5. Fate and Transport

CONTENTS

FIGURE

TABLES

5. FATE AND TRANSPORT

Fate and transport of contaminants in the environment can be modeled to predict the potential spread of contamination. The possible transport of contaminants from surface and subsurface sources through the vadose zone and into the Snake River Plain Aquifer (SRPA) is of particular concern at the INEEL. All WAG 5 sites were reviewed for the BRA as potential sources of groundwater contamination. The criteria that were developed and applied to identify sites for quantitative evaluation in the RI/BRA are described in Section 3.4. It was concluded in a review of previous evaluations that most sources of potential groundwater contamination had been investigated adequately. All groundwater modeling for WAG 5 used the GWSCREEN code developed for INEEL applications (Rood 1994). Highly sophisticated two- or three-dimensional predictive modeling of contaminant movement was not justified because (1) GWSCREEN generates bounding estimates of concentrations in groundwater and (2) the risks associated with WAG 5 sites were generally well below levels of concern. Therefore, the scope for the assessment of fate and transport of contaminants from sources located within ARA and PBF was limited. A careful review of previous groundwater modeling for consistency and verification of input variables was completed. In addition, some sites were evaluated with GWSCREEN modeling to ensure that all modeling conducted for the risk assessment was performed with currently accepted input parameters.

5.1 Modeling Overview

The potential sources of groundwater contamination in WAG 5 include injection wells and surface-and near-surface-contaminated soils. These potential contaminant sources were evaluated using the computer code GWSCREEN (Rood 1994). GWSCREEN was used to simulate groundwater concentrations versus time for specified time periods. Groundwater concentrations resulting from surface and near-surface sources were estimated for each COPC at each release site.

The maximum 30-year average groundwater concentration of each COPC was calculated at 100, 1,000, and up to 10,000 years in the future. A period of 10,000 years was the maximum time period for groundwater analysis, as recommended in the INEEL guidance for cumulative risk assessment (LMITCO 1995).

The contaminant concentrations used in GWSCREEN probably overestimate the true aquifer concentrations that may be produced by leaching and transport of contaminants to the aquifer beneath WAG 5. Because of the complexity of the subsurface and limited information about factors that influence flow and transport of contaminants in groundwater, the uncertainty about potential contaminant concentrations associated with the groundwater pathway exposure routes is greater than the uncertainty associated with any other exposure pathway in this BRA. To compensate for this relatively large uncertainty, conservative input parameters and assumptions were used in the groundwater pathway analysis. Some of the conservative assumptions that were applied in the GWSCREEN analysis include the following:

- The one-dimensional plug flow model used by GWSCREEN adequately represents contaminant transport through the unsaturated zone, though the model conservatively represents a more rapid transport of contaminants to the SRPA than actually occurs. GWSCREEN does not simulate contaminant dispersion in the unsaturated zone, which would increase the transport times significantly and reduce the concentrations of contaminants arriving in the SRPA.

- Groundwater flow through fractured basalt in the unsaturated zone occurs very rapidly in comparison to flow through sedimentary interbeds. This assumption is incorporated into the GWSCREEN modeling by using the cumulative thickness of the sedimentary interbeds present beneath each site area to represent the vadose zone thickness. Using the relatively small thickness results in a shorter unsaturated zone travel time in which radioactive decay can occur. Therefore, the GWSCREEN estimates of radionuclide concentrations are expected to be conservatively high.

- All COPC mass contained in surface soils at each release site contributes to groundwater contamination. No adjustment is made for loss of COPC mass caused by mechanisms such as volatilization, wind erosion, surface water erosion, and contaminant uptake into plants. The only contaminant loss mechanism considered in the groundwater pathway evaluation was radioactive decay.

- Contaminants are uniformly distributed within the groundwater modeling source volume. Estimates of COPC mass that may be transported to groundwater are based on upper-limit estimates of COPC soil concentrations.

5.2 Description of the GWSCREEN Model

Groundwater fate and transport modeling predicted the maximum contaminant concentrations that could occur in the SRPA from leaching and transport of radionuclide and nonradionuclide constituents from the injection wells or surface- and near-surface-contaminated soils. The GWSCREEN model (Rood 1994) simulated the potential release of contaminants from the release sites and subsequent transport in the vadose zone and the SRPA. The basis for using GWSCREEN is discussed in Track 2 guidance for the INEEL (DOE-ID 1994).

GWSCREEN uses a mass conservation approach to model (1) contaminant release from a source volume, (2) contaminant transport in the unsaturated zone, and (3) contaminant transport in the SRPA. Release from the source volume is modeled as a first-order leaching process and considers the solubility and sorptive properties of the contaminant. Unsaturated zone transport is described using a plug-flow model. Transport in the saturated zone is calculated with a semi-analytical solution to the advection-dispersion equation for transient mass flux input. The source model, the unsaturated zone model, and the saturated zone model are linked together by the contaminant flux across model boundaries as illustrated in Figure 5-1.

GWSCREEN models the leaching process using the approach of Baes and Sharp (1983), which is described mathematically by a first-order leach-rate constant. This leach rate constant, λ_L (year^{-1}), is defined as

$$\lambda_L = \frac{q}{\theta_c R_d T}$$

where

q = net water infiltration rate (m/year)

θ_c = volumetric moisture content in the source volume (m^3/m^3)

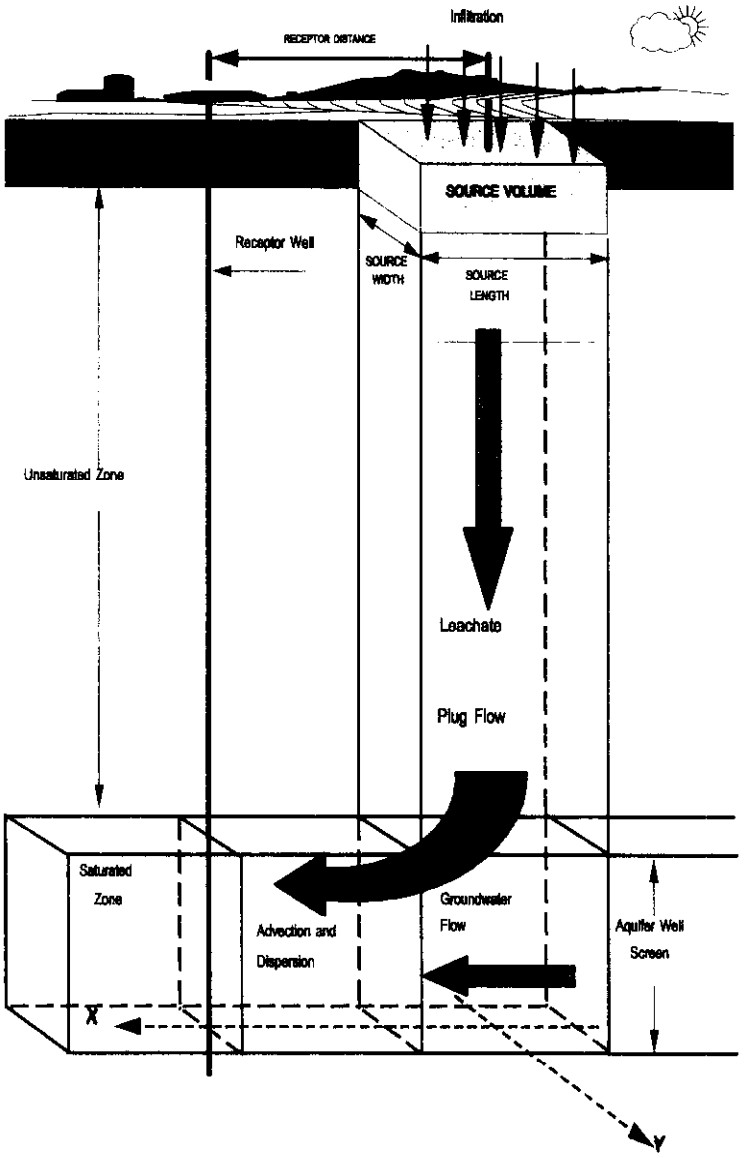

Figure 5-1. Conceptual model of flow and transport implemented in GWSCREEN (Rood 1994).

R_d = retardation factor in the source volume (dimensionless)

T = thickness of the contaminated volume (m).

The contaminant is assumed in the source term model to be uniformly mixed in the finite source volume. For cases in which the initial concentration of the leachate exceeds the solubility of the contaminant, the solubility is used as the limiting concentration in leachate. For WAG 5, however, maximum contaminant concentrations in the groundwater were calculated assuming infinite solubility (i.e., the contaminant release was not solubility limited).

GWSCREEN models the unsaturated zone as a homogeneous, isotropic, porous medium with constant unidirectional flow in the vertical (downward) direction. Water velocity is calculated assuming a unit gradient condition. In the unsaturated zone model, nonsorbing contaminants move with the vertical velocity of the water in the unsaturated zone. Sorbing contaminants move at a slower velocity, but maintain a sharp front because dispersion is not considered. The unsaturated zone water velocity, u_u (m/year), is given by

$$u_u = \frac{q}{\theta_u}$$

where

q = net water infiltration rate (m/year)

θ_u = volumetric moisture content in the unsaturated zone (dimensionless).

Transport in the saturated zone is calculated using an analytic solution to the advection-dispersion equation for contaminants in a saturated porous medium. This mass balance equation is written as

$$\frac{\partial C}{\partial t} + \frac{U}{R_d}\frac{\partial C}{\partial x} = \frac{D_x}{R_d}\frac{\partial^2 C}{\partial x^2} + \frac{D_y}{R_d}\frac{\partial^2 C}{\partial y^2} - \lambda_d C$$

where

C = contaminant concentration in groundwater (g/m^3)

U = groundwater pore velocity (m/year)

D_x, D_y = dispersion coefficients in the x and y directions (m^2/year)

R_d = retardation factor in the aquifer (dimensionless)

λ_d = decay or degradation constant ($year^{-1}$)

t = time variable (year)

x = distance from center of source parallel to groundwater flow direction (m)

y = distance from center of source perpendicular to groundwater flow direction (m).

The solutions to the above equation (Rood 1994) are used for assessment of transport in groundwater for both radiological and nonradiological contaminants.

The assumptions used in the saturated zone transport model are listed below:

- Flow is uniform and unidirectional with no sources (recharge) or sinks (discharge).
- The aquifer is adequately modeled as an isotropic, homogeneous, porous medium.
- The contaminant is vertically mixed in a zone defined by the well screen thickness. In GWSCREEN, the well screen thickness defines the depth over which contaminants are allowed to mix.
- The source to the aquifer is rectangular.
- Dispersion is constant throughout the domain.
- Sorption is linear and instantaneous.
- Molecular diffusion is negligible.
- Contaminant solubility limits are infinite (represented by a value of 1E+6, meaning the leachate concentration is allowed to exceed the solubility limit).

For vertical mixing, concentrations are averaged over the thickness of the well screen. This assumption is reasonable for wells in close proximity to the source. Under such conditions, the bottom of the well screen is more likely to coincide with the base of the plume.

5.3 Model Input Parameters

5.3.1 Contaminant Sources

The injection wells, PBF-5 and PBF-15, were simulated using the pond release source model based on discharge quantities of liquid waste. For the two injection wells, the source zones were defined by the area that would be created when the injected flow passed through the sedimentary interbeds. The area was determined mathematically as the average annual injection flow rate divided by the representative saturated hydraulic conductivity of the sedimentary interbed material:

Flow Rate/Saturated Hydraulic Conductivity = $(m^3/year)/(m/year) = m^2$.

Dimensionally, the above corresponds to units of area. The method is considered acceptable for determining the extent of lateral subsurface spreading[1]. The source zone width and length were set equal to the square root of the area. A vertical source zone thickness of 1.0 m was assumed in the analysis of both wells. Known contaminant quantities based on liquid-waste concentrations were used as input for the well simulations. A complete discussion of the modeling for the two PBF injection wells is given in Appendix J (see Rohe, Sondrup, and Whitaker [1996]).

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a. Henry, R., Parsons Infrastructure and Technologies Group, Inc., 1996, Personal Communication with A. S. Rood, Lockheed Martin Idaho Technologies Company.

The remaining release sites were simulated as buried soil waste sources that leach contaminants via natural percolation of precipitation. The source zone areas (see Table B-19 in Appendix B) were determined from past records and site investigations. The source length and width were determined by taking the square root of this area. The source zone thickness was generally based on the average thickness of the surface and near surface soils overlying the basalt bedrock. The value was determined from boreholes drilled in each area.

In the absence of reliable disposal inventory data, measured contaminant concentrations were used to estimate the mass available for leaching. The contaminant masses at each site were derived by multiplying the contaminant concentrations by the source volume. The 95% upper confidence level (UCL) estimate of the mean concentration (or maximum concentration for maximums less than the 95% UCL) for the depth interval to 10 ft, defined in Table B-21 of Appendix B, was used for each source. The total mass of each contaminant considered in the GWSCREEN modeling was calculated for each individual constituent at each retained release site. Using detected concentrations to represent historical disposals for sites such as ponds may tend to underestimate the risk. However, the relationship of risk to mass is linear in GWSCREEN, and the consequences of underestimating the mass are probably not significant.

The contaminants were assumed to be uniformly distributed throughout the contaminated soil source volume. The total amount of contaminant mass or activity at each release site was estimated using the following equation:

$$M = \rho V C$$

where

ρ = soil density in source (1,500 kg/m^3)

V = source volume (m^3)

C = soil concentration (mg/kg) or activity (Ci/kg).

5.3.2 Unsaturated Zone Thickness

For the GWSCREEN simulations, the unsaturated zone was assumed to consist only of the sedimentary interbeds between the contaminant release point and the top of the aquifer. Ignoring the travel time for water to move vertically through basalt layers separating the sedimentary interbeds is recommended in INEEL Track 2 guidance (DOE-ID 1994). Lithologic logs of wells in the vicinity of the release sites were used to estimate the total interbed thicknesses.

5.3.3 Common Input Parameters

Because the intent of the GWSCREEN modeling for WAG 5 was to determine upper-bound groundwater concentrations, many of the parameters used to run GWSCREEN are default values from INEEL Track 2 guidance (DOE-ID 1994) and are common input parameters for each release site. Soil, interbed, and basalt material and hydraulic properties used in this analysis were either derived from Track 2 defaults (DOE-ID 1994; Dicke 1997) or obtained from INEEL-specific data presented in the GWSCREEN documentation (Rood 1994). The input parameters common to the simulations are shown below in Table 5-1.

Table 5-1. Common GWSCREEN parameters.

Parameter	Code Variable	Value	Unit
Net infiltration rate	PERC	0.10	m/year
Moisture content (source)	THETAS	0.3	m^3/m^3
Evaporation loss rate constant	EVAP	0	1/year
Other loss rate constant	RC2	0	1/year
Moisture content (unsaturated)	THETAU	0.3	m^3/m^3
Solubility limit	SL	1E+6	mg/L
Soil density (source)	RHOS	1.5	g/cm^3
Soil density (unsaturated)	RHOU	1.9	g/cm^3
Aquifer density (saturated)	RHOA	1.9	g/cm^3
Porosity (saturated)	PHI	0.1	m^3/m^3
Longitudinal dispersivity (saturated)	AX	9	m
Transverse dispersivity (saturated)	AY	4	m
Vertical dispersivity (saturated)	AZ	0.4	m
Aquifer pore velocity (saturated)	VX	570	m/year
Well screen thickness	THICK	15	m
Integration time	INTIME	30	year
Body weight	BW	70	kg
Averaging time (radionuclides)	AT	25,560	day
Averaging time (nonradionuclides)	AT	10,950	day
Water intake rate	WI	2	L/day
Exposure frequency	EF	350	day/year
Exposure duration	ED	30	year
Radiological dose limit	DLIM	4E-3	rem/year
Carcinogenic risk criteria	CRISK	1E-7	unitless
Hazard quotient	HQ	0.1	unitless

The infiltration rate of 10 cm/year (4 in./year) is a Track 2 default value (DOE-ID 1994). The value is conservative compared to data from two other studies. Magnuson and McElroy (1993) estimated 10 cm/year (4 in./year) to be the upper-bound value of an estimated infiltration range based on measurements at depth in sedimentary interbeds beneath the Subsurface Disposal Area (SDA) at the RWMC. Miller, Hammel, and Hall (1990) estimated average annual infiltration rates of 2.5 to 5.2 cm (0.99 to 2.05 in.) at the CFA Landfill II based on meteorological data collected at CFA.

The moisture content in the source and unsaturated zone sediments was based on a calculation using the default moisture contents for soils and interbeds presented in INEEL Track 2 guidance (DOE-ID 1994). The default values were based on a geometric average of fitted moisture characteristic curves presented in Rood (1994). Sediment and aquifer densities were assigned Track 2 default values.

In addition to the moisture values, the longitudinal and transverse dispersivities and the equivalent well screen thickness were assigned Track 2 default values. The values are appropriate for a potential well located near the release site. The aquifer porosity and average linear velocity, or pore velocity, also were assigned Track 2 default values. The average linear velocity of 570 m/year (1,870 ft/year) is a conservative estimate that was developed based on INEEL-wide data (DOE-ID 1994).

Solubility limits were ignored in the release and transport calculations. Solubility limits of the contaminants were assumed to be essentially infinite and were represented by a value of 1E+6, which means that the leachate concentration was allowed to exceed the solubility limit.

5.3.4 Contaminant-Specific Parameters

Half lives and slope factors for radionuclides were obtained from the most recent supplement to the HEAST tables (EPA 1995a). Radionuclide progenies were determined from the Table of Radioactive Isotopes (Brown and Firestone 1986). Doses for nonradiological contaminants were obtained from EPA Region 3 risk tables (EPA 1995b) and from the EPA Integrated Risk Information System (IRIS) database.

Distribution coefficients for the organic compounds were estimated using the following equation:

$$K_d = K_{oc} \frac{\%OC}{100}$$

where

K_d = distribution coefficient (mL/g)

K_{oc} = organic carbon distribution coefficient (mL/g)

$\%OC$ = percent organic carbon (dimensionless).

K_{oc} values were taken from INEEL Track 2 guidance (DOE-ID 1994). Percent organic carbon (%OC) was assigned a Track 2 default value of 0.3%, which is the lower bound of a range given by the Department of Agriculture for Montana soils (DOA 1975). It is assumed that the %OC for WAG 5 is not greater than the lower-bound estimate for Montana soils. For inorganic compounds, the distribution coefficients (K_d) were assigned Track 2 default values or values from Dicke (1997).

5.4 Results of GWSCREEN Simulations

The results of the GWSCREEN runs for the surface soil release sites are presented in Table 5-2, Table B-31 in Appendix B, and Appendix D. The output files for the injection wells at PBF-05, and PBF-15 are presented in Appendix J (see Rohe, Sondrup, and Whitaker [1996]).

The source of what may be elevated lead in groundwater at WAG 5 (see Section 4.3.3) is not clearly defined. Transport modeling for sites with lead contamination in soils at WAG 5 indicates that the known lead concentrations in soils are not sufficient to increase groundwater concentrations above background levels. Excluding the possibility that sources of lead contamination in the vadose zone have not been sufficiently characterized, WAG 5 does not appear to be the source of elevated lead concentrations in groundwater.

Table 5-2. Summary of GWSCREEN simulation results for the WAG 5 surface release sites.

Group	COPC	Limiting Groundwater Concentration (mg/L or pCi/L)	Maximum Groundwater Concentration (mg/L or pCi/L)	Average Groundwater Concentration (mg/L or pCi/L)	Time of Peak Groundwater Concentration (year)	Maximum Contaminant Level (mg/L)
1	Aroclor-1242	2.13E-04	8.33E-09	8.33E-09	1.80E+04	5.00E-04
	Arsenic	5.68E-05	3.62E-04	3.25E-04	6.03E+01	5.00E-02
	Cadmium	1.83E-02	1.44E-05	1.32E-05	9.63E+01	5.00E-03
	Chloride	NA	2.35E-06	9.08E-07	2.43E+01	NA
	Chromium	1.83E-01	1.15E-03	9.03E-04	3.63E+01	1.00E-01
	Copper	1.35E+00	1.16E-04	1.10E-04	2.64E+02	1.30E+00
	Diethylether	7.30E+00	1.03E-07	3.98E-08	2.43E+01	NA
	Lead	NA	2.18E-05	2.18E-05	1.22E+03	1.50E-02
	Nickel	7.30E-01	3.21E-05	3.21E-05	1.22E+03	1.40E-01
	Silver	1.83E-01	5.00E-06	4.99E-06	1.10E+03	NA
	Sulfate	NA	1.09E-05	4.23E-06	2.43E+01	NA
	Thallium	NA	**6.42E-03**	**2.48E-03**	2.43E+01	2.00E-03
	Ag-108m	7.87E+00	2.60E-09	2.59E-09	1.10E+03	NA
	Am-241	1.45E-01	2.00E-07	2.00E-17	4.11E+03	NA
	Co-60	2.52E+00	6.52E-06	5.85E-06	1.44E+02	NA
	Cs-134	1.01E+00	1.08E-09	1.08E-09	6.03E+03	NA
	Cs-137	1.51E+00	1.15E-04	1.15E-04	6.03E+03	NA
	Eu-152	8.31E+00	1.85E-08	1.85E-08	7.83E+03	NA
	Eu-154	5.08E+00	2.63E-09	2.63E-09	7.83E+03	NA
	Np-237	1.59E-01	5.97E-08	5.42E-08	1.20E+02	NA
	Pu-238	1.61E-01	3.95E-10	3.95E-10	1.80E+04	NA
	Pu-239/240	1.51E-01	5.99E-09	5.99E-09	1.80E+04	NA
	Ra-226	1.61E-01	3.14E-02	1.22E-02	2.43E+01	5[a]
	Sr-90	8.52E-01	1.73E-03	1.68E-03	3.12E+02	NA
	Tc-99	3.40E+01	1.52E-04	5.89E-05	2.43E+01	NA

Table 5-2. (continued).

Group	COPC	Limiting Groundwater Concentration (mg/L or pCi/L)	Maximum Groundwater Concentration (mg/L or pCi/L)	Average Groundwater Concentration (mg/L or pCi/L)	Time of Peak Groundwater Concentration (year)	Maximum Contaminant Level (mg/L)
	Th-230	1.27E+00	3.92E-05	3.91E-05	1.22E+03	NA
	U-234	1.07E+00	1.40E-04	1.28E-04	9.63E+01	NA[b]
	U-235	1.01E+00	4.70E-05	4.30E-05	9.63E+01	NA[b]
2	Chromium	1.83E-01	8.46E-02	6.63E-02	3.57E+01	1.00E-01
	Lead	NA	3.38E-04	3.38E-04	1.19E+03	1.50E-02
	Manganese	5.11E+00	4.53E-03	4.49E-03	6.07E+02	NA
	Ag-108m	7.87E+00	1.44E-04	1.44E-04	1.07E+03	NA
	Am-241	1.45E-01	6.31E-07	6.30E-07	3.99E+03	NA
	Co-60	2.52E+00	4.81E-04	4.49E-04	1.41E+02	NA
	Cs-137	1.51E+00	1.05E-06	1.05E-06	5.85E+03	NA
	Pu-238	1.61E-01	9.81E-08	9.81E-08	1.75E+04	NA
	U-234	1.07E+00	1.02E-04	9.47E-05	9.41E+01	NA[b]
	U-238	7.68E-01	1.06E-04	9.91E-05	9.41E+01	NA[b]
3	Chromium	1.83E-01	1.00E-01	7.92E-02	3.63E+01	1.00E-01
	Co-60	2.52E+00	3.47E-08	3.11E-08	1.45E+02	NA
	Cs-137	1.51E+00	1.55E-06	1.55E-06	6.04E+03	NA
	Pu-238	1.61E-01	2.97E-09	2.97E-09	1.81E+04	NA
	Sr-90	8.52E-01	6.53E-08	6.36E-08	3.13E+02	NA
	U-234	1.07E+00	2.84E-06	2.59E-06	9.63E+01	NA[b]
	U-235	1.01E+00	1.74E-07	1.58E-07	9.63E+01	NA[b]
	U-238	7.68E-01	2.13E-07	1.94E-07	9.63E+01	NA[b]
4	Lead	NA	3.03E-04	2.78E-04	1.14E+03	1.50E-02
5	Chloride	NA	7.80E-04	3.26E-04	2.38E+01	NA
	Phosphate	NA	8.33E-04	3.48E-04	2.38E+01	NA
	Sulfate	NA	1.56E-03	6.52E-04	2.38E+01	NA
	Co-60	2.52E+00	1.77E-05	2.05E-05	1.35E+02	NA
	Cs-137	1.51E+00	1.17E-06	1.15E-06	5.56E+03	NA
	U-234	1.07E+00	1.53E-05	1.71E-05	9.03E+01	NA[b]
	U-235	1.01E+00	7.01E-07	7.84E-07	9.03E+01	NA[b]
	U-238	7.68E-01	1.36E-05	1.53E-05	9.03E+01	NA[b]
6	Aroclor-1254	2.13E-04	2.60E-07	2.60E-07	1.69E+04	5.00E-04
	Arsenic	5.68E-05	3.80E-03	3.61E-03	5.76E+01	5.00E-02
	Lead	NA	2.16E-04	2.08E-04	1.15E+03	1.50E-02
	Manganese	5.11E+00	9.15E-03	8.50E-03	5.86E+02	NA
	Am-241	1.45E-01	2.35E-06	2.34E-06	3.84E+03	NA

Table 5-2. (continued).

Group	COPC	Limiting Groundwater Concentration (mg/L or pCi/L)	Maximum Groundwater Concentration (mg/L or pCi/L)	Average Groundwater Concentration (mg/L or pCi/L)	Time of Peak Groundwater Concentration (year)	Maximum Contaminant Level (mg/L)
	Cs-137	1.51E+00	2.61E-06	2.61E-06	5.64E+03	NA
	Pu-238	1.61E-01	5.32E-07	5.32E-07	1.69E+04	NA
	Pu-239/240	1.51E-01	2.34E-07	2.34E-07	1.69E+04	NA
	Th-228	2.06E-01	1.29E-03	1.24E-03	1.15E+03	NA
	Th-230	1.27E+00	3.69E-05	3.56E-05	1.15E+03	NA
	Th-232	1.45E+00	2.91E-05	2.80E-05	1.15E+03	NA
	U-234	1.07E+00	5.92E-04	5.86E-04	9.13E+01	NA [b]
	U-235	1.01E+00	1.62E-05	1.60E-05	9.13E+01	NA [b]
	U-238	7.68E-01	4.01E-04	3.97E-04	9.13E+01	NA [b]

Bolded numbers indicate values in excess of the associated maximum contaminant level (MCL).

a. The value shown represents the combined Ra-226 and Ra-228 MCL.

b. The non-isotope-specific MCL for uranium is 20 g/L.

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