutyl phthalate/L,
~1% organic content, 25°C (Sullivan et al. 1982)

Material	Freundlich Adsorption, μg
Texas Shelf Montmorillonite	3,930 $\mu\text{g/L}$ solution - 44 μg adsorption 22 $\mu\text{g/L}$ solution - 1.9 μg adsorption
Kaolinite	3,840 $\mu\text{g/L}$ solution - 20 μg adsorption 19 $\mu\text{g/L}$ solution - 4 μg adsorption
Ca-Montmorillonite	3,440 $\mu\text{g/L}$ solution - 4 μg adsorption 27 $\mu\text{g/L}$ solution - 36 μg adsorption

Water Solubility: 11.2 mg/L at 25°C (Howard et al. 1985)
400 mg/L at 25°C (Verschuere 1983)

K_{OC} : 1,800 (Russell and McDuffie 1986)
170,000 (Streng and Peterson 1989)

Henry's Law Constant: $1.81 \times 10^{-6} \text{ atm}\cdot\text{m}^3/\text{mol}$ at 23°C (Atlas et al. 1983)
 $2.8 \times 10^{-7} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Streng and Peterson 1989)

Degradation Rate: $t_{1/2}$ <14 days in freshwater sediment (Johnson et al. 1984)

$t_{1/2}$ = 15.4 days soil/activated sludge (pH=7) after 14-day acclimation period (Sugatt et al. 1984)

$t_{1/2}$ = 7 to 14 days in freshwater sediment (pond), mixed 9 parts water, 1 part sediment (Johnson and Lulves 1975; Johnson et al. 1984)

$t_{1/2}$ = 1 to 3 days in freshwater at 0.5 mg/L concentration after 2- to 7- day acclimation period (Walker et al. 1984)

$t_{1/2}$ = 2 to 4 days in freshwater/sediment environment at 0.5 mg/L loading of phthalate (Walker et al. 1984)

$t_{1/2}$ = 60 to 70 days in sandy soil, pH = 6.2 in dissolved organic contents = 1.4% when original conc. 1,000 mg/L phthalate (Inman et al. 1984)

$t_{1/2}$ = 30 to 50 days in silt loam saturated with water containing 1.96% dissolved organic carbon when original conc. 1,000 mg/L phthalate (Inman et al. 1984)

Di-n-Octyl Phthalate

CAS No. 117-84-0

Synonym: 1,2-benzenedicarboxylic acid di-n-octyl ester

$K_{O/W}$: 165,900 (Hansch and Leo 1985) (not a recommended value)
 7.4×10^9 (Streng and Peterson 1989)

Water Solubility: 3 mg/L at 25°C (Wolfe et al. 1980)
0.34 mg/L (Streng and Peterson 1989)
0.285 mg/L (Verschuere 1983)

K_{OC} : 2,385 (Syracuse Research Corp. 1988) calculated value
 3.6×10^9 (Streng and Peterson 1989)

Henry's Law Constant: 4.45×10^{-7} atm•m³/mol at 25°C,
(Syracuse Research Corp. 1988)
 5.5×10^{-6} atm•m³/mol (Streng and Peterson 1989)
 1×10^{-6} atm•m³/mol (Petrasek et al. 1983)

Degradation Rate: $t_{1/2}$ = 5 days in freshwater/sediment environment with
initial concentration 5 mg/L (Sanborn et al. 1975)

Bis(2-ethylhexyl)phthalate

CAS No. 117-81-7

Synonyms: di(2-ethylhexyl)phthalate
dioctyl phthalate
1,2-benzenedicarboxylic acid bis(2-ethylhexyl)ester octoil

$K_{O/W}$: 128,800 (OECD 1981)
 4.1×10^9 (Streng and Peterson 1989)

Soil Sorption: Linear isotherm on kaolinite, montmorillonites, and sediments;
more adsorption than dibutyl phthalate, less adsorption in
distilled water than in seawater (Sullivan et al. 1981, 1982)

Summary of phthalate sorption results in seawater at 25°C (Sullivan et al. 1982).

Adsorbate	Adsorbent	Wt. Range of Adsorbent, mg	Initial Phthalate conc., $\mu\text{g/L}$	K
BEHP	montmorillonite	6-80	377	11.4 ± 1.1
[^{14}C]BEHP	montmorillonite	5-77	13	12.7 ± 0.8
[^{14}C]BEHP	kaolinite	6-126	13	12.1 ± 1.8
BEHP	calcite	23-178	208	1.8 ± 0.8
[^{14}C]BEHP	calcite	3-210	7	1.8 ± 0.4
[^{14}C]BEHP	calcium montmorillonite	6-80	16	1.3 ± 0.3
[^{14}C]BEHP	sediment	11-83	6	5.1 ± 1.0
[^{14}C]BEHP	montmorillonite (distilled water)	6-80	9	4.6 ± 0.3
DBP	montmorillonite	55-687	3,930	0.044 ± 0.005
[^{14}C]DBP	montmorillonite	6-58	22	0.019 ± 0.002
DBP	kaolinite	25-621	3,840	0.020 ± 0.003
[^{14}C]DBP	kaolinite	4-64	19	0.004 ± 0.001
DBP	calcite	30-435	3,710	0.005 ± 0.001
[^{14}C]DBP	calcite	8-94	25	0.010 ± 0.002
DBP	calcium montmorillonite	26-542	3,440	0.004 ± 0.001
[^{14}C]DBP	calcium montmorillonite	7-90	27	0.036 ± 0.017
DBP	sediment	9-79	19	0.149 ± 0.017

BEHP = Bis(ethylhexyl)phthalate

DBP = Di-n-butyl phthalate

K = partition coefficient = ng of phthalate/mg of adsorbent divided by the ng
of phthalate/mL of seawater

For kaolinite, calcite, and Ca-montmorillonite, adsorption = desorption over 12 hours.

Water Solubility: 0.40 mg/L at 25°C (Wolfe et al. 1980)
0.34 mg/L at 25°C (Howard et al. 1985)
0.4 mg/L (Streng and Peterson 1989)

K_{oc}: 87,000 (Streng and Peterson 1989)

Henry's Law Constant: 1.47×10^{-5} atm•m³/mol at 25°C (Syracuse Research Corp. 1988)
 4.4×10^{-7} atm•m³/mol (Streng and Peterson 1989)

Degradation Rate: t_{1/2} ~5 days in seawater near Japanese factory
(Haltori et al. 1975)

t_{1/2} ~14 days in seawater away from pollution
(Haltori et al. 1975)

t_{1/2} ~14 days in river water in Japan
(Haltori et al. 1975)

t_{1/2} = 15 to >30 days in freshwater pond with 1 mg/L
starting conc. (Johnson and Lulves 1975)

t_{1/2} = <7 to 30 days in seawater when initial conc. = 0.001
to 0.1 mg/L (Perez et al. 1985)

t_{1/2} = 28 days in eutrophic lake at conc. 10⁻⁶ to 1 mg/L
(Rubin et al. 1982; Subbo-Rao et al. 1982)

t_{1/2} >> 14 days in freshwater/sediment at
1-70 mg/L (Schwartz et al. 1979)

t_{1/2} < 140 days in sandy loam inoculated with sludge with
2-20 mg/L phthalate (Fairbanks et al. 1985)

t_{1/2} ~ 15 garden soil at 60% moisture, pH 8.2, 500 mg/L
phthalate (Shanker et al. 1985)

Butyl Benzyl Phthalate

CAS No. 85-68-7

$K_{O/W}$: 81,280 (Hansch and Leo 1985)
104.78 (Verschueren 1983)

Soil Sorption: Three soils with organic carbon contents of 0.70 to 2.0%,
influent concentration between 0 and 1.0 mg/L. Freundlich
adsorption from 68 to 350 mg butyl benzyl phthalate
(Gledhill et al. 1980)

Water Solubility: 2.69 mg/L at 25°C (Howard et al. 1985)
2.90 mg/L at 25°C (Verschueren 1983)

K_{OC} : 17,000 (Russell and McDuffie 1986)

Henry's Law Constant: 1.26×10^{-6} atm•m³/mol (Syracuse Research Corp. 1988)
at 25°C (calculated value)

Degradation Rate: $t_{1/2} < 2$ days in Mississippi River water when added at
1 mg/L conc. (Saeger and Tucker 1976)

A.5 ALDEHYDES

Butyraldehyde

CAS No. 123-72-8

Synonym: butanal

$K_{O/W}$: 7.586 (Hansch and Leo 1985)

Water Solubility: 30 to 71 g/L at 25°C (Smith and Bonner 1951)

K_{OC} : 9.4 (Syracuse Research Corp. 1988) calculated value

Henry's Law Constant: 1.15×10^{-4} atm•m³/mol at 25°C (Buttery et al. 1969)

Degradation Rate: degrades fast in sewage (in BIoDEG summary database, no reference given)

Benzaldehyde

CAS No. 100-52-7

Synonym: benzoic aldehyde

$K_{O/W}$: 30.2 (Hansch and Leo 1981)

Water Solubility: 3 g/L at 25°C (Sherman 1978).

Degradation Rate: degrades fast in sewage (in BIODEG summary database, no reference given)

A.6 KETONES

Acetone

CAS No. 67-64-1

Synonyms: β -ketopropane
2-propanone
dimethylketone

$K_{o/w}$: 0.575 (Hansch and Leo 1985)
0.581 (Streng and Peterson 1989)

Soil Sorption: No sorption on montmorillonite, kaolinite, stream sediments,
local stream algae, and local stream mold (Rathbun et al. 1982)

Water Solubility: miscible (Riddick et al. 1986),
1,000 g/L (Streng and Peterson 1989)

K_{oc} : 18 (Syracuse Research Corp. 1988) calculated value
2.2 (Streng and Peterson 1989)

Henry's Law Constant: $3.88 \times 10^{-5} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Snider and Dawson 1985)
 $2.10 \times 10^{-5} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Streng and Peterson 1989)

Degradation Rate: in seawater with 3-10 mg/L acetone added with wastewater
 $t_{1/2} \sim 7$ days (Price et al. 1974)
in soils $t_{1/2} = 4.8$ days (Streng and Peterson 1989)

Methyl Ethyl Ketone (MEK)

CAS No. 78-93-3

Synonyms: 2-butanone
2-oxobutane

K_{ow} : 1.069 (Hansch and Leo 1985)
1.9 (Streng and Peterson 1989)

Core Sorption: Freundlich $1/N=1.00$ at 60°C , 500 to 5,000 mg methyl ethyl ketone/L; Freundlich $1/N=0.99$ at 38°C , 500 to 5,000 mg methyl ethyl ketone/L, all on a cleaned core of Cottage Grove sandstone (Donaldson et al. 1975)

Water Solubility: 223 g/L at 25°C (Taft et al. 1985)
270 g/L (Streng and Peterson 1989)

K_{oc} : 5.2 (Syracuse Research Corp. 1988) calculated value
4.5 (Streng and Peterson 1989)

Henry's Law Constant: $5.59 \times 10^{-5} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Park et al. 1987)
 $2.7 \times 10^{-5} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Streng and Peterson 1989)

Degradation Rate: $t_{1/2} \sim 7.5$ days in seawater at 3-10 mg/L MEK when wastewater laden with MEK added (Price et al. 1974)
 $t_{1/2} \leq 1$ day in Polish river water at 10 mg/L loading, with 200 to 400 ppm up to 9 days (Dojlido 1979)
 $t_{1/2} = 16$ days in soil (Streng and Peterson 1989)

Methyl n-Butyl Ketone

methyl butyl ketone

CAS No. 591-78-6

Synonym: 2-hexanone

$K_{\text{O/W}}$: 23.99 (Hansch and Leo 1981)
24 (Streng and Peterson 1989)

Water Solubility: 17.5 g/L at 20°C (Papa and Sherman 1981)
14 g/L (Streng and Peterson 1989)

K_{OC} : 15 (Streng and Peterson 1989)

Henry's Law Constant: $1.1 \times 10^{-5} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Streng and Peterson 1989)

MIBK

CAS No. 108-10-1

Synonyms: methyl isobutyl ketone
hexanone
4-methyl-2-pentanone

$K_{O/W}$: 15.48 (Syracuse Research Corp. 1988) calculated value
5.3 (Streng and Peterson 1989)

Water Solubility: 19 g/L (Streng and Peterson 1989)
19.0 g/L (Verschuere 1983)

K_{OC} : 19 (Syracuse Research Corp. 1988) calculated value
19 (Streng and Peterson 1989)

Henry's Law Constant: $1.38 \times 10^{-4} \text{ atm}\cdot\text{m}^3/\text{mol}$ at 25°C (Syracuse Research Corp. 1988) calculated value
 $4.2 \times 10^{-5} \text{ atm}\cdot\text{m}^3/\text{mol}$ at 25°C (Streng and Peterson 1989)

Degradation Rate: $t_{1/2} = 15$ days in seawater when present at 3-10 mg/L
concentration added to seawater as wastewater
(Price et al. 1974)

Methyl n-Propyl Ketone

CAS No. 107-87-9

Synonyms: 2-Pentanone
ethyl acetone

$K_{O/W}$: 8.129 (Hansch and Leo 1985)

Water Solubility: 43 g/L at 25°C (Yalkowsky et al. 1987)

Henry's Law Constant: $6.36 \times 10^{-5} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Hine and Mookerjee 1975)

Degradation Rate: biodegrades fast in sewage after system acclimates to presence of compound (in BIODÉG summary database, no references given)

Acetophenone

CAS No. 98-86-2

Synonyms: 1-phenylethanone
phenyl methyl ketone
acetylbenzene

K_{ow} : 38.01 (Hansch and Leo 1985)
48 (Strenger and Peterson 1989)

Selected chemical and physical properties of the sediments and soils

Soil	pH (1 : 1)	CEC meq/100g)	Organic carbon, %	Sand, %	Silt, %	Clay, %	$K_p^{(a)}$	K_{oc}
1	7.79	23.72	2.07	3.0	41.8	55.2	0.89	43
2	7.44	19.00	2.28	33.6	35.4	31.0	0.56	24
3	7.83	33.01	0.72	0.2	31.2	68.6	0.68	95
4	8.32	3.72	0.15	82.4	10.7	6.8	0.07	48
5	8.34	12.40	0.11	7.1	75.6	17.4	0.09	82
6	4.45	18.86	0.48	2.1	34.4	63.6	0.12	25
7	7.79	11.30	0.95	15.6	48.7	35.7	0.27	28
8	7.76	15.43	0.66	34.6	25.8	39.5	0.30	46
9	5.50	8.50	1.30	0.0	71.4	28.6	0.29	22
10	7.60	8.33	1.88	50.2	42.7	7.1	0.85	45
11	7.55	8.53	1.67	26.2	52.7	21.2	0.53	31
12	6.70	31.15	2.38	17.3	13.6	69.1	0.68	29
13	7.75	20.86	1.48	1.6	55.4	42.9	0.66	45
14	6.35	3.72	1.21	67.6	13.9	18.6	0.44	36

(a) Modified Freundlich partition coefficient, $1/n=1$, $K_p=0.04 + 0.32$ (organic carbon percentage)

Influent contained 138 - 1,108 mg acetophenone/L, 25°C (Khan et al. 1979), sorption correlates with organic carbon content.

$R_d = 0.14$ Soil with 11.2% clay but no other characterization (Gerstl and Mingelgrin 1984)
 $R_d = 0.05$ Soil with 6.9% clay but no other characterization (Gerstl and Mingelgrin 1984)
 $R_d = 0.37$ Soil with 61.1% clay but no other characterization (Gerstl and Mingelgrin 1984)
 $R_d = 0.15$ Soil with 23.8% clay but no other characterization (Gerstl and Mingelgrin 1984)
 $R_d = 0.30$ Soil with 72.5% clay but no other characterization (Gerstl and Mingelgrin 1984)
 $R_d = 0.22$ Soil with 10.6% clay but no other characterization (Gerstl and Mingelgrin 1984)

Water Solubility: 6.13 g/L at 25°C (Southworth and Keller 1986)
 5.5 g/L (Streng and Peterson 1989)

K_{oc} : average of 14 soils, 45 (Khan et al. 1979)
 23 (Streng and Peterson 1989), $10^{0.81}$ to $10^{1.26}$

Henry's Law Constant: 1.07×10^{-5} atm•m³/mol at 25°C (MacKay et al. 1982)
 3.2×10^{-5} atm•m³/mol (Streng and Peterson 1989)

Degradation Rate: $t_{1/2} = 4$ days based on field observations (Dragun 1986)

$t_{1/2} = 3.6$ days based on field observations in soil in The Netherlands, redox condition not specified (Zoeteman et al. 1981)

$t_{1/2} = <11$ days (~4 days) in Ohio River; compound added in sewage overall concentration 20.5 mg/L, system pH 7.2 (Ludzack and Ettinger 1963)

A.7 CARBOXYLIC ACIDS

Pelargic Acid perhaps Westinghouse Hanford (1989) used this to mean pelargonic acid, which has the following data

$\text{H}_3\text{C}(\text{CH}_2)_7\text{COOH}$

CAS No. 112-05-0

Synonym: nonanoic acid

Melting Point: 15°C (Buckingham 1982, V4:4310)

Boiling Point: 255°C (Buckingham 1982, V4:4310)

Water Solubility: insoluble (Grasselli and Ritchey 1975, III:n610)

Hexadecanoic Acid

CAS No. 57-10-3

Synonym: palmitic acid

Melting Point: 64°C (Buckingham 1982, V3:2895)

Boiling Point: 390°C (Buckingham 1982, V3:2895)

Water Solubility: insoluble (Grasselli and Ritchey 1975, III:h284)

Benzoic Acid

CAS No. 65-85-0

$K_{O/w}$: 74.13 (Chiou et al. 1977)
74 (Streng and Peterson 1989)

Dissociation Constant: 4.205 (Sarjeant and Dempsey 1979)
(see also Mabey and Mill 1978)

Soil Sorption: No sorption (Bailey et al. 1968). 25°C;
Na-montmorillonite, CEC of 87 meq/100 g, solution pH 6.8,
100 μ mol benzoic acid/L; H-montmorillonite, CEC of 73.5
meq/100g, solution pH 3.35, 100 μ mol benzoic acid/L

Water Solubility: 2.70 g/L at 18°C (Chiou et al. 1977; MacKay et al. 1980)
3.4 g/L at 25°C (Streng and Peterson 1989)

K_{OC} : 46 (Streng and Peterson 1989)

Henry's Law Constant: 0.287×10^{-5} atm•m³/mol (U.S. EPA 1981)
 1.3×10^{-7} atm•m³/mol (Streng and Peterson 1989)

A.8 AMINES

-NH₂

Dimethylnitrosamine

CAS No. 62-75-9

Synonyms: n-nitrosodimethylamine
2,2'-(nitrosoimino)-bisethanol
2,2'-nitrosiminodiethanol

$K_{O/W}$: 0.269 (Hansch and Leo 1985)

	<u>% Organic</u>	<u>pH</u>	<u>Appearance in Column Effluent</u>
Soil Column Transport:			
Williamson silt loam	1.9	5.8	50 mL
Lima loam	3.8	7.8	40 mL
Deerfield sand	2.5	5.1	30 mL
Scarboro sand	14.8	5.6	45 mL
Influent: 5 mg dimethylnitrosamine/L, 25°C.			
Conclusion: Dimethylnitrosamine moves as rapidly in the soil column as chloride (Dean-Raymond and Alexander 1976). (~ no adsorption).			

Water Solubility: miscible (Callahan et al. 1979)

K_{OC} : 12 (Syracuse Research Corp. 1988) calculated value

Henry's Law Constant: 2.63×10^{-7} atm•m³/mol at 20°C (Syracuse Research Corp. 1988) calculated value

Degradation Rate: $t_{1/2}$ = 10 days in uncharacterized soil, pH 6.4 in laboratory batch study. Breaks down to methylamine and formaldehyde (Kaplan and Kaplan 1985)

17% percent degradation over a 10-30 day period in a sandy loam with 2.2% OC moistened to field capacity and pH 4.8, rate is fast initially, then levels off (Mallik et al. 1981)

no degradation in 2 days in a silt loam (Tate and Alexander 1976)

N-Methoxymethanamine

CAS No.

Compound not found in the literature.

3,5-Dimethylpyridine

CAS No. 591-22-0

Synonym: 3,5-lutidine

Boiling Point: 171°C (Buckingham 1982, V2:2217)

Moderately soluble in water (Buckingham 1982, V2:2217)

Density: 0.942 at 20°C (Grasselli and Ritchey 1975, IV:p3725)

Morpholine

CAS No. 110-91-8

Synonyms: tetrahydro-2H-1,4-oxazine
diethylene imidoxide
diethylene oximide

$K_{O/W}$: 0.138 (Hansch and Leo 1985)

Water Solubility: miscible (Nieneker 1971; Riddick et al. 1986)

Henry's Law Constant: $1.41 \times 10^{-7} \text{ atm}\cdot\text{m}^3/\text{mol}$ at 25°C (Syracuse Research Corp. 1988) calculated value

Degradation Rate: $t_{1/2} \gg 14$ days (only 2% degraded in 14 days) in river mud, pH=7.5 at morpholine conc. of 10-100 mg/L (Calamari et al. 1980)

A.9 HALIDES

F, Cl, Br, or I

Dichlorofluoromethane

Cl_2CHF

CAS No. 75-43-4

Synonyms: Freon 21
alcofrene type 5
arcton 7
dichloromonofluoromethane
genetron 21

Heavy, colorless gas

Boiling Point: 8.9°C

Melting Point: -135°C

Vapor Pressure: 2 atm at 28.4°C

Vapor Density: 3.82 compared to 1.00 for air

Use: refrigerant (Sax and Lewis 1989)

Water Solubility: insoluble (Grasselli and Ritchey 1975, III:m326)

Tetrachloroethylene

CAS No. 127-18-4

Synonyms: ethylene tetrachloride
perchloroethylene

$K_{\text{O/W}}$: 2,512 (Hansch and Leo 1979)
400 (Munz and Roberts 1987)

Soil Sorption: Willamette silt loam; 3.3% sand, 69% silt, 26% clay, 1.6% organic carbon content; isotherms are linear, Freundlich 1/N is 1.0; calculated K_{OC} was 210 (Chiou et al. 1977)

	Materials	Sorption
Sediment Sorption:	1. Granular bentonite clay	10% in 10 min
	2. Dolomite limestone	Slight
	3. Ottawa sand	None
	4. Peat moss	40% in 10 min
	(Dilling et al. 1975) in 1 mg tetrachloroethylene/L influent, 25°C, closed system.	

Lincoln fine sand, 92% sand, 0.087% organic carbon, CEC of 3.5 meq/100 g pH 6.4, 20°C; Freundlich adsorption was 0.2, K_{OC} calculated at 200, retardation factor of 2.5 (Wilson et al. 1981).

Water Solubility: 200 mg/L at 25°C (Coca and Diaz 1980)
150 mg/L (Streng and Peterson 1989)

K_{OC} : 238 at 25°C (Friesel et al. 1984)
360 (Streng and Peterson 1989)

Henry's Law Constant: $1.84 \times 10^{-2} \text{ atm}\cdot\text{m}^3/\text{mol}$ at 25°C (Munz and Roberts 1987)
 $2.6 \times 10^{-2} \text{ atm}\cdot\text{m}^3/\text{mole}$ (Streng and Peterson 1989)

Degradation Rate: $t_{1/2} = 300$ days based on field observations in soil/groundwater (Dragun 1986)

$t_{1/2} = 13$ days in lab when soil inoculated with microbial flora (Dragun 1986)

Chloroform

CHCl_3

CAS No. 67-66-3

Synonym: Trichloromethane

$K_{o/w}$: 93.3 (Chiou et al. 1977)
93 (Streng and Peterson 1989)

Freundlich 1/N: 0.77 to 0.95 (Hutzler et al. 1983) (sands, sandy loam, loamy sand and silt loam); no appreciable sorption on soils of lower organic carbon content.

Soil Sorption: Retardation factor <1.5 (Wilson et al. 1981); column movement per day in Lincoln fine sand was 41% in effluent, 54% volatilized, 5% degraded with 0.90 mg CHCl_3/L ; 31% in effluent, 61% volatilized and 8% degraded with 0.25 mg CHCl_3/L influent; Lincoln fine sand organic content was 0.087%, 92% sand, 5.9% silt and 2.1% clay, CEC was 3.5 meq/100 g.

Water Solubility: 7.95 g/L at 25°C (Chiou et al. 1977; MacKay et al. 1980),
8.00 g/L at 25°C (Wilson et al. 1981)
10.62 g/L at 0°C (Deshon 1979)
8.2 g/L (Streng and Peterson 1989)
7.9 to 8.2 g/L at 20°C (MacKay and Shiu 1981).

K_{oc} : 80 (Wilson et al. 1981)
31 (Streng and Peterson 1989)

Henry's Law Constant: $3.67 \times 10^{-3} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Gossett 1987)
 $2.9 \times 10^{-3} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Streng and Peterson 1989)
 $3.8 \pm 0.3 \times 10^{-3} \text{ atm}\cdot\text{m}^3/\text{mol}$ (MacKay and Shiu 1981)

Melting Point: -63.5°C (MacKay and Shiu 1981)

Boiling Point: -61.7°C (MacKay and Shiu 1981)

Vapor Pressure: $2.0 \text{ to } 3.3 \times 10^1 \text{ kPa}$ (0.2 to 0.3 atm at 20°C)
(MacKay and Shiu 1981)

Methylene Chloride

CAS No. 75-09-2

Synonyms: dichloromethane
              methylene dichloride
              Freon 30

$K_{\text{O/w}}$: 17.38 (Hansch and Leo 1985)
          20 (Streng and Peterson 1989)

	Materials	Sorption
Sediment Sorption:	1. Granular bentonite clay	10% in 10 min
	2. Dolomite limestone	Slight
	3. Ottawa sand	None
	4. Peat moss	40% in 10 min
	(Dilling et al. 1975)	

Water Solubility: 13.7 g/L at 20°C (Horvath 1982)
                  20 g/L (Streng and Peterson 1989)
                  16.7 g/L (Verschueren 1983)

K_{oc} : 28 (Sabljić 1984)
          8.8 (Streng and Peterson 1989)

Henry's Law Constant: $2.19 \times 10^{-3} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Gossett 1987)
                           $2.0 \times 10^{-3} \text{ atm}\cdot\text{m}^3/\text{mol}$ (Streng and Peterson 1989)

Degradation Rate: $t_{1/2} = 35 \text{ to } 50 \text{ days}$ at 5 mg/L present in Rhine River
                          (Zoeteman et al. 1980)

$t_{1/2} = 3.3 \text{ days}$ (Streng and Peterson 1989)

Degrades rapidly under anaerobic soil conditions
(Cline and Viste 1985)

A.10 NITRO COMPOUNDS

Methyl nitrate

H_3CONO_2

CAS No. 598-58-3

Synonym: nitric acid methyl ester

Boiling Point: 65°C (Buckingham 1982, V4:3930)

Density at 25°C : 1.20 (Buckingham 1982, V4:3930)
Vapor explodes upon heating
Highly irritant

Melting Point: -82.3°C (Grasselli and Ritchey 1975, III:n534)

Water Solubility: slightly soluble (Grasselli and Ritchey 1975, III:n534)

Butyl nitrate

CAS No. 928-45-0

Synonyms: nitric acid butyl ester
n-butylnitrate

Boiling Point: 136°C (Buckingham 1982, VI:938)

Flammable liquid; reacts explosively with Lewis acids (aluminum chloride, boron trifluoride, etc.) (Sax and Lewis 1989, VII:642)

Water Solubility: insoluble (Grasselli and Ritchey 1975, III:n530)

A.11 POLYHYDRIC ALCOHOLS

Two or more hydroxyl groups (may be substitutions for hydrogens).

Methoxydiglycol

$\text{H}_3\text{COCH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{OH}$

CAS No. 111-77-3

Synonyms: 2-(2-methoxyethoxy)ethanol
diethylene glycol methyl ether
diethylene glycol monomethyl ether

Water Solubility: 25°C miscible (Kirk-Othmer 1983, 21:382-383)

Boiling Point: 1 atm 194°C (Kirk-Othmer 1983, 21:382-383)

Vapor Pressure at 25°C: 0.024 kPa (Kirk-Othmer 1983, 21:382-383)

Freezing Point: -76°C (Kirk-Othmer 1983, 21:382-383)

Specific Gravity at 20°C: 1.021 (Kirk-Othmer 1983, 21:382-383)
(see also Dow Chemical Co. 1981)

Methoxytriglycol

CAS No. 112-35-6

Synonyms: 2-[2-(2-methoxyethoxy)ethoxy]ethanol
triethylene glycol monomethyl ether
methoxy triethylene glycol

Little information located

Boiling Point: 249°C (Grasselli and Ritchey 1975, III: e532)

Butoxyglycol

CAS No. 111-76-2

Synonym: ethylene glycol mono-n-butyl ether
same as 2-butoxyethanol (see page A.18)

Water Solubility at 25°C: miscible (Kirk-Othmer 1983, 21:384-385)

Boiling Point at 1 atm: 170°C (Kirk-Othmer 1983, 21:384-385)

Vapor Pressure at 25°C: 0.11 kPa (Kirk-Othmer 1983, 21:384-385)

Specific Gravity at 20°C: 0.90075 (Kirk-Othmer 1983, 21:384-385)

Butoxydiglycol

CAS No. 112-34-5

Synonyms: 2-(2-butoxyethoxy) ethanol
diethylene glycol monobutyl ether
diethylene glycol mono-n-butyl ether

Degradation Rate: In sewage, biodegrades fast once the system acclimates to presence of the compound in some instances (results inconsistent) (in BIODÉG summary database; no references cited)

Water Solubility at 25°C: miscible (Kirk-Othmer 1983, 21:384-385)

Boiling Point at 1 atm: 231°C (Kirk-Othmer 1983, 21:384-385)

Vapor Pressure at 25°C: 0.003 kPa (Kirk-Othmer 1983, 21:384-385)

Specific Gravity at 20°C: 0.9553 (Kirk-Othmer 1983, 21:384-385)

Freezing Point: -68°C (Kirk-Othmer 1983, 21:382-383)

Ethoxytriethylene glycol

$\text{C}_2\text{H}_5\text{OCH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{OH}$

CAS No. 112-50-5

Synonyms: 2-[2-(2-ethoxyethoxy)ethoxy]ethanol
triethyleneglycol monoethyl ether
ethoxytriethylene glycol

Degradation Rate: $t_{1/2} > 20$ days (only 22% degraded after 20 days) in seawater
spiked with 3-10 mg/L glycol (Price et al. 1974)

Little information located

Boiling Point: 256°C (Grasselli and Ritchey 1975, IV: t1388)

A.12 POLYNUCLEAR AROMATIC HYDROCARBONS

Benzene Rings with Common Ortho Positions

Phenanthrene

CAS No. 85-01-8

Synonym: isometric with anthracene

$K_{o/w}$: 28,840 (Hansch and Leo 1985)
29,000 (Streng and Peterson 1989)

Freundlich 1/N: 1.0 (Karickhoff et al. 1979), DOE Run and Hickory Hill coarse silts 3.27% and 2.78% organic carbon content, respectively, 20- to 50- μ m particle size range, 20 mg phenanthrene/mL, 25°C

Water Solubility: 1.15 mg/L at 25°C (Schwarz 1977)
1.3 mg/L (Streng and Peterson 1989)

K_{oc} : 230,000 (Karickhoff et al. 1979)
140,000 (Streng and Peterson 1989)

Henry's Law Constant: 2.28×10^{-5} atm $\cdot$ m³/mol (Syracuse Research Corp. 1988)
calculated value,
 1.6×10^{-4} atm $\cdot$ m³/mol (Streng and Peterson 1989)
 $4.0 \pm 0.8 \times 10^{-5}$ atm $\cdot$ m³/mol (MacKay and Shiu 1981)

Melting Point: 101°C (MacKay and Shiu 1981)

Boiling Point: 339°C (MacKay and Shiu 1981)

Solid at environmental conditions

Vapor Pressure: 2.67×10^{-7} atm (MacKay and Shiu 1981)

Adsorption: no adsorption on bentonite clay from seawater
(Meyer and Quinn 1973)

R_d = 50 for sandy loam, pH 7.9, CEC = 10.10 meq/100g, OC = 0.5%
(Sims et al. 1988)

R_d = 160 for sandy loam, pH 4.8, CEC = 6.35 meq/100g, OC = 0.94%
(Sims et al. 1988)

Degradation Rate: in sandy loam, pH 7.9, partially saturated (80%),
 $t_{1/2}$ = 16 days at 900 ppm loading in soil (Sims et al. 1988)

in sandy loam, pH 4.8, partially saturated (80%),
 $t_{1/2}$ = 35 days at 900 ppm loading in soil (Sims et al. 1988)

A.13 PHENOLS

Phenol

CAS No. 108-95-2

Synonyms: carbolic acid
phenic acid
phenylic acid
phenyl hydroxide
hydroxybenzene
oxybenzene

K_{ow} : 28.84 (Hansch and Leo 1985)
29 (Gaffney et al. 1987)

Soil Sorption: No adsorption in silty clay (Greskovich 1974), adsorbed mainly by soil humus (Mozheiko and Solod 1969), no adsorption on kaolinite or montmorillonite with 1 to 100 mg phenol/L in the influent (Luh and Baker 1970)

Captina Silt Loam   Palouse Silt Loam
(Scott et al. 1983)

Percent sand	33	17
Percent silt	55	59
Percent clay	12	24
CEC	6	22
pH	5.4	5.4
Temperature	25°C	25°C
% Organic carbon	1.1	3.6
Freundlich adsorption	0.57	11.9
Freundlich 1/N	0.96	0.76
K_{oc} calculated	91	38.8

No phenol adsorption on goethite (Yost and Anderson 1984). Phenol sorption can vary significantly with pH and soil from oxide content- K_{oc} of 16 (Boyd 1982). No adsorption on aquifer materials (Eholich et al. 1982)

K_{OC} : 14 (Streng and Peterson 1989).

Water Solubility: 82.8 g/L at 25°C (Southworth and Keller 1986)
93 g/L (Streng and Peterson 1989)

Henry's Law Constant: 3.33×10^{-7} atm•m³/mol at 25°C (Gaffney et al. 1987),
 4.5×10^{-7} atm•m³/mol (Streng and Peterson 1989)

K_{OC} : $10^{3.46}$ based on Connecticut Lake sediments with 4.2 to 10.2% OC
(Isaacson and Frink 1984)

$10^{1.43}$ based on various soils (Dragun 1986)

Biodegradation Rate: $t_{1/2}$ = 1 to 2.2 days in silt loams with 1.1 to 3.6%
organic carbon, pH 5.4, and an extremely low
concentration of phenol (Sims and Overcash 1983)

$t_{1/2}$ = 0.11 to 0.15 days (Scott et al. 1982, 1983)

$t_{1/2}$ = <1 day in soil suspensions when present at
25-50 mg/L (Alexander and Aleem 1961; Alexander and
Lustigman 1966)

$t_{1/2}$ = ~100 days when present in landfill leachate at
concentrations between 30-90 parts per trillion (ng/L)
in soils in Oklahoma (Deeley et al. 1985)

$t_{1/2}$ = 2 to 3 days when present in soil at 100 mg/L
conc. from oil refinery settling pond (Meyer et al.
1984)

$t_{1/2}$ = ~5 days in seawater when present at 3-10 mg/L
added as wastewater (Price et al. 1974)
(see also Baker and Mayfield 1980; Haider et al. 1974)

A.14 PHOSPHATES

PO₄

Tributyl Phosphate

CAS No. 126-73-8

$K_{\text{O/w}}$: 9,800 (Streng and Peterson 1989) (calculated)
10,100 (Saeger et al. 1979)

Water Solubility: 280 mg/L (Streng and Peterson 1989; Saeger et al. 1979)

K_{OC} : 6,000 (Streng and Peterson 1989) calculated

Henry's Law Constant: $0.019 \text{ atm}\cdot\text{m}^3/\text{mol}$ (Streng and Peterson 1989) calculated

Degradation Rate: $t_{1/2}$ ~4 to 7 days in Mississippi River water when
concentration 1 mg/L (Saeger et al. 1979)

$t_{1/2}$ >67 days (Streng and Peterson 1989)

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APPENDIX B

EXAMPLES OF HANFORD SEDIMENT COLUMN LEAKAGE OF ORGANIC
COMPOUNDS AND RADIONUCLIDES

APPENDIX B

EXAMPLES OF SEDIMENT COLUMN LEAKAGE OF ORGANIC COMPOUNDS AND RADIONUCLIDES AT THE HANFORD SITE

This appendix lists examples of probable sediment column leakage of organic compounds and radionuclides. Only positive values (greater than the analytical detection limit) for organics and radionuclides in the groundwater were used as indicators of sediment column leakage because inorganics are present in the groundwater naturally and may even be leached from the soil column by the wastewater. Inorganic analytical results for the groundwater samples were not, therefore, used in the following examples.

The distribution of major contaminants on the Hanford Site (Figure B.1) is given in Figure B.2. A single waste stream has not been identified with each disposal facility because many facilities have received several wastes or been taken in and out of operation one or more times. Several facilities have, however, been associated with a single wastewater. For example, the 216-W-LCW crib has always received laundry waste waters from the 2724-W and 2723-W buildings.

The various specific disposal facilities are associated with the major unconfined aquifer contaminants as shown in Figure B.2. Available data are best used as indicative of the type of radionuclides leaking through the sediment column. Cesium-137 and strontium-90 leakage is generally low; groundwater contains low activities in the tenths of a picocurie per liter to less than 5 pCi/L. Tritium, on the other hand, is often present in quantities as high as millions of picocuries per liter. Cobalt-60, ruthenium-106, and antimony-125 are often present at levels of 10 to 800 pCi/L. These leakage levels generally agree well with the sediment column distribution coefficients expected for these radionuclides, as discussed in Section 5. In this appendix, monitoring well locations relative to each disposal unit are given first, followed by tables of the wastewater components analytically identified in the groundwater. Organic components were generally low in concentration, but methylene chloride and TOX (total organic halogens) values can

occasionally be found into the 10,000-ppb range. The period during which these samples were taken was March 1985 to March 1989.

Our presumption is that the detection of organics and radionuclides in the monitoring wells is an indication that liquid disposal in the designated facility (or a neighboring one) has lead to the migration of the designated constituents to the upper unconfined aquifer.

FIGURE B-1. Hanford Site

CCl_4 = carbon tetrachloride
 TCE = 1,1,1-trichloroethane; tetrachloroethylene
 CHCl_3 = chloroform
 CN = cyanide

FIGURE B-2. Distribution of Major Contaminants in the Unconfined Aquifer at the Hanford Site

FIGURE B.3. Monitoring Well Locations at 1324-N/NA Pond

TABLE B.1. Sediment Column Leakage of Waste Components Disposed to 1324-N/NA Pond (120-N-1)

Monitoring Well	Organics Identified in Groundwater
199-N-58	Methylene chloride, TOX
199-N-59	Chloroform, TOX
199-N-60	Chloroform, TOX
199-N-61	Chloroform, Bis(2-ethylhexyl)phthalate, TOH
	Radionuclides Identified in Groundwater
199-N-58	None
199-N-59	None
199-N-60	None
199-N-61	None

FIGURE B.4. Monitoring Well Locations around 1325-N Crib

TABLE B.2. Sediment Column Leakage of Waste Components Disposed to 1325-N Crib (120-N-2)

Monitoring Well	Organics Identified in Groundwater
199-N-27	Acetone, chloroform, TOX
199-N-29	Chloroform, TOX
199-N-31	Chloroform, TOX
199-N-32	Chloroform, TOX
199-N-33	Chloroform, bis(2-ethylhexyl)phthalate
199-N-36	Acetone, chloroform
199-N-41	Methylene chloride, TOX
199-N-42	Acetone, methylene chloride, TOX
199-N-52	TOX
199-N-70	TOX
	Radionuclides Identified in Groundwater
199-N-27	Cobalt-60, antimony-125, technetium-99, tritium
199-N-29	Antimony-125, cobalt-60, iodine-129, ruthenium-106, strontium-90, tritium, technetium-99
199-N-31	Antimony-125, cobalt-60, ruthenium-106, strontium-90, technetium-99, tritium
199-N-32	Cobalt-60, antimony-125, ruthenium-106, strontium-90, technetium-99, tritium
199-N-33	Antimony-125, cobalt-60, iodine-129, ruthenium-106, strontium-90, tritium
199-N-36	Antimony-125, cobalt-60, ruthenium-106, strontium-90, tritium
199-N-41	Cobalt-60, tritium
199-N-42	Cobalt-60, tritium
199-N-52	Cobalt-60, technetium-99, tritium
199-N-70	Cobalt-60, ruthenium-106, tritium

N42,000

FIGURE B.5. Monitoring Well Locations at 216-A-8 Crib

TABLE B.3. Sediment Column Leakage of Waste Components Disposed to 216-A-8 Crib (216-A-8)

Monitoring Well	Organics Identified in Groundwater
299-E25-6	None
299-E25-9	None
	Radionuclides Identified in Groundwater
299-E25-6	Ruthenium-106, tritium
299-E25-9	Ruthenium-106, tritium

FIGURE B.6. Monitoring Well Locations Around the 216-A-29 Ditch

TABLE B.4. Sediment Column Leakage of Waste Components Disposed to 216-A-29 Ditch (216-A-29)/216-B-3 Pond

<u>Monitoring Well</u>	<u>Organics Identified in Groundwater</u>
299-E25-26	None
299-E25-28	TOX
299-E25-32	None
299-E25-34	TOX
299-E25-35	TOX
	<u>Radionuclides Identified in Groundwater</u>
299-E25-26	Cobalt-60, cesium-137, ruthenium-106, tritium
299-E25-28	Cesium-137, cobalt-60, ruthenium-106, technetium-99, tritium
299-E25-32	Technetium-99, tritium
299-E25-34	Tritium
299-E25-35	Tritium

FIGURE B.7. Monitoring Well Locations at 216-A-30 Crib

TABLE B.5. Sediment Column Leakage of Waste Components Disposed to 216-A-30 Crib (216-A-30)

Monitoring Well	Organics Identified in Groundwater
299-E16-2	None
299-E25-11	None
	Radionuclides Identified in Groundwater
299-E16-2	Cesium-137, cobalt-60, ruthenium-106, strontium-90, tritium
299-E25-11	Cesium-137, cobalt-60, ruthenium-106, strontium-90, tritium

FIGURE B.8. Monitoring Well Locations at 216-A-36B Crib

TABLE B.6. Sediment Column Leakage of Waste Components Disposed to 216-A-36B Crib

Monitoring Well	Organics Identified in Groundwater
299-E17-5	TOX
299-E17-9	2-propanol, acetone
299-E17-14	TOX
299-E17-15	Bis(2-ethylhexyl)phthalate, methylene chloride, TOX
299-E17-16	Acetone, methylene chloride, TOX
299-E17-17	Trichlorofluoromethane
	Radionuclides Identified in Groundwater
299-E17-5	Carbon-14, cesium-137, cobalt-60, iodine-129, ruthenium-106, strontium-90, tritium
299-E17-9	Cesium-134, cobalt-60, iodine-129, ruthenium-106, strontium-90, technetium-99, tritium
299-E17-14	Cobalt-60, iodine-129, ruthenium-106, strontium-90, technetium-99, tritium
299-E17-15	Cobalt-60, ruthenium-106, strontium-90, technetium-99, tritium
299-E17-16	Cobalt-60, iodine-129, technetium-99, tritium
299-E17-17	Cobalt-60, iodine-129, ruthenium-106, technetium-99, tritium

FIGURE B.9. Monitoring Well Locations at 216-A-37-1 Crib

TABLE B.7. Sediment Column Leakage of Waste Components Disposed to 216-A-37-A Crib (216-A-37-1)

Monitoring Well	Organics Identified in Groundwater
299-E25-17	None
299-E25-18	Acetone, TOX
299-E25-19	Methyl ethyl ketone, TOX
299-E25-20	None
	Radionuclides Identified in Groundwater
299-E25-17	Cesium-137, cobalt-60, strontium-90, tritium
299-E25-18	Cesium-137, cobalt-60, ruthenium-106, strontium-90, technetium-99, tritium
299-E25-19	Cesium-137, cobalt-60, ruthenium-106, strontium-90, tritium
299-E25-20	Cesium-137, cobalt-60, ruthenium-106, technetium-99, tritium

FIGURE B.10. Monitoring Well Locations at 216-A-37-2 Crib

TABLE B.8. Sediment Column Leakage of Waste Components Disposed to 216-A-37-2 Crib (216-A-37-2)

Monitoring Well	Organics Identified in Groundwater
299-E25-21	None
299-E25-22	None
299-E25-23	Styrene
299-E25-24	None
	Radionuclides Identified in Groundwater
299-E25-21	Cesium-137, cobalt-60, ruthenium-106, strontium-90, tritium
299-E25-22	Cesium-137, cobalt-60, ruthenium-106, technetium-99, tritium
299-E25-23	Cesium-137, cobalt-60, ruthenium-106, strontium-90, tritium
299-E25-24	Cesium-137, cobalt-60, ruthenium-106, strontium-90, tritium

FIGURE B.11. Monitoring Well Locations at 216-A-45 Crib

TABLE B.9. Sediment Column Leakage of Waste Components Disposed to 216-A-45 Crib (216-A-45)

Monitoring Well	Organics Identified in Groundwater
299-E17-12	None
299-E17-13	None
	Radionuclides Identified in Groundwater
299-E17-12	Cesium-137, cobalt-60, iodine-129, plutonium-239/40, ruthenium-106, technetium-99, tritium
299-E17-13	Cesium-137, cobalt-60, plutonium-239/40, ruthenium-106, strontium-90, technetium-99, tritium

FIGURE B.12. Monitoring Well Locations at B Pond

TABLE B.10. Sediment Column Leakage of Waste Components Disposed to B Pond System

<u>Monitoring Well</u>	<u>Organics Identified in Groundwater</u>
699-42-40A	TOX
699-42-40B	TOX
699-42-42B	TOX
699-42-42J	Acetone
699-43-43	TOX
699-44-42	TOX
	<u>Radionuclides Identified as Groundwater</u>
699-42-40A	Cesium-137, cobalt-60, ruthenium-106, tritium
699-42-40B	Cesium-137, cobalt-60, ruthenium-106, strontium-90, tritium
699-42-42B	Tritium
699-42-42J	Tritium
699-43-43	Tritium
699-44-42	Tritium

FIGURE B.13. Monitoring Well Locations At 216-B-55 Crib

TABLE B.11. Sediment Column Leakage of Waste Components Disposed to 216-B-55 Crib (216-B-55)

Monitoring Well	Organics Identified in Groundwater
299-E28-12	None
299-E28-13	TOX
	Radionuclides Identified in Groundwater
299-E28-12	Cesium-137, cobalt-60, ruthenium-106, tritium
299-E28-13	Cesium-137, cobalt-60, ruthenium-106, tritium

FIGURE B.14. Monitoring Well Locations at 216-B-62 Crib

TABLE B.12. Sediment Column Leakage of Waste Components Disposed to 216-B-62 Crib (216-B-62)

Monitoring Well	Organics Identified in Groundwater
299-E28-18	None
299-E28-21	TOX
	Radionuclides Identified in Groundwater
299-E28-18	Cesium-137, cobalt-60, ruthenium-106, strontium-90, tritium
299-E28-21	Cesium-137, cobalt-60, ruthenium-106, strontium-90, tritium

FIGURE B.15. Monitoring Well at 216-S-26 Crib

TABLE B.13. Sediment Column Leakage of Waste Components Disposed to 216-S-26 Crib (216-S-26)

<u>Monitoring Well</u>	<u>Organics Identified in Groundwater</u>
299-W27-1	Chloroform
	<u>Radionuclides Identified in Groundwater</u>
299-W27-1	Cesium-137, cobalt-60, ruthenium-106, strontium-90, tritium

FIGURE B.16. Monitoring Well Locations at 216-U-14 Ditch

TABLE B.14. Sediment Column Leakage of Waste Components Disposed to 216-U-14 Ditch (216-U-14)

Monitoring Well	Organics Identified in Groundwater
299-W19-1	None
299-W19-21	None
299-W19-27	None
	Radionuclides Identified in Groundwater
299-W19-1	Technetium-99
299-W19-21	Cesium-137, plutonium-239/40, ruthenium-106
299-W19-27	Ruthenium-106

FIGURE B.17. Monitoring Well Locations at 216-U-17 Crib

TABLE B.15. Sediment Column Leakage of Waste Components Disposed to 216-U-17 Crib (216-U-17)

Monitoring Well	Organics Identified in Groundwater
299-W19-19	None
299-W19-20	TOX
299-W19-23	None
299-W19-24	TOX
299-W19-25	None
299-W19-26	None
	Radionuclides Identified in Groundwater
299-W19-19	Cesium-137, cobalt-60, ruthenium-106, strontium-90, technetium-99, tritium
299-W19-20	Cesium-137, cobalt-60, ruthenium-106, strontium-90, technetium-99, tritium
299-W19-23	Cesium-137, plutonium-238, plutonium-239/40, ruthenium-106, technetium-99, tritium
299-W19-24	Cobalt-60, plutonium-238, plutonium-239/40, ruthenium-106, strontium-90, technetium-99, tritium
299-W19-25	Cesium-137, cobalt-60, plutonium-238, plutonium-239/40, ruthenium-106, technetium-99, tritium
299-W19-26	Cesium-137, cobalt-60, technetium-99, tritium

FIGURE B.18. Monitoring Well Location at 216-W-LCW Crib

TABLE B.16. Sediment column Leakage of Waste Components Disposed to 216-W-LCW Crib (216-W-LC)

Monitoring Well	Organics Identified in Groundwater
299-W14-10	None
	Radionuclides Identified in Groundwater
299-W14-10	Cesium-137, cobalt-60, ruthenium-106, strontium-90, tritium

FIGURE B.19. Monitoring Well Locations at 216-Z-20 Crib

TABLE B.17. Sediment Column Leakage of Waste Components Disposed to 216-Z-20 Crib (216-Z-20)

Monitoring Well	Organics Identified in Groundwater
299-W18-17	Acetone, carbon tetrachloride, TOX, chloroform
299-W18-18	None
299-W18-19	None
299-W18-20	None
	Radionuclides Identified in Groundwater
299-W18-17	Cobalt-60, ruthenium-106, tritium
299-W18-18	Cesium-137, cobalt-60, ruthenium-106, tritium
299-W18-19	Cesium-137, cobalt-60, ruthenium-106, tritium
299-W18-20	Cesium-137, cobalt-60, ruthenium-106, tritium

FIGURE B.20. Monitoring Well Locations at 2101-M Pond

TABLE B.18. Sediment Column Leakage of Waste Components Disposed to 2101-M Pond

Monitoring Well	Organics Identified in Groundwater
299-E18-1	None
299-E18-2	Acetone, TOX
299-E18-3	TOX
299-E18-4	TOX
	Radionuclides Identified in Groundwater
299-E18-1	None
299-E18-2	None
299-E18-3	None
299-E18-4	None

Note all wells 399-x-x or 399-x-xx

FIGURE B.21. Monitoring Well Locations at the 300 Area Process Trenches

TABLE B.19. Sediment Column Leakage of Waste Components Disposed to 300 Area Process Trenches (316-5)

Monitoring Well	Organics Identified in Groundwater
399-1-1	Chloroform, methylene chloride, TOX
399-1-2	Chloroform, hexane, methylene chloride, tetrachlorethane, TOX
399-1-4	Chloroform, methylene chloride, TOX
399-1-6	Chloroform, methylene chloride, thiourea, TOX
399-1-7	Acetone, chloroform, methylene chloride, tetrachloroethylene, tetraethylpyrophosphate, TOX
399-1-8	2,6-bis(1,1-dimethylethyl)-4-methyl phen, chloroform, methylene chloride, phenol, TOX
399-1-10	Chloroform, methylene chloride, 1,1,1-trichloroethane, 1,2-dichloroethane, TOX
399-1-11	Chloroform, 1,2-dichloroethane, methylene chloride, TOX, 1,1,1-trichloroethane
399-1-12	Chloroform, TOX
399-1-13	Methyl ethyl ketone, TOX
399-1-14	Chloroform, methylene chloride, TOX
399-1-15	Acetone, chloroform, methylene chloride, TOX
399-1-16A	Chloroform, methyl ethyl ketone, TOX
399-1-16B	Methyl ethyl ketone, TOX, trans-1,2-dichloroethene, trichloroethylene
399-1-16C	Trans-1,2-dichloroethene, trichloroethylene
399-1-17A	Chloroform, 1,1,1-trichloroethane, tetrachloroethylene, TOX
399-1-17B	Methylene chloride, trans-1,2-dichloroethene, TOX
399-1-17C	TOX

TABLE B.19. (contd)

<u>Monitoring Well</u>	<u>Organics Identified in Groundwater</u>
399-1-18A	Carbon tetrachloride, methyl ethyl ketone
399-1-18B	Methyl ethyl ketone
399-1-18C	Methyl ethyl ketone
399-1-19	Chloroform, tetrachloroethylene, trichloroethylene, 1,1,1-trichloroethane, TOX
399-2-1	Chloroform, methylene chloride, tetrachloroethylene, tetrahydrofuran, TOX
399-2-2	Chloroform, methylene chloride, trichloroethylene, TOX
399-3-7	Chloroform, methylene chloride, tetrachloroethylene, 1,1,1-trichloroethane, TOX
399-3-9	Chloroform, TOX
399-3-10	Bis(2-ethylhexyl)phthalate, chloroform, methylene chloride, phenol, tetrachloroethylene, TOX
399-4-1	Acetone, chloroform, 2-hexanone, phenol, TOX, 1,1,2-trichloroethane, trichloroethylene
399-4-7	1,2-benzene dicarboxylic acid, chloroform, hexane, methylene chloride, phenol, TOX
399-4-11	Chloroform, TOX, trichloroethylene
399-8-1	TOX
399-8-2	Methylene chloride, phenol, tetrachloroethylene, TOX, 1,1,1-trichloroethane
399-8-3	Chloroform, methylene chloride, TOX
699-S19-E13	Chloroform, methylene chloride, tetrachloroethylene, TOX, 1,1,1-trichloroethane
699-S30-E15A	Methyl ethyl ketone, phenol, tetrahydrofuran, TOX
	<u>Radionuclides Identified in Groundwater</u>
399-1-1	Cobalt-60, ruthenium-106, technetium-99, tritium
399-1-2	Cobalt-60, ruthenium-106, technetium-99, tritium

TABLE B.19. (contd)

<u>Monitoring Well</u>	<u>Radionuclides Identified in Groundwater</u>
399-1-4	Cobalt-60, tritium
399-1-6	Cesium-137, cobalt-60, tritium
399-1-7	None
399-1-8	None
399-1-10	None
399-1-11	None
399-1-12	None
399-1-13	Tritium
399-1-14	Tritium
399-1-15	Tritium
399-1-16A	Tritium
399-1-16B	None
399-1-16C	None
399-1-17A	None
399-1-17B	Cobalt-60, strontium-90
399-1-17C	None
399-1-18A	Tritium
399-1-18B	Tritium
399-1-18C	Tritium
399-1-19	None
399-2-1	Cobalt-60, technetium-99, tritium
399-2-2	Cobalt-60, strontium-90, ruthenium-106, technetium-99
399-3-7	Cesium-137, cobalt-60, tritium
399-3-9	Cobalt-60, strontium-90, technetium-99, tritium

TABLE B.19. (contd)

<u>Monitoring Well</u>	<u>Radionuclides Identified in Groundwater</u>
399-3-10	Cesium-137, cobalt-60, strontium-90, tritium
399-4-1	Cesium-137, cobalt-60, ruthenium-106, tritium
399-4-7	Cesium-137, cobalt-60, technetium-99, tritium
399-4-11	Tritium
399-8-1	Cesium-137, cobalt-60, ruthenium-106, tritium
399-8-2	Cobalt-60
399-8-3	Cesium-137, cobalt-60, ruthenium-106, tritium
699-S19-E13	Cesium-137, cobalt-60, ruthenium-106, tritium
699-S30-E15A	Tritium

FIGURE B.22. Monitoring Well Location at 400 Area Percolation Ponds

TABLE B.20. Sediment Column Leakage of Waste Component Disposed to 400 Area Percolation Ponds (400 Area Process Pond and Sewer System)

Monitoring Well	Organics Identified in Groundwater
699-2-7	None
	Radionuclides Identified in Groundwater
699-2-7	Tritium

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