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Release Data Package for the 2004 Composite Analysis

R. G. Riley
C. A. Lo Presti

August 2004

Prepared for the U.S. Department of Energy
under Contract DE-AC06-76RL01830

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Summary

A composite analysis is required by U.S. Department of Energy (DOE) Order 435.1 to ensure public safety through the management of active and planned low-level radioactive waste disposal facilities associated with the Hanford Site. The original Hanford Site composite analysis of 1998 must be revised and submitted to DOE Headquarters in 2004 because of revisions to waste site information in the 100, 200, and 300 Areas, updated performance assessments and environmental impact statements, changes in inventory estimates for key sites and constituents, and a change in the definition of offsite receptors.

Beginning in fiscal year (FY) 2003, the DOE Richland Operations Office initiated activities, including the development of data packages, to support the 2004 Composite Analysis. This report describes the data compiled in FY 2003 to support the Release Module of the System Assessment Capability for the 2004 Composite Analysis. This work was conducted as part of the Characterization of Systems Task of the Groundwater Remediation Project (formerly the Groundwater Protection Program) managed by Fluor Hanford, Inc., Richland, Washington.

The Release Module applies release models to waste inventory data from the Inventory Module and accounts for site remediation activities as a function of time. The resulting releases to the vadose zone, expressed as time profiles of annual rates, become source terms for the Vadose Zone Module. Radioactive decay is accounted for in all inputs and outputs of the Release Module. The Release Module is implemented as the VADER (VADose zone Environmental Release) computer code. Key components of the Release Module are numerical models (i.e., liquid, soil-debris, cement, saltcake, reactor block and glass) that simulate contaminant release from the different waste source types found at the Hanford Site. The Release Module also handles remediation transfers to onsite and offsite repositories.

Each numerical model requires key parameter data to perform simulations of contaminant release from the different waste sources. This data package contains all the key parameter data necessary for implementation of the Release Module for conduct of the 2004 Composite Analysis.

A number of decisions were made that affect Release Module implementation for the 2004 Composite Analysis:

- Naval reactor compartments are excluded as a source of contaminant release (Appendix A).
- Chlorine-36 is excluded as a subsurface source of release to the atmosphere (Appendix B).
- Carbon-14 and iodine-129 release to the atmosphere is accounted for from buried waste.
- Contaminant release from immobilized low-activity waste (ILAW) waste is to be simulated using a numerical simulation of release outputs of the Subsurface Transport Over Reactive Multiphases (STORM) code.
- Contaminant release from tank high-level waste residuals is to be simulated using the cement model as opposed to the saltcake model used in previous assessments. This allows for some basis of

comparison with release modeling associated with ongoing tank farm closure assessments. Simulations may be conducted with the saltcake model as a sensitivity analysis.

- No consideration is given to the effects of any form of containment on the initiation of contaminant release from waste sources.

Acronyms

CSTF	Containment Systems Test Facility
CWS	Cooling water system
DOE	U.S. Department of Energy
ERDF	Environmental Restoration Disposal Facility
ETF	Effluent Treatment Facility
FY	fiscal year
GOSPL	Geographic and Operational Site Parameters List
GTF	Grout Treatment Facility
HICs	High Integrity Containers
HLW	High-level waste
HWVP	Hanford Waste Vitrification Plant
ILAW	immobilized low-activity waste
LLW	Low-level waste
RCRA	Resource Conservation and Recovery Act of 1976
RL	Richland Operations Office
SAC	System Assessment Capability
STOMP	Surface Transport Over Multiple Phases
STORM	Subsurface Transport Over Reactive Multiphases
TRUSAF	Transuranic Waste Storage and Assay Facility
VADER	VADose zone Environmental Release
WIDS	waste information data system
WTF	Waste Treatment Facility

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1.0 Introduction

The composite analysis for the Hanford Site (composite analysis) is a radiological assessment to estimate doses to hypothetical future members of the public from radionuclides from low-level waste disposal and all other sources of radioactive contamination at the Hanford Site. This analysis is required under U.S. Department of Energy (DOE) Order 435.1. Results of the first composite analysis were reported in Kincaid et al. (1998) and a 2004 update of the composite analysis is underway this fiscal year (Hildebrand et al. 2003). The composite analysis will simulate radionuclide release from all Hanford sources over a period beginning in 1944 and continuing through 10,000 years post-closure.

This document contains the data package for the Release Module of the System Assessment Capability (SAC) that will be used to conduct the composite analysis. The document includes a description of the Release Module and its association to the other SAC modules, a conceptual model for contaminant release from engineered waste systems represented by the Release Module, an implementation model that describes key input parameters and outputs of the numerical models that make up the Release Module, and descriptions of the numerical models used to simulate contaminant release from specific waste sources. The input parameters for the numerical model are described and the data to be used in the composite analysis assessment are summarized in tables. Parameter uncertainty is discussed along with technical issues needing resolution to continue to improve the release model capability.

2.0 Background

The Release Module of SAC (known hereafter as Release Module) applies release models to waste inventory data from the SAC Inventory Module and accounts for waste transfers conducted in the context of site remediation activities as a function of time. The resulting releases to the vadose zone, expressed as time-profiles of annual rates, become source terms for the SAC Vadose Zone Module. Radioactive decay is accounted for in all inputs and outputs of the Release Module. The Release Module is implemented as the VADER (VADose zone Environmental Release) Revision 1 computer code (Figure 2.1).

2.1 General Conceptual Model of Contaminant Release from Engineered Waste Systems

The Release Module simulates contaminant releases from Hanford during operational periods (i.e., during years of plutonium production and radioactive waste reprocessing) and post operational periods (i.e., during cleanup and closure of the Hanford Site). During operational periods, large volumes of liquid waste were discharged to the ground or released to the Columbia River. Hanford waste containing contaminants of concern was also disposed in engineered systems during operational and post-operational periods.

Engineered waste systems have a number of features that influence the rate at which contaminants can be released from waste. Those features are illustrated in Figure 2.2. The waste may be placed in some form of trench or reside in a tank. The trench, tank, or other form of engineered structure (repository) serves as a barrier to infiltrating water so that the water does not make contact with the waste and transport contaminants from the waste to the vadose zone. Waste inside an engineered system (e.g.,

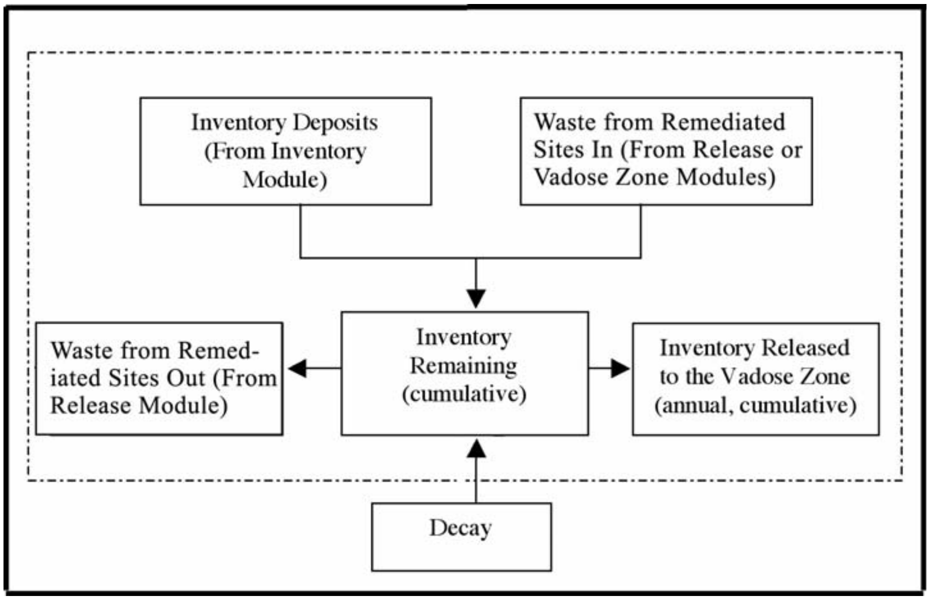

Figure 2.1. Data Input and Output from the Release Module (VADER)

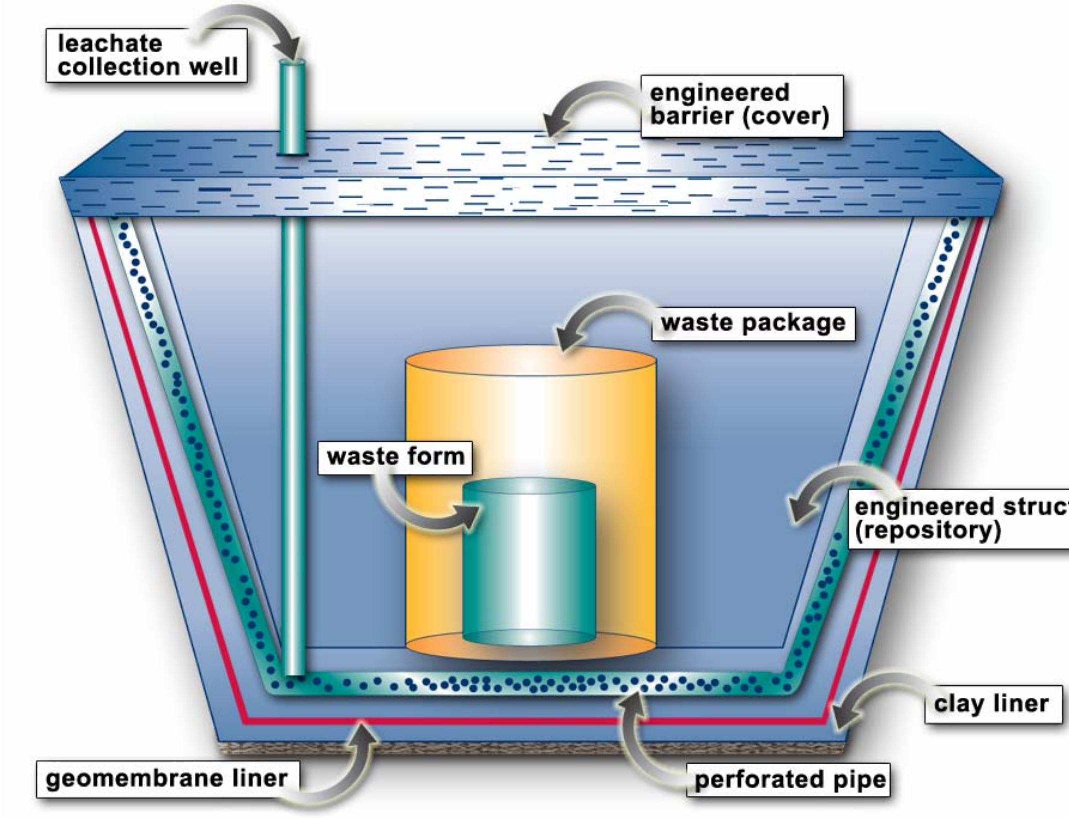

Figure 2.2. Basic Features of a Waste Containment Facility

trench) may also be contained in a waste package (e.g., metal drum, cardboard or wooden boxes or high integrity concrete container; Duncan et al. 1995). Drums or concrete containers, in particular, act as barriers to transport of the contaminants from the waste. Major containment materials for Hanford waste are concrete, steel, and bituminous layers and coatings. The stability of containment materials influences the length of time before infiltrating water contacts the waste and contaminants become available for release. Surface covers atop an engineered system (Meyers and Duranceau 1994; DOE 1996) and liners (geomembrane and clay) and leachate collection systems at the bottom of engineered systems further restrict the ability of infiltrating water to transport contaminants to the vadose zone (40 CFR 258.40; EPA 1997). Surface covers play a particularly important role because migration of infiltrating pore water may be limited to a diffusion-controlled process as long as the cover maintains its integrity.

A number of key physico-chemical processes govern how much contaminant at any given time is released from the waste to the infiltrating water (Serne and Wood 1990). One process is the affinity of contaminants to be retained by the waste (e.g., by sorption to soil or waste material). Another process involves the ability of waste or waste forms to dissolve and, in some cases, form new precipitates allowing some contaminants to be released to the infiltrating water while other contaminants remain trapped in the precipitated solids. Release from the waste may also be limited by the solubility of the contaminant in the infiltrating water. Abiotic and biotic degradation of organic contaminants may occur while part of the waste or during transport limiting the amount of contaminant reaching the vadose zone.

Water infiltrating an engineered system (e.g., high-level waste tank) may contact and react with fill materials (e.g., soil, basalt, grout) (McGrail et al. 2001) and with containment materials in various states of degradation, and with different types of waste. Reaction with these materials will result in changes to the chemistry of the water over time. Its composition, pH, and redox state at any given time will influence the extent to which the processes described in the previous paragraph influence contaminant release from the waste.

Pore water migration in an engineered system is controlled by the permeability of a critical layer comprising the cover atop the engineered system. Critical layers include synthetic geomembranes associated with regulatory compliant covers or layers that overcome some of the deficiencies associated with these covers (i.e., asphalt layers with bituminous coatings). Migration of pore water under a stable cover is diffusion controlled. The ability of the cover to minimize pore water migration will be a function of the quality of the installation (no leakage as the desirable feature) and the stability of the critical layer over time. The long-term stability of these covers is unknown (Meyers and Duranceau 1994).

Contact between migrating water and the waste is delayed if the waste is contained in a repository (e.g., tank, vault, high integrity container) or waste package. Containment materials include concrete, steel, bituminous coatings, wood and cardboard. The corrosive characteristic of the soil is a key factor in determining concrete and steel stability (Pihlajavaara 1994; Escalante 1989). The potential for carbonate mineral formation in the waste material also influences concrete stability (Walton et al. 1997). The stability of lignocellulosic containment materials (wood and cardboard) is controlled by the susceptibility of these materials to abiotic and biotic degradation processes or imposed physical processes (i.e., indiscriminate disposal practices and subsidence control that lead to loss of containment integrity). Crude disposal practices have resulted in significant loss of containment integrity for waste disposed in wood and cardboard containers (Duncan et al. 1995). However, subsurface conditions at Hanford would suggest that some containment materials (concrete and steel) would be relatively stable over time (i.e., thousands to tens of thousands of years); therefore, important features to consider in modeling contaminant release from such systems in long-term assessments. Exceptions to this rule would be where reaction of the waste with containment materials (e.g., high-level waste in tanks) would lead to acceleration of the containment degradation process.

Release of contaminants from waste to migrating pore water is influenced by specific waste features. Important features include such things as waste stability or ability to maintain structural integrity; structural and compositional makeup of the waste (i.e., the degree of homogeneity or heterogeneity); number, type, concentration of contaminants; and permeability. Processes that influence release from the waste to the migrating pore fluid include desorption, diffusion (e.g., diffusion out of permeable waste such as sludge or grout), solubility, solid phase dissolution/precipitation, chemical affinity, and corrosion.

Pore water (leachate) containing contaminants released from the waste eventually reaches the engineered system boundary with the vadose zone. At the boundary, a leachate collection system, followed by a geomembrane liner followed by a synthetic clay liner are the final barriers to release of the contaminants from the engineered system to the vadose zone. Collected leachate moves into a sump where it is pumped out of the engineered system. For an optimized system, migration of the contaminated pore water is controlled by the very low hydraulic conductivity properties of the geomembrane liner and the effective diffusion of contaminants through the geomembrane materials (e.g., diffusion in the pore-water moderated by sorption) (40 CFR 258.40). Leakage in the geomembrane liner component of such systems is known to occur often during their installation (predominantly at seams) (Bonaparte and Gross 1990). Under these conditions migration of contaminants that pass through these breaches is then controlled by restricted migration in the geosynthetic clay layer (EPA 1997).

2.2 Implementation Model

The Release Module accounts for releases that occurred in the early years of Hanford Site operations and those that may be expected while the Hanford Site is remediated over the next several decades and beyond. The Release Module relies on several sources of input (Figure 2.3). Input from the Inventory Module consists of contaminant mass and activity deposits, year of deposit, and waste volume. Some of the release models (i.e., soil-debris, cement) require site-specific or waste feature information (i.e., site cross sectional area, site volume or waste surface area or volume). Recharge rate is an important parameter to the saltcake and soil-debris models and the empirical LAWABP1 glass model. Key process parameters are retardation factor (soil-debris model), contaminant solubility (soil-debris model), matrix solubility (saltcake model), diffusion coefficient (cement model) and fractional release rate (reactor block model).

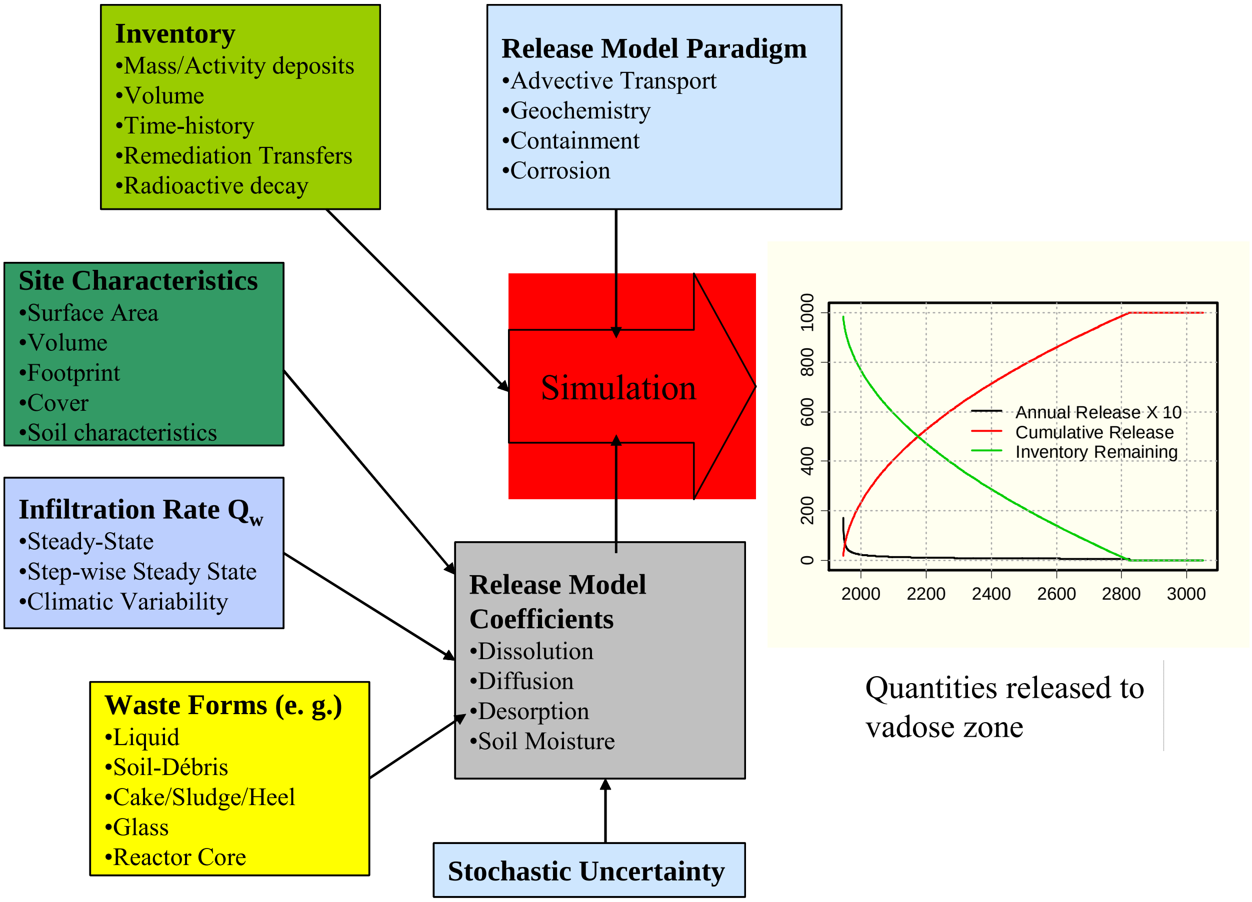

Figure 2.3. Characteristics of Release Implementation Model

A delay in the initiation of contaminant release can be applied to those waste types in some form of metal or concrete containment structure. For both types of containment, simple corrosion models are used to estimate the length of the delay.

2.2.1 Assumptions and Limitations

For the composite analysis, a number of assumptions have been made in the implementation model that result in a simplification of the model:

- Beyond the timing and magnitude of infiltration rates, the implementation model will not include the effects of waste containment (e.g., steel liners in tanks, drums, High Integrity Containers [HICs] or geomembrane and/or geosynthetic clay liners) on contaminant release from waste. It is expected that this assumption will result in more conservative (faster release) estimates.

- Contaminant release for most contaminants from surplus production reactor waste cores is assumed to occur according to a simple linear fractional release rate, ignoring the complex features of the core and their influence on contaminant release. One exception is the option of time/temperature dependent release of carbon-14 from the cores.

- Contaminants will be released from tank waste by the diffusion-controlled mechanism (cement model) assuming all the waste is sludge or hard heel because saltcake waste was removed during the sluicing process. It is expected that this assumption will result in less conservative (slower release) but more realistic estimates.

- The waste source requiring the application of a model to simulate the release of contaminants from Naval reactor compartments is excluded because it was determined that the contaminants would not release from this waste during the length of time of this assessment (see Appendix A for details).

- All release model parameters except infiltration are treated as constant (within each realization) over the full simulation period. Consequently, the possibility of parameters such as soil moisture content distributions changing over time is not considered.

- Infiltration rate time-profiles for soil-debris waste will be varied over simulation realizations to reflect uncertainty in water infiltration. However, time periods representing ground cover will be held constant over all realizations to reflect the current Hanford Disposition Schedule.

- The glass model consists of a numerical expression that simulates release outputs based on results from the immobilized low-level waste STORM code (Bacon et al. 2000) as input to the vadose zone module of SAC. Generation of stochastics in SAC simulations of contaminant release from glass waste will be made through variation of recharge rate over time. The empirical glass release model is based on LAWABP1 glass (Bacon and McGrail 2001). Another model for LAWA44 glass, which is closer to the type of glass to be made for ILAW waste, may be implemented in the future.

- Liquid and river releases will be treated as instantaneous releases at time of deposit (pass-through model) to the vadose zone and the Columbia River, respectively.

- Remediation transfers will be treated as if they were completed within one year, even though in practice they could require multiple years. When actual remediation transfers at a site require multiple years to complete, the convention is to assign the transfer to the year the entire remediation transfer is completed or scheduled to be completed.

- Waste sources that apply the cement model assume a waste form that maintains structural integrity over the period of release (i.e., the surface area-to-volume ratio of the waste remains constant). Calculated surface areas are external and structures are assumed to be solid i.e., there is no distinguishing between a waste that is a true waste form or hollow concrete structure (e.g., buildings or tunnels that contain contamination).

2.3 Numerical Models

In this section, analytical solutions for each release model are described. Information is also provided on the issues of atmospheric release and containment.

2.3.1 Assignment of Numerical Models to Specific Waste Types

Table 2.1 summarizes the release models to be applied to the various waste site types identified in the composite analysis. Specific conditions for modeling some of the sites are described in the footnotes. Data sets are applied site-specifically. Equations are shown without a radioactive decay term for conceptual simplicity.

Table 2.1. Summary of Release Model Assignments to Waste Source Types

Release Model	Waste Source Type
Liquid	Single-shell tanks,[a] unplanned releases[b], trenches, cribs, drain/tile fields, radioactive process sewers, French drains, retention basins, ponds, ditches, sumps, injection/reverse wells, storage tanks, diversion boxes, catch tanks, valve pits, settling tanks, receiving vaults, neutralization tanks, and releases direct to the Columbia River
Soil-Debris	Unplanned releases,[b] burial grounds, laboratories, storage, stacks, landfills, surplus production sites (i.e., the soil below and surrounding a site), sand filters[c]
Cement	Process unit/plants, control structures, storage tunnels, cemented waste in burial grounds, single-shell tanks,[a] double-shell tanks[e]
Saltcake	Single-shell tanks,[d] double-shell tanks[e]
Reactor Block[f]	Decommissioned surplus production reactor cores
Glass[g]	Vitrified ILAW waste from single-shell tanks

(a) Releases from single-shell tanks will be modeled using a combination of liquid and cement models. Releases include past tank leaks, liquid released during retrieval and contaminant release from dissolution of residual solids following waste retrieval completion.
(b) Modeled as initial liquid release, release from a surface contaminated soil or a combination of both.
(c) Site 116-C-2C uses the liquid release model.
(d) Simulations of contaminant release from tank residuals may be conducted with the saltcake model as a sensitivity analysis.
(e) Double-shell tanks are assumed not to leak prior to and during retrieval. Release of contaminants from residual solids modeled using cement model.
(f) B reactor release occurs entirely in the 100 Area, following a specified period of time (75 years). Remaining inventories for all other reactors moved to 200 West Area burial ground (218-W-5) where release continues using the reactor block model.
(g) An empirical model that simulates the release curves for LAWABP1 glass from the ILAW STORM model, allowing SAC (VADER) to maintain generation of stochastics through variation of recharge rate.

2.3.2 Analytical Solution: Liquid Release Model

Liquid releases are modeled as being dumped to the ground and instantly available to go into the vadose zone without retardation the year they enter the inventory (Eslinger et al. 2002). This is a pass-through, no decay, instantaneous release, and complete depletion release model. The loss of contaminant from the waste source as a function of time is given by:

$$dM/dt = -MF \tag{1}$$

where M = current quantity of contaminant in the source zone (Ci or kg) or site inventory at time t
F = fractional release rate (y^{-1})

When the fractional release rate is assigned the value of 1, the entire contaminant quantity is instantaneously released into the ground. The dumping of the contaminant quantity can be retarded by assigning a fractional release rate between 0 and 1. The minus sign indicates that the quantity dM/dt is to be subtracted from the inventory quantity M(t).

2.3.3 Analytical Solution: Soil-Debris Model

The soil-debris model postulates release of contaminants from inventory soil wastes into a "source zone." The complete soil-debris model implemented in VADER Revision 1 has two régimes: solubility-driven and desorption-driven. When desorption would yield a contaminant concentration greater than the solubility limit, the model operates in the "solubility-controlled" model and the release rate depends on the magnitude of the solubility limit. When the concentration of a contaminant is less than the capacity of infiltrating water to dissolve, the quantity released depends on the infiltration rate, a partition coefficient (i.e., K_d) and soil characteristics (i.e., moisture content and bulk density), and is considered "desorption-controlled."

As an option, the soil-debris model as implemented in VADER can be operated in the solubility-driven régime without switching into desorption-driven mode (C_{sol} model).

The rate of release of contaminant for a given contaminant by the soil-debris model is given by:

$$dM/dt = -QAC_w \tag{2}$$

where $C_w = C_{sol}$ effective concentration when the release process is solubility-controlled
$C_w = M/(\theta RAh)$ effective concentration when the release process is desorption-controlled.

where $R = 1 + (\beta K_d)/\theta$

Switching régimes is controlled by comparing the remaining mass M(t) in the waste form with the maximum mass ($M_{max} = \theta RC_{sol}Ah$) possible to dissolve without a precipitated phase, consistent with an aqueous phase saturated with the contaminant.

If M(t) is larger than M_{max}, the release process is considered to be solubility controlled; otherwise it is desorption controlled. Under solubility-control, with constant Q_w and A, dM/dt is constant. Under desorption-control, with constant Q_w and A, dM/dt is steadily decreasing as M(t) is depleted:

where M_{max} = the maximum quantity of contaminant theoretically possible in the source zone (in Ci or kg) without a precipitated phase

M = M(t) is current quantity of contaminant contained in the source zone (Ci or kg)

Q_w = infiltration rate for the site in cm/yr; Q_w can be considered constant, or considered to be time-dependent based on site climate, cover, and remediation activities

A = surface area of the soil waste form exposed to the release mechanism (cm^2)

h = depth thickness or height of the soil waste form at the site (cm)

C_w = a coefficient expressing the effective release concentration of the contaminant (Ci/cm^3 or kg/cm^3)

C_{sol} = expresses aqueous solubility of the contaminant in Ci/cm^3 or kg/cm^3

R may be considered either a retardation factor or a soil apportionment factor (unitless) which depends on several factors:

ß Soil bulk density in g/cm^3
K_d Sorption factor (cm^3/g)
θ Volumetric content of water in soil (unitless fraction)

dM/dt = the rate of loss of contaminant from the source zone (the rate contaminant crosses the soil waste form boundary and enters the environment)

t = the elapsed time (years) from the beginning of release from containment

2.3.4 Analytical Solution: Cement Model

The cement model is applied to waste that has the characteristics of cement, with the contaminant embedded homogeneously in the cement waste form. For the composite analysis, the cement model (Section 5.3) will be used to simulate contaminant release from tank residuals. A surface area to volume ratio of 1.21×10^{-2} cm^{-1} (V/A = 0.825 m) will be applied to all tanks. A diffusion coefficient of 6×10^{-7} cm^2/s will be applied to all tanks (Khaleel and Connelly 2004). The total external surface area and volume of the waste form must be known. The ratio of surface area to waste volume is assumed to be constant, implying that the cement waste form maintains structural shape integrity over time. The structure is assumed to be a solid cementitious material. The most important term in the model is the diffusion coefficient. It describes the rate at which the contaminant migrates from the interior of the cement form to its surface. Once at the surface, 100% of the contaminant is assumed to be leached into the migrating pore water. Release continues at a steadily decreasing rate until M(t) is completely depleted.

The rate of loss of contaminant for a given contaminant is given by:

$$\boldsymbol{dM/dt = -M_o\ (A/V)\ (D/\pi t)^{1/2}} \tag{3}$$

where M_0 = the original quantity of the contaminant contained in the cement (Ci or kg). This can be seen as a function of concentration (kg/cm^3 or Ci/cm^3) and volume (cm^3)
M(t) = current quantity of the contaminant contained in the cement (Ci or kg)
A = the geometric surface area of the cement structure (cm^2)
V = the volume of the cement structure (cm^3)
D = the diffusion coefficient of the contaminant (cm^2/yr)
t = the elapsed time (years) from the beginning of release from containment
dM/dt = the rate of loss of contaminant from the cement waste form as it is leached into the environment by infiltrating water

2.3.5 Analytical Solution: Saltcake Model

The saltcake model is used to simulate contaminant release from tank waste solid residuals. For the composite analysis, simulations may be conducted with the saltcake model as a sensitivity analysis. Contaminants are assumed to be contained within a waste matrix termed saltcake, which is composed of saltcake, sludge, and heel without differentiation. The waste is assumed to be homogeneously distributed throughout the tank and the saltcake matrix is assumed to be mostly composed of nitrate salts (e.g., sodium nitrate). This saltcake is assumed to contain the contaminants that dissolve in percolating water congruently with the matrix. The saltcake model consists of a simple analytical solution containing a term for infiltration, matrix (nitrate) solubility, and the cross-sectional area of the waste source.

The release rate for a given contaminant is given by:

$$\boldsymbol{dM/dt = -M_o\ A\ Q_w\ C_{wo}^{sol}/M_{wo}} \tag{4}$$

where M_{wo} = the original mass of saltcake (kg). M_{wo} may also be derived by the product of tank waste volume and waste density such that M_{wo} equals M_o
M_o = the original quantity of contaminant in Ci or kg embedded in the saltcake.
M = M(t) is the current quantity of the contaminant contained in the saltcake (Ci or kg) at time t
A = the surface area of saltcake exposed to the release mechanism (cm^2)
C_{wo}^{sol} = the aqueous solubility of the saltcake simulated as the concentration of nitrate (as nitrate salts) in tank supernate (g/cm^3)
Q_w = the site recharge rate in cm/yr, also termed infiltration rate
dM/dt = the rate of loss of contaminant from the saltcake waste form per unit time t (the rate at which the contaminant leaks from the tank into the environment)

2.3.6 Analytical Solution: Reactor Block Model

The reactor block model is used to simulate the release of contaminants from decommissioned production reactor cores on the Hanford Site. Reactor cores are composed of graphite, a material extremely resistant to corrosion and highly impermeable. The mechanism of contaminant release from reactor cores is not well understood. The analytical solution is simple, consisting of only a contaminant mass and fractional release term.

The rate of loss of contaminant for a given contaminant is given by:

$$\boldsymbol{dM/dt = -M_o F_{rrr}} \tag{5}$$

where M_o = the initial quantity in Ci or kg of contaminant in the graphite core
F_{rrr} = the fractional release rate in yr^{-1}. F_{rrr} is analyte specific, and ranges from 0 to 1

This model generates a family of curves such that the smaller the value of F_{rrr}, the more elapsed time is required until a specific contaminant inventory is completely depleted from the graphite block. M_o serves as a multiplier to calculate annual quantity released.

Carbon-14 is a special case because its release from graphite has been found to be strongly temperature-dependent. Therefore, a release model has been developed to allow the carbon-14 fractional release rate to vary as a function of time and reactor temperature during reactor operation, shutdown and cooling (ten year time frame), cocooning, and disposal on the Central Plateau. The analytical solution for the time and temperature dependent release of carbon-14 from reactor cores is represented numerically in the following expression (Kincaid et al. 1998):

$$\mathbf{dM/dt = -M_o (365)[565(1+100e^{-(0.08)(365)t})e^{-6440/T}]} \tag{7}$$

where M_o = the initial quantity in Ci of carbon-14 in the core
T = the absolute temperature of the reactor block (°K)
t = elapsed time in years since deposit year

2.3.7 Analytical Solution: Glass Model

For the composite analysis, simulation of contaminant release from immobilized low-activity waste will consist of generating annual release curves from the SAC Release Module (i.e., VADER) based on numerical modeling of individual normalized release flux output curves produced by STORM as part of past performance assessment test cases. This approach allows the generation of stochastics in SAC simulations through variation of infiltration rate. The infiltration rate has been determined to have the greatest effect on uncertainty in contaminant release from immobilized low-activity waste. It is recognized that exact numerical simulations of STORM release outputs, that is, capturing fine-structure from the STORM runs, are not feasible given available resources. Efforts have been made to minimize and allow quantification of the uncertainty for each simulation of release in the composite analysis.

A number of functional forms (e.g., exponentials and n-order polynomials) were evaluated for their ability to capture the general shape of the release curves generated by STORM. The functional form that provided the best fit for the range of release curves associated with the test cases (0.1 through 50 mm/yr) is based on combining a logistic curve to represent the influence of infiltration rate with a polynomial (cubic) to represent the combined influence of elapsed time and infiltration rate.

The empirical model functional form that embodies these characteristics is:

$$f(R,t)=[a/(b+e^{-c*log_{10}(R)})]*[e^{-1x10^{-7}(w+xR+yR^2+zR^3)t}]$$

$$dM/dt = -M_o\, f(R,t) \tag{7}$$

where $f(R,t)$ = normalized flux at time t elapsed years for infiltration rate R. Normalized flux is defined as the fraction of total contaminant inventory released during a given year t. Units are ppm/year. In the STORM runs, $f(R,t)$ranges from 10^{-11} to 1.

R = recharge rate (or infiltration rate) at year t in mm/year. R can be treated either as constant or stochastic over the simulation period.

a, b, c, w, x, y, z = estimated parameters from the empirical model fit process based on LAWABP1 glass (i.e., Table 5.14)

M_o = initial quantity of contaminant embedded in glass in Ci or kg

$1x10^{-7}$ = a scaling factor for time in years that enhances numerical stability in the model fitting process due to the differences in scaling of the predictor (year) and response (flux) variables.

It should be recognized that infiltration rates for immobilized low-activity glass waste forms are expected to vary from 0 up to 110 mm/yr or more. Since the empirical release model is based on curves ranging from R = 0.1 mm/yr to 50 mm/year, use of this function for infiltration rates greater than 50 mm/yr will generate extrapolated release rates which may not be as reliable as interpolated rates.

2.3.8 Modeling Release to the Atmospheric Pathway

Atmospheric release for the composite analysis will be managed through the Inventory, Release (VADER) and Vadose Zone Modules (STOMP). Atmospheric releases during operational time periods are simulated through the Inventory Module. Outputs of the Inventory Module are directed into an atmospheric dispersion model (Napier 2002). VADER will simulate the post-operational release of carbon-14 from above-ground surplus production reactor sources to the dispersion model. STOMP will simulate the release of carbon-14 and iodine-129 to the soil surface from buried waste. Chlorine-36 was evaluated and excluded as a subsurface source of release to the atmosphere (Appendix B).

2.3.9 Modeling the Effects of Waste Containment

The Release Module has the capability to account for the effects of metal and concrete containment on release of analytes from waste. Containment at Hanford include steel liners in high-level waste tanks and low carbon steel drums, Naval reactor compartments and reactor vessels, immobilized low-activity waste canisters, and concrete high integrity containers. Containment in the release module is expressed as a delay in the time of initiation of release of an analyte from the waste. The delay in release is calculated off-line using a corrosion model for both metal and concrete materials. The delay can be varied between simulation runs to account for stochastic variability.

For the composite analysis, the effects of containment will not be a consideration for any of the waste sources. This is expected to result in more conservative (faster) release rates.

3.0 Data Gathering Methods

Mathematical formulas that express the release of contaminants from various waste sources, the parameters important to those formulations and associated parameter data, and their application in past Hanford assessments are documented in many reports published since 1987. Preparation and publication of an initial data catalog (Riley and Lo Presti 2001) was conducted under the Vadose Zone Groundwater Integration Project managed by Bechtel Hanford, Inc. for the DOE Richland Operations Office (RL). The initial report 1) provided a summary of descriptions and uses of release models used in assessments from 1987 to 2001, 2) described analytical solutions for contaminant release from various types of waste sources and assessed their commonality, 3) linked release models to data on various waste sources found on the Hanford Site, and 4) provided listings of sources of parameter information and parameter data used in the models. For purpose four, the report provided links to specific pages, figures, and tables for locating specific information and data within documents. Information and data from the initial report (Riley and Lo Presti 2001) was used in the preparation and application of a release data package in conduct of the SAC initial assessment (Bryce et al. 2002).

The initial report (Riley and Lo Presti 2001), with support provided by the Groundwater Remediation Project managed by Fluor Daniel Hanford, Inc. for DOE/RL, has been updated (Riley and Lo Presti 2003). This updated report presents a conceptual model of release that informs the reader of some of the key features and processes that influence contaminant release from Hanford waste sources. Additional applications of release models to assessments pertaining to immobilized low-activity waste and solid waste disposal sites are summarized. A section on the effects of containment on contaminant release from selected waste sources is included. The report (Riley and Lo Presti 2003) excludes information on release by way of the atmospheric pathway. Information on release to the atmospheric pathway from near-surface waste sources was acquired from number of reports that summarized previous Hanford assessments (Kincaid et al. 1998; Wood et al. 1995; Wood et al. 1996; Kincaid et al. 1995; DOE 1989; DOE 1996; Streile et al. 1996). Information and data from these reports and the most recent data catalog (Riley and Lo Presti 2003) were sources for data summarized in Chapter 5.

4.0 Model Input Parameter Requirements

Table 4.1 summarizes the key parameters associated with the numerical models described in Section 2.3. Parameter values for each of the models are discussed in Chapter 5.

Table 4.1. Summary of Input Parameter Requirements for Release Models

Model Parameter	Release Model Type					
	Liquid	Soil-Debris	Cement	Saltcake	Reactor Block	Glass
Cross sectional area of source zone		X		X		
Depth of waste or distance from soil surface to bottom of contaminant source zone		X				
Distribution coefficient		X				
Bulk density of soil		X				
Volumetric moisture content of soil		X				
Contaminant solubility		X				
Matrix solubility				X		
Fractional release rate	X				X	
Infiltration rate		X		X		X
Waste density(a)				X		
Waste surface area			X			
Waste volume			X			
Diffusion coefficient			X			
Mass of structural component in source zone(a)				X		
Mass or activity of contaminant	X	X	X	X	X	X
Temperature(b)					X	

(a) Because the Inventory Module provides the saltcake matrix of each tank as a volume, a saltcake matrix density value is required to convert tank waste volumes to equivalent masses. Recent applications of the saltcake model within SAC have used a statistically derived value of density for tank solids (Chen et al. 1998) based on tank characterization data. Typical density values are around 1.5 g/cm^3.

(b) For release of carbon-14 from graphite reactor cores.

5.0 Proposed Input Parameter Values and Distributions

This section summarizes the parameters and parameter data and other waste source data for the six numerical models described in Chapter 2.

5.1 Liquid Release Model

Liquid releases are modeled as being dumped to the ground and instantly available to go into the vadose zone without retardation and decay the year they enter the inventory (Eslinger et al. 2002). The instantaneous release is accomplished by assigning the model a fractional release rate of one. The liquid release model is also used to account for instantaneous releases directly to the Columbia River.

5.2 Soil-Debris Model

For the composite analysis, contaminant release from all burial grounds will be simulated using the soil-debris model. At some burial grounds, the cement model will be used in combination with the soil-debris model. This recognizes that one or more burial grounds will be assigned an inventory of stabilized waste (e.g., technetium, iodine, and uranium in high integrity concrete vaults or other form of concrete waste). Accounting for these inventories in this manner maintains consistency with the initial composite analysis assessment (Kincaid et al. 1998) and past low-level waste performance assessments (Wood et al. 1995, 1996).

Contaminant inventory in the soil is provided by the Inventory Module. Source zone depth/height information is also needed for all burial ground sites to run the soil-debris model. Some depth/height information has been obtained from the waste information data system (WIDS) as provided by the Geographic and Operational Site Parameters List (GOSPL) (Last et. al. 2004a). An average depth/height (5.349 m) has been calculated based on the available WIDS data and applied to all burial ground sites that do not have a depth/height value. In a few instances, cross-sectional area values were not available, in which case a value of 999m^2 is applied. These data are summarized in Table 5.1.

The soil-debris model will be applied to laboratory, storage, and stack-type waste sources. Available dimensional data on these sites are from the WIDS database. When waste source dimension information was missing, the waste source with missing data was compared to waste sources where dimension data were available to calculate and assign dimensions from which depths/heights and cross-sectional areas could be estimated. The soil-debris model has been applied to some of the unplanned release sites. Where cross-sectional area and depth/height information were missing, values of 0.999 m^2 or 9.99 m^2 and 0.999 m were assigned for cross-sectional area and depth/height, respectively. This data set is summarized in Table 5.2.

Values for bulk density and volumetric moisture content for the 100, 200, and 300 Areas were calculated from available data (Peterson et al. 1996; Schalla et al. 1988; Fayer et al. 1999) at depths no greater than 6 m (i.e., the approximate maximum depth observed for burial grounds on the Hanford Site). Those data are summarized in Table 5.3.

Table 5.1. Summary of Cross-Sectional Area and Depth/Height Data for Burial Grounds

Site	Cross-Sectional Area (m^2)	Depth/Height (m)
100-B-3	999	5.3
118-B-1	2,982	6.1
118-B-2	167	3.0
118-B-3	8,942	6.1
118-B-4	139	4.6
118-B-5	232	6.1
118-B-6	13.9	6.1
118-B-7	6.0	2.4
118-C-1	18,952	6.1
600-33	37.2	5.3
100-D-3	999	5.3
100-D-32	231	5.3
100-D-40	117	6.1
100-D-42	277	5.3
100-D-43	163	4.6
100-D-45	181	5.2
100-D-47	3,961	5.3
118-D-1	15,677	6.1
118-D-2	33,445	6.1
118-D-3	23,226	6.1
118-D-4	11,148	5.3
118-D-5	149	3.0
118-DR-1	871	8.8
118-F-1	2,787	6.1
118-F-2	11,148	6.1
118-F-3	813	4.6
118-F-5	6,968	4.6
118-F-6	7,432	5.5
132-F-5	223	8.2
100-H-5	1,585	4.6
118-H-1	24,387	6.1
118-H-2	650	5.3
118-H-3	8,210	6.1
118-H-4	418	3.0
118-H-5	5.6	3.0

Table 5.1. (contd)

Site	Cross-Sectional Area (m^2)	Depth/Height (m)
100-K-2	975	4.6
118-K-1	66,890	6.1
218-C-9	16,983	5.3
218-E-1	7,441	5.3
218-E-RCRA	44,792	12.2
218-E-LLW	44,792	12.2
218-E-Cores	10,000	5.3
GTFL	581	10.4
CS-Resin	211,677	5.3
ILAW-HLW-Solid	211,677	5.3
TC-Resin	211,677	5.3
U.S. Ecology	409,300	5.3
218-E-10	442,102	4.9
218-E-12A	4,415	5.3
218-E-12B	878,649	4.9
218-E-2	22,165	5.3
218-E-2A	1,368	5.3
218-E-4	14,493	5.3
218-E-5	6,433	5.3
218-E-5A	1,115	5.3
218-E-7	27	5.3
218-E-8	4,274	5.3
218-E-9	3,967	5.3
218-W-4C	231,886	5.3
218-W-1	22,168	5.3
218-W-11	9,290	4.6
218-W-1A	25,686	5.3
218-W-2	28,509	5.3
218-W-2A	182,214	5.3
218-W-3	33,924	5.3
218-W-3A	211,677	5.3
218-W-3AE	226,500	5.3
218-W-4A	73,496	5.3
218-W-4B	29,952	5.3
218-W-5	364,626	5.3
618-1	3,300	5.3

Table 5.1. (contd)

Site	Cross-Sectional Area (m^2)	Depth/Height (m)
618-13	581	7.6
618-2	6,991	5.3
618-3	6,243	4.6
618-4	12,173	5.3
618-5	5,376	5.3
618-7	43,737	5.3
618-8	5,574	5.3
618-9	687	4.6
618-10	23,226	5.3
618-11	34,839	5.3
600-148 (ERDF)	98,942	5.3

ERDF = Environmental Restoration Disposal Facility.
HLW = High-level waste.
LLW = Low-level waste.
RCRA = Resource Conservation and Recovery Act of 1976.

Table 5.2. Summary of Depth/Height and Cross-Sectional Areas for Application of the Soil-Debris Release Model to Selected Source Terms in the 2004 Composite Analysis

Site	Diameter (m)	Length (m)	Width (m)	Depth/Height (m)	Cross-Sectional Area (m^2)
100-K-42 (Storage)		41.5	21.3	6.7	884
100-K-43 (Storage)		41.5	21.3	6.7	884
100-F-36 (Laboratory)				17.7	447
100-F-38 (UPR)				0.999	0.999
100-H-31 (UPR)				0.999	0.999
100-K-78 (UPR)				0.999	318
100-N-66 (Reactor-Soil)				0.999	19,526
116-D-8 (Storage)				0.999	0.999
118-B-8 (Reactor-Soil)				0.999	3,948
118-B-9 (Storage)		7.3	3.7	3.0	26.8
118-C-3 (Reactor-Soil)				0.999	6,039
118-C-4 (Storage)		1.2	7.6	1.2	92.9
118-D-6 (Reactor-Soil)				0.999	3,948
118-DR-2 (Reactor-Soil)				0.999	3,948
118-F-4 (Crib)		3.0	3.0	4.6	9.3
118-F-7 (Storage)		4.9	2.4	2.4	11.9
118-F-8 (Reactor-Soil)				0.999	4,113

Table 5.2. (contd)

Site	Diameter (m)	Length (m)	Width (m)	Depth/Height (m)	Cross-Sectional Area (m^2)
118-H-6 (Reactor-Soil)				0.999	5,760
118-KE-1 (Reactor-Soil)				0.999	5,344
118-KE-2 (Storage)(a)		12.2	7.6	9.1	92.9
118-KW-1 (Reactor-Soil)				0.999	4,568
118-KW-2 (Storage)(a)		12.2	7.6	9.1	92.9
120-D-2 (Surface Impoundment)		28.1	28.1	4.3	792
132-DR-2 (Stack)	5.1			60.1	20.4
141-C (Laboratory)(b)				18.2	431
200-W-40 (Laboratory)(c)		15.2	7.0	20.4	107
200-W-43 (Sand Filter)		25.9	25.9	4.0	676
200-W-44 (Sand Filter)		29.3	29.3	6.7	856
200-W-45 (Sand Filter)		33.6	15.2	4.9	511
200-W-69 (Laboratory)(b)		99.9	48.7	18.2	4,866
200-E-30 (Sand Filter)		33.5	15.2	4.9	511
200-E-103 (UPR)				0.999	17,326
200-E-107 (UPR)		115	34.8	0.999	3,982
200-E-115 (UPR)		9.1	8.1	0.999	83.5
200-E-124 (UPR)		64	4.6	0.999	294
200-E-125 (UPR)		6.8	4.4	0.999	30.3
200-E-41 (UPR)		150	150	0.999	22,500
200-E-42 (UPR)		94.0	95.0	0.999	26,000
200-E-44 (UPR)				0.999	9.99
200-E-117 (UPR)		3.1	3.1	0.999	9.3
200-E-121 (UPR)		200	24.4	0.999	4,876
200-E-122 (Storage)(d)		44	20	6.7	880
200-E-123 (UPR)		7.1	4.5	0.999	32.0
200-E-128 (UPR)				0.15	0.018
200-E-129 (UPR)		6.1	3.7	0.999	22.3
200-E-130 (UPR)				0.999	0.999
200-E-137 (Stack)	4.3			61	14.5
200-W-104 (Storage)				0.999	0.999
200-W-15 (UPR)		12.2	2.4	0.999	29.7
200-W-67 (UPR)		100	18	0.999	1,800
200-W-76 (Storage)		18.3	7.6	0.999	9.99
200-W-83 (UPR)		6.1	6.1	0.999	139
200-W-85 (UPR)		3.1	3.1	0.999	37.2
200-W-86 (UPR)		36.6	9.1	0.999	9.3

Table 5.2. (contd)

Site	Diameter (m)	Length (m)	Width (m)	Depth/Height (m)	Cross-Sectional Area (m^2)
200-W-87 (UPR)		6.1	3.1	0.999	334
200-W-90 (UPR)				0.999	18.6
202-A-WS-1 (Storage)				0.999	9.99
212-N (Storage)(a)				9.1	555
212-P (Storage)(a)				9.1	555
212-R (Storage)(a)				9.1	555
216-Z-1A (Tile Field)		84.0	35.0	5.8	2,940
216-Z-9 (Trench)		36.6	27.4	6.4	1,003
216-Z-19 (Crib)		63.1	3.0	5.5	192
218-E-14 (Storage Tunnel)		109	5.8	6.9	632
218-E-15 (Storage Tunnel)		515	10.4	6.7	5,332
221-B-WS-2 (Storage)		5.4	4.0	6.7	21.4
222-SD (Storage)		5.8	4.9	2.6	27.8
300-16 (UPR)				0.999	0.999
300-24 (UPR)				0.999	2,752
300-25 (Laboratory)		71.5	61.9	13.7	4,423
300-251 (UPR)		30	25	0.999	450
300-264 (Laboratory)(e)		70	40	22.6	2,800
300-28 (UPR)		168	6.5	0.999	1,055
300-33 (UPR)		116	48.8	0.999	5,649
300-39 (Storage)		27.4	10.1	10.4	276
300-4 (UPR)		19.5	21.3	0.999	415
303-K_CWS (Storage)		24.1	28.7	4.1	690
303-M-SA (Storage)		13.7	10.6	0.13	145
305-B-SF (Storage)		36.9	11.6	5.5	427
313-ESSP (Storage)				0.999	99.9
4843 (Storage)(f)		12.2	12.2	5.0	149
600-108 (Storage)		12.2	3.7	2.4	44.6
600-259 (Laboratory)(e)		25	25	22.6	625
600-59 (Storage)(g)		6.1	4.6	2.6	27.9
RMWSF (Storage)(h)		12.3	6.7	9.1	56,345
TRUSAF (Storage)(d)		60	18.3	6.7	1,098
HLW-Store (Storage)				5.3	100,000
1224B Plant Filter (Process Unit/Plant)	0.79			2.3	0.49
3712USSA (Storage)				0.999	99.9
GTF (Process Unit/Plant)		9.99	9.99	2.4	99.9

Table 5.2. (contd)

Site	Diameter (m)	Length (m)	Width (m)	Depth/Height (m)	Cross-Sectional Area (m^2)
UPR-100-F-3		3.0	3.0	0.999	9.3
UPR-200E-10				0.999	0.999
UPR-200-E-119				0.999	0.999
UPR-200-E-99				0.999	0.999
UPR-200-E-106				0.999	0.999
UPR-200-E-140				0.999	0.999
UPR-200-E-45		91.4	30.5	0.999	2,787
UPR-200-E-55		30.5	30.5	0.999	929
UPR-200E-74				0.999	4.6
UPR-200W-10				0.999	0.999
UPR-200W-113				0.999	0.999
UPR-200-W-134				0.999	0.999
UPR-200-W-164				0.999	283
UPR-200-W-44		7.6	6.1	0.999	46.5
UPR-200-W-51		17.1	7.2	5.5	122
UPR-200-W-52				0.999	0.999
UPR-200-W-55				0.999	0.999
UPR-200-W-6				0.999	0.999
UPR-200-W-75		21.3	21.3	0.999	455
UPR-200-W-78				0.999	3.7
UPR-200-W-8		129.5	30.5	0.999	3,948
UPR-200-W-83				0.999	0.999
UPR-200-W-90				0.999	6.5
UPR-300-FF-1				0.999	0.999

(a) Same height as 118-B-9.
(b) Height is the average of the heights of 221-T-CSTF and 300-25 laboratories.
(c) Same volume as 221T CSTF.
(d) Same height as 100-K-42 and 100-K-43 facilities.
(e) Same dimensions as Lab 221-T-CSTF.
(f) Same volume as 118-B-9.
(g) Same height as 222SD facility.
(h) Same dimensions as 118-B-9.
CWS = Cooling water system.
TRUSAF = Transuranic Waste Storage and Assay Facility.
GTF = Grout Treatment Facility.
CSTF = Containment Systems Test Facility.
HLW = High-level waste.

Table 5.3. Calculated Values[a] of Bulk Density and Volumetric Moisture Content for 2004 Composite Analysis Release Model Runs of the Soil-Debris Model

Area	Bulk Density (g/cm^3)	Volumetric Moisture Content (θ_w)
100[b]	2.16 ± 0.20	0.0830 ± 0.0497
200 West[c]	1.535 ± 0.1085	0.0594 ± 0.0310
200 East[d]	1.535 ± 0.1085	0.0594 ± 0.0310
300[e]	2.16 ± 0.20	0.0657 ± 0.0174

(a) Values are based on a statistical treatment of individual data points measured or calculated over a depth range from 0 to 20 feet.
(b) Bulk density and volumetric moisture content values calculated from bulk density and moisture content data from Peterson et al. 1996. Volumetric moisture content (θ) = volume of water in sample divided by ([dry weight of soil/bulk density] + volume of water).
(c) Bulk density and volumetric moisture content values for 200 East Area also used for the 200 West Area.
(d) Bulk density and volumetric moisture content values calculated from bulk density and moisture content data from Fayer et al. (1999).
(e) The same value of bulk density used in the 100 Area was assigned to the 300 Area. The volumetric moisture content value for the 300 Area was calculated from using the moisture content data found in Appendix B (page B.2) of Schalla et al. (1988).

Site recharge rates, site cross-sectional areas, and sorption factors are the same as those used by the vadose zone module (see the vadose zone data package for the composite analysis, Last et al. 2004b). Recharge rates vary based on current or predicted site conditions (e.g., soil type, presence or absence of vegetation or a cover) (Fayer et al. 1999; Riley and Lo Presti 2001) and the precipitation record of the Hanford Site. In the case of the sorption factors (K_ds) , the soil-debris model uses values recently assigned as a result of an assessment of contaminant transport in Hanford sediments (Cantrell et al. 2002; Last et al. 2004b). The most commonly used K_d category is that associated with sites that are low organic, low salts, and near neutral pH in chemistry (Table 5.4). Exceptions are six unplanned release sites (UPR-200-E-19, UPR-200-E-99, UPR-200-E-45, UPR-200-W-51, UPR-200-W-52, UPR-200-W-75) where a category 2 high-impact K_d is used (Table 5.5).

Values of aqueous solubility (C_{sol}) for analytes were derived from experimental measurements or estimated based on geochemical calculations (e.g., using the MINTEQA2 computer code). For radionuclides where no specific solubility values were available, the aqueous solubility has been fixed at an arbitrarily high default value (1 x 10^{10} mg/L) so that the soil-debris release model automatically selects algorithms for sorption (K_d) control in these cases (Kincaid et al. 1998). Radionuclides that have been assigned default values are tritium, technetium, iodine, strontium, and cesium. Uranium and plutonium solubility were calculated starting from values of uranium and plutonium estimated in Hanford groundwater (Wood et al. 1995) (Table 5.6). The solid phases assumed to control dissolved uranium and plutonium for these calculations were $UO_2(OH)_2 \cdot H_2O$ and $PuO_2 \cdot H_2O$. The solubility of chromic anhydride (CrO_3) is used to represent the solubility of Cr^{+6} (Dean 1999).

Table 5.4. Waste Chemistry/Source Category 4: Low Organic/Low Salt/Near Neutral

Analyte	High Impact (F1)		
	K_d Estimate (mL/g)		
	Best	Min	Max
Non-Adsorbing Radionuclides			
Tritium	0	0	0
Technetium-99	0	0	0.1
Chlorine-36	0	0	0
Moderately Adsorbing			
Iodine-129	0.2	0	2
Uranium-238	0.8	0.2	4
Selenium-79	5	3	10
Neptunium-237	10	2	30
Carbon-14	50	0	100
Highly Adsorbing			
Strontium-90	22	10	50
Cesium-137	2,000	200	10,000
Plutonium-239	600	200	2,000
Europium-152	200	10	1,000
Organic Elements			
Carbon Tetrachloride	0.2	0.1	0.6
Inorganic Elements			
Chromium VI	0	0	0.3

Table 5.5. Waste Chemistry/Source Category 2: Very High Salt/Very Basic

Analyte	High Impact (D)		
	K_d Estimate (mL/g)		
	Best	Min	Max
Non-Adsorbing Radionuclides			
Tritium	0	0	0
Technetium-99	0	0	0.1
Chlorine-36	0	0	0
Moderately Adsorbing			
Iodine-129	0.02	0	0.2
Uranium-238	0.8	0.2	4
Selenium-79	0	0	0.1
Neptunium-237	200	100	500
Carbon-14	50	0	100
Highly Adsorbing			
Strontium-90	22	10	50
Cesium-137	10	0	500
Plutonium-239	200	70	600
Europium-152	200	10	1,000
Organic Elements			
Carbon Tetrachloride	0.2	0.1	0.6
Inorganic Elements			
Chromium VI	0	0	0.3

Table 5.6. Aqueous Solubility for Analytes in the Soil-Debris Model

Analyte	Values (Ci/m^3)	Source
Tritium	9.7 x 10^7	Kincaid et al. 1998
Technetium	1.7 x 10^2	
Iodine	1.77 x 10^0	
Strontium	1.37 x 10^6	
Cesium	8.67 x 10^5	
Chlorine	3.30 x 10^2	
Carbon	4.47 x 10^4	
Selenium	6.98 x 10^2	
Europium	1.77 x 10^6	
Uranium	2.95 x 10^{-11}	Wood et al. 1995
Plutonium	3.58 x 10^{-10}	
Neptunium	5.7 x 10^{-9}	
Carbon Tetrachloride	8 x 10^{-4} g/cm^3	Rohay 2000
Chromium VI	6.17 x 10^{-4} g/cm^3	Dean 1999

5.3 Cement Model

The original quantity of contaminant contained in the cement is provided by the Inventory Module. Waste source dimensions (see Table 2.1 for waste source types) to calculate source volumes and surface areas are primarily from the WIDS database. When source dimension information was missing, the source with missing data was compared to a source of similar type to obtain or calculate dimensions from which volumes and surface areas could be estimated. For each site or aggregated site, the surface area to volume ratio is assumed to be constant for all time periods during any given realization of the assessment run.

Table 5.7 summarizes source dimensional data for application of the cement model for the composite analysis.

Diffusion coefficients are from several sources. A default value is used when specific data are lacking (Table 5.8). Most diffusion coefficients are derived from experiments performed under saturated moisture conditions (Serne et al. 1992). Diffusion coefficients for selected radionuclides have been determined for unsaturated conditions (Mattigod et al. 2001).

Table 5.7. Summary of Waste Source Volumes and Surface Areas for Sources Requiring Cement Release Model for 2004 Composite Analysis Runs

Waste Source	Length (m)	Width (m)	Height (m)	Volume (m^3)	Surface Area (m^2)
100-D-53 (Process Unit/ Plant)(a)	20.7	11.9	2.44	601	652
100-K-6	2.7	2.7	0.999	7.3	25.4
100-K-61(a)	9.99	9.99	2.4	244	297
100-K-62(a)	9.99	9.99	2.4	244	297
116-KE-5 (Process Unit/Plant)	9.99	9.99	2.4	244	297
116-KE-6D (Process Unit/ Plant)(a)	9.99	9.99	2.4	244	297
116-KW-4 (Process Unit/ Plant)(a)	9.99	9.99	2.4	244	297
218-W-4C (Cement in Burial Ground)	482	482	5.4	124 x 10^6	474 x 10^5
200 ETF (Process Unit/Plant)(a)	9.99	9.99	2.4	244	297
200-E-136 (Process Unit/Plant)	306	36.3	30.5	338,651	43,106
201C (Process Unit/Plant)(b)	42.7	24.4	6.7	6,971	2,980
202S (Process Unit/Plant)	142	49.1	25.0	174,546	23,536
203-S_%_205-S (Process Unit/ Plant(d)	84	68	22.8	130,005	18,343
205A (Process Unit/Plant)	3.7	3.0	2.4	27.2	55
218-E-14 (Storage Tunnel)	109	5.8	6.9	4,334	2,840
218-E-15 (Storage Tunnel)	515	10.4	67.7	35,766	17,704
218-E-RCRA	205	219	12.2	5.46 x 10^5	9.99 x 10^4
218-W-3AE (cement in burial ground)				1.21 x 10^6	4.63 x 10^5
218-W-4B (cement waste in burial ground)				1.60 x 10^5	6.36 x 10^4
221B (Process Unit/Plant)(c)	195	34.6	24.2	163,161	24,576
221T (Process Unit/Plant)(c)	195	34.6	24.2	163,161	24,576
221U (Process Unit/Plant)	247	20.1	23.5	116,586	22,468
224B (Process Unit/Plant)	60.1	18.3	21.4	23,471	5,546
224T(Process Unit/Plant)	60.1	18.3	18.3	20,088	5,063
224U (Process Unit/Plant)(e)	60.1	18.3	19.8	21,780	5,304
231Z (Process Unit/Plant)(f)	66	66	22.8	99,142	14,720
232-Z (Process Unit/Plant)	17.4	11.3	9.8	1,135	724

Table 5.7. (contd)

Waste Source	Length (m)	Width (m)	Height (m)	Volume (m^3)	Surface Area (m^2)
233-S (Process Unit/Plant)	26.2	11.3	9.8	2,883	1,322
234-5Z (Process Unit/Plant)(c)	195	34.6	24.2	163,161	24,576
241-A-431 (Process Unit/Plant)	6.1	4.9	0.999	29.7	81.4
241-C-801 (Process Unit/Plant)	9.8	7.9	7.6	588	424
241-SX-401 (Process Unit/ Plant)	11.0	7.3	2.1	171	236
241-SX-402 (Process Unit/ Plant)	11.0	7.3	2.1	171	236
276-S (Process Unit/Plant)	17.7	13.1	10.7	2,472	1,120
276U (Process Unit/Plant)	20.2	16.5	2.4	810	842
291C (Process Unit/Plant)(a)	13.6	13.6	2.4	454	505
291U (Process Unit/Plant)	5.8	5.5	4.3	136	160
292S (Process Unit/Plant)	8.2	4.3	0.999	35.1	95.2
293S (Process Unit/Plant)	8.8	4.9	0.999	43.1	114
300VTS (Process Unit/Plant)(g)	104	85.3	25.0	221,021	27,134
300-249 (Plant Unit/Process)(a)	9.99	9.99	2.4	244	297
303-M-UOF(a)	9.99	9.99	2.4	244	297
309-WS-1 (Process Unit/Plant)	4.3	4.3	4.9	88.8	120
309-WS-2 (Process Unit/Plant)	8.0	4.8	4.9	188	202
325-WTF (Process Unit/ Plant)(a)	9.99	9.99	2.4	244	297
600-117 (Process Unit/Plant)(g)	143	91.4	25.0	327,352	37,929
600-148 (Cement Component in ERDF)	433	229	5.0	4.95×10^5	2.04×10^5
618-11 (Cement Waste in Burial Ground)	3.0	2.5	7.6	68.9	199
WRAP (Process Unit/Plant)(d)	73.1	61.0	22.8	101,495	15,023
GTF (Process Unit/Plant)(a)	9.99	9.99	2.4	244	297
GTFL (Cement Component in Burial Ground)	38.1	15.2	10.4	6,017	2,267
HWVP (Process Unit/Plant)(a)	9.99	9.99	2.4	244	297
CS Resin (Cement Component in Burial Ground)	460	460	5.3	1.13×10^6	4.33×10^5
ILAW-HLW-Solid (Cement Component in Burial Ground)	460	460	5.3	1.13×10^6	4.33×10^5

Table 5.7. (contd)

Waste Source	Length (m)	Width (m)	Height (m)	Volume (m^3)	Surface Area (m^2)
TC-Resin (Cement Component in Burial Ground)	460.08	460.08	5.3	1.13 x 10^6	4.33 x 10^5
2711-S (Process Unit/Plant)	4.2672	3.81	2.4384	39.64	71.91
2718-S (Process Unit/Plant)	4.2672	3.81	2.4384	39.64	71.91
2904-SA (Process Unit/Plant)	2.4384	2.4384	2.1336	12.69	32.70
1224B Plant Filter (Process Unit/Plant)			2.29[(h)]	1	6.7

(a) Same height as 276U facility.
(b) Same height as 100-K-42 and 100-K-43 facilities.
(c) Data generated from averages of 202S and 211U facility dimensions.
(d) Same height as 231Z facility.
(e) Data generated from dimensions of 224B and 224T facilities including the averaging of the height for those two facilities.
(f) Dimensions estimated knowing that the facility is shaped like a square (60 m x 60 m) with attached rectangular area (23 m x 23 m) (Aaberg memo). We took the square root of the sum of the cross sectional surface areas depicting the facility shape (4,336 m^2) to yield an average dimension of 66 m x 66 m. The height of the facility was estimated using the average of heights of the 202A, 202S, 221B, 221T, 221U, 224B, 224T, 224U, and 234-5Z facilities (22.76 m).
(g) Same height as 202S facility.
(h) Diameter of filter (0.79 m).

ERDF = Environmental Restoration Disposal Facility, GTF = Grout Treatment Facility, ILAW = Immobilized low-activity waste, HLW = High-level waste, WTF = Waste Treatment Facility, ETF = Effluent Treatment Facility, RCRA = Resource Conservation and Recovery Act of 1976, HWVP = Hanford Waste Vitrification Plant.

Table 5.8. Diffusion Coefficients for the Cement Release Model

Analyte	Min (cm^2/yr)	Max (cm^2/yr)	Source
Technetium-99	1.58 x 10^{-4}	1.89 x 10^{-3}	Recent laboratory work (Mattigod et al. 2000)
Iodine-129	3.5 x 10^{-5}	3.5 x 10^{-5}	
Tritium	1.58 x 10^0	1.58 x 10^0	Default values (Serne et al. 1992)
Uranium-238	3.15 x 10^{-5}	3.15 x 10^{-5}	
Strontium-90	1.58 x 10^{-3}	1.58 x 10^{-3}	
Plutonium-239/240	1.58 x 10^{-5}	1.58 x 10^{-5}	
Cesium-137	1.58 x 10^{-2}	1.58 x 10^{-2}	
Carbon-14	3.15 x 10^{-5}	3.15 x 10^{-5}	
Europium-152	1.58 x 10^{-3}	1.58 x 10^{-3}	
Neptunium-237	3.15 x 10^{-4}	3.15 x 10^{-4}	
Selenium-79	6.30 x 10^{-3}	6.30 x 10^{-3}	
Chromium-VI	3.15 x 10^{-3}	3.15 x 10^{-3}	From cement (Serne et al. 1992)

5.4 Saltcake Model

In the past, the saltcake model has been used to simulate the release of contaminants from radioactive mixed waste in tanks. The sluicing process used to remove waste from these tanks likely removes all of the solid material known as saltcake. Thus, it does not seem reasonable to use the saltcake model to simulate contaminant release from solids remaining in a tank after sluicing.

For the composite analysis, simulations may be conducted with the saltcake model as a sensitivity analysis. In this case, a value of 0.36 g/cm^3 for saltcake solubility will be applied to all high-level waste tank solids. The value is based on the highest nitrate concentration found in high-level waste tank drainable liquors (Serne and Wood 1990). The same value was used in the application of release modeling in the tank waste remediation system final environmental impact statement (DOE 1996). The model takes the original tank waste volume(s) and converts it to original mass M_{wo} using a tank solid waste density of 1.58 ± 0.20 g/ml obtained by random sampling from a Gaussian distribution. This value was obtained from the analysis of 525 core samples collected from the 177 high-level waste tanks (Chen et al. 1998). Waste volumes and analyte quantities are provided by the Inventory Module. Sequences of recharge rates are those used by the vadose zone module. Tank cross-sectional areas used by the saltcake model are summarized in Table 5.9.

5.5 Reactor Block Model

The same model used to simulate release of radionuclides from decommissioned surplus production reactors in the initial composite analysis will be used in the 2004 Composite Analysis. Two scenarios are envisioned for simulating release from the reactor sources. Scenario 1 consists of those eight reactors that are being subjected to cocooning in the 100 Area for up to 75 years and then transported to the Central Plateau for final burial. Scenario 2 involves the release of contaminants from B Reactor that remains on the ground surface in the 100 Area and is not transported to the Central Plateau for burial. In both of these scenarios, analyte release to the vadose zone will be simulated in the same way. Radionuclide fractional release rates (DOE 1989, p. C.3) available for composite analysis release modeling is summarized in Table 5.10. With the exception of carbon-14, these release rates have been calculated from experimental leach rates (White et al. 1984) taking into account Hanford reactor configurations.

The constant carbon-14 fractional release rate was calculated using a time dependent equation (DOE 1989, p. D.4) assuming a constant reactor temperature of 22°C for inclusion in Table 5.10. The fractional release rate for carbon-14 can be made time/temperature dependent (see Section 2.3.6). A previous study has indicated temperatures at the graphite reflector edge may reach temperatures up to 900°C (Corlett 1958). At such a core temperature, temperature on the external face of the cast iron thermal shield is at a temperature of approximately 200°C (Haugland 1958). White et al. (1984) used a 10-year cool-off period for assessments involving reactor decommissioning. Therefore, one can envision an analytical solution where the fractional release rate of carbon-14 (at the time of each reactor shut down) is allowed to cool from 200°C to 22°C (linearly) over a period of 10 years.

Table 5.9. High-Level Waste Tank Cross-Sectional Areas for 2004 Composite Analysis[(a)]

Tank Group	Type 1[(b)] (cm^2)	Type 2[(c)] (cm^2)	Type 3[(d)] (cm^2)	Type 4[(e)] (cm^2)	Type 5[(f)] (cm^2)
T-101 to T-112				4,102,270	
T-201 to T-204					291,716
TY-101 to TY-106			4,102,270		
TX-101 to TX-118			4,102,270		
SY-101 to SY-103	4,102,270				
S-101 to S-110			4,102,270		
SX-101 to SX-115		4,102,270			
U-101 to U-112				4,102,270	
U-210 to U-204					291,716
B-101 to B-112				4,102,270	
B-201 to B-204					291,716
BY-101 to BY-112			4,102,270		
BX-101 to BX-112				4,102,270	
C-101 to C-112				4,102,270	
C-201 to C-204					291,716
AN-101 to AN-107	4,102,270				
AZ-101 to AZ-102	4,102,270				
AY-101 to AY-102	4,102,270				
AX-101 to AX-104		4,102,270			
A-101 to A-106		4,102,270			
AP-101 to AP-108	4,102,270				
AW-101 to AW-106	4,102,270				

(a) Data from WHC 1994.
(b) Double-shell tanks of this type are 22.8 m in diameter. The bottoms of the tanks are located 16.8 m below the ground surface and the top of their domes are located 2.2 m below the ground surface.
(c) Single-shell tanks of this type are 22.8 m in diameter. The bottoms of the tanks are located 15.2 m below the ground surface and the top of their domes are located 1.8 m below the ground surface.
(d) Single-shell tanks of this type are 22.8 m in diameter. The bottoms of the tanks are located 13.8 m below the ground surface and the top of their domes are located 2.4 m below the ground surface.
(e) Single-shell tanks of this type are 22.8 m in diameter. The bottoms of the tanks are located 11.3 m below the ground surface and the top of their domes are located 2.3 m below the ground surface.
(f) Single-shell tanks of this type are 6 m in diameter. The bottoms of the tanks are located 11.4 m below the ground surface and the top of their domes are located 3.4 m below the ground surface.

For the eight reactor cores destined for eventual disposal on the Central Plateau, the following scenario will be implemented for time/temperature dependent carbon-14 release:

- Reactor temperature at time of shutdown: 200ºC
- Linear decrease in reactor temperature from 200ºC to 22ºC for a 10-year period of time following reactor shutdown
- Reactor temperature constant at 22ºC for an additional 65 years while reactors remain in the 100 Area
- Reactor temperature dropped to 16ºC at the time of their burial on the 200 Area plateau and stays at this temperature for the remainder of any simulations.

Table 5.10. Fractional Release Rates Available for Use in Reactor Block Model for 2004 Composite Analysis

Analyte	Fractional Release Rate (y^{-1})
Americium-241	2.92×10^{-2}
Carbon-14[(a)]	6.9×10^{-5}
Cesium-137	1.10×10^{-2}
Chlorine-36	3.65×10^{-4}
Cobalt-60	1.10×10^{-2}
Europium-152	2.92×10^{-2}
Iodine-129	3.65×10^{-4}
Iron-55	3.65×10^{-3}
Nickel-59	3.65×10^{-3}
Nickel-63	3.65×10^{-3}
Plutonium 239/240	2.92×10^{-2}
Selenium-79	2.92×10^{-2}
Strontium-90	1.10×10^{-2}
Technetium-99	2.92×10^{-2}
Tritium	3.65×10^{-4}

(a) The fractional release rate for carbon-14 was calculated using the temperature dependent equation in Section 2.4.6 $(365)[565(1+100e^{-0.08(365)0.3})e^{-6440/295.15}] = 6.9 \times 10^{-5}\ y^{-1})$ and assuming EIS conditions of steady-state release flux (time [t] at steady-state flux conditions (at 0.3 yr) and constant temperature of 22°C (295.15°K) representative of conservative subsurface temperature at burial depths on the 200 Area plateau.

(b) Fractional release rate for europium-154 used for europium-152 isotope.

The basis for the above assumptions was that it was noted that in using this equation for the composite analysis (Kincaid et al. 1998) that the release flux falls within 1% of its ultimate steady-state flux value at approximately 0.3 year. Compared to the length of the initial composite analysis simulations (1,000 to 2,000 years), the initial period of transient release was assumed to be insignificant. By assuming steady-state and constant temperature conditions, the above equation reduces to the form of the analytical solution used for the other radionuclides and a constant fractional release value rate for carbon-14 can be calculated.

For B Reactor, the simulation is slightly different:

- Reactor temperature at time of shutdown: 200ºC
- Linear decrease in reactor temperature from 200ºC to 22ºC for a 10-year period of time following reactor shutdown
- Reactor temperature stays at 22ºC for the remainder of any simulation.

Carbon-14 fractional release rates for conduct of these scenarios are summarized in Table 5.11. The results of both of these simulations can be compared to the corresponding simulations that are made using a constant fractional release rate for carbon-14.

Table 5.11. Carbon-14 Fractional Release Rates for Scenarios A and B

Time (y)	Temperature (°C)	Temperature (°K)	Fractional Release Rate (y^{-1})(a)
1	200	473.15	2.5×10^{-1}
2	182.2	455.35	1.5×10^{-1}
3	164.4	437.55	8.4×10^{-2}
4	146.6	419.75	4.5×10^{-2}
5	128.8	401.95	2.3×10^{-2}
6	111.0	384.15	1.1×10^{-2}
7	93.2	366.35	4.8×10^{-3}
8	75.4	348.55	2.0×10^{-3}
9	57.6	330.75	7.2×10^{-4}
10	39.8	312.95	2.4×10^{-4}
11	22.0	295.15	6.9×10^{-5}
76	16.0	289.15	4.4×10^{-5}

(a) Calculated using the following equation: $F = (365)[565(1+100e^{-(0.08)(365)t})e^{-6440/T}]$.

Implementation of the above scenario requires dates of reactor shutdown or standby. These data are provided in Table 5.12 and signify the onset of release from each of the reactor cores for each of the above scenarios.

Table 5.12. Shutdown Dates for Hanford Production Reactors(a)

Reactor	Date of Shutdown
DR Reactor	12-30-64
H Reactor	4-21-65
F Reactor	6-25-65
D Reactor	6-26-67
B Reactor	2-12-68
C Reactor	4-25-69
KW Reactor	2-1-70
KE Reactor	1-28-71
N Reactor	3-87 (standby)

(a) Ballinger and Hall 1991.

5.6 Glass Model

Curve fitting was performed using six STORM curves (i.e., outputs from the 2001 immobilized low-activity waste test cases (Table 5.13) from year 3 to 20,000 pooled, so as to develop an optimal solution over the entire available range of recharge rates represented in the test cases. Coefficient values with standard errors from the curve fitting process are shown in Table 5.14.

Table 5.13. STORM Cases Used to Develop Empirical Glass Model for Release of Technetium from Glass Waste Forms in the RH Trench. Also applies to total Uranium and Iodine release (cf., pg 23-24) Based on LAWABP1 glass. (Bacon and McGrail 2001)

STORM Case	Recharge Rate (mm/yr)	Asymptotic Normalized Flux at 20,000 Years (ppm/yr)
WFD	0.1	0.000381
WF7	0.5	0.00347
WF4	0.9	0.0124
WFA (Base case)	4.2	0.926 (at 100,000 years)
WF8	10	1.9004
WF6	50	2.5094

Table 5.14. Parameter Estimates from Model Fitting Process for the Glass Release Empirical Model for Technetium (G1 run)

Parameter	Value from Modeling Fitting Process	Standard Error
A	0.13378	0.001465
B	0.052915	0.0005578
C	3.9664	0.01591
W	103.75	2.327
X	-75.729	2.111
Y	88.631	0.4882
Z	-0.61862	0.01285

Currently parameter estimates have been developed only for technetium releases from the base French glass waste form, using the LAWABP1 Waste Glass formulation (Bacon and McGrail 2001, pg. 4 and 10). However, assuming congruent release of other analytes for a given waste form, this equation would apply to any similar embedded analyte in a glass with the LAWABP1 composition. Analytes released congruently with the dissolution of the waste glass include technetium, uranium, iodine, and selenium (Bacon and McGrail 2001, pg. 24).

Plutonium release from this glass has a similar time-flux profile but is about four orders of magnitude lower than the profile for technetium. Plutonium release is congruent with dissolution of PuO_2 rather than with the waste glass. For purposes of the composite analysis, plutonium releases will be accounted for using predicted releases from the empirical equation multiplied by 0.0001.

Because the release model calculates normalized flux, it will be necessary to calculate the instantaneous annual quantity released by multiplication of the annual flux by the initial inventory of analyte. Values for the predictor variable, infiltration rate, are to be provided either through the INFILTRATION keyword in VADER (table of constant recharge rates for periods of time) or through a special input file with annual realizations of recharge rate as generated by an off-line stochastic process. Release is congruent with dissolution of the glass waste form. In this manner, inventory remaining is accounted for, and when it is exhausted upon complete dissolution of the glass waste form, release stops. The release rates are slow enough that this does not happen for millions of years. The STORM model accounts for a change in surface area because of dissolution, but this effect is small, again because of the slow dissolution rates. The empirical model coefficients implicitly account for this change in surface area.

Currently there is no plan to implement a delay of release for immobilized low-activity waste for the composite analysis simulations to account for containment integrity. This is so contaminant releases to the water table from composite analysis simulations can be compared to results obtained in the immobilized low-activity waste 2001 performance assessment, where the effects of canister containment were not taken into consideration.

5.7 Atmospheric Release Modeling

The approach to post operational release of carbon-14 to the atmosphere from above-ground surplus production reactor sources is summarized in Appendix C. Carbon-14 release to the atmosphere from reactor cores located on the ground surface is assumed to be governed by its rate of conversion to carbon dioxide as a result of reaction with chronic ingress of air and moisture into the graphite matrix. The effects of cocooning on carbon-14 releases to the atmosphere were not taken into consideration.

Annual amounts of carbon-14 released from each reactor are obtained by VADER applying the release rate as a function of temperature found in column 3 of Table 5.15 to the times representative of reactor cooling followed by the remaining time periods that the reactors remain on the Hanford surface at an average temperature of 22°C. The application of the annual release rate at 22°C listed in Table 2.1 to eight reactors gives an annual release of 1.92 Ci/y that is consistent with the estimated annual release rate of 2 Ci/year for eight reactors cited in the SPRD EIS (DOE 1989, Appendix G, p. G.27).

For buried waste, VADER releases carbon-14 input from the Inventory Module to the Vadose Zone Module (STOMP) using the appropriate release model. STOMP partitions the VADER input into atmospheric and groundwater pathway components. As in the Inventory Module, STOMP assigns the amount of carbon-14 directed to the atmospheric pathway based on a carbon-14 to CO_2 rate as a function of temperature. For atmospheric release, the STOMP code requires data for distribution of the analyte between solid and liquid phases (K_d), liquid and gas phases (Henry's law constant), and effective diffusion coefficients in the liquid and gas phases (Table 5.16). For the composite analysis, STOMP will

Table 5.15. Reaction and Atmospheric Release Rates for Carbon-14 (as CO_2) from Surplus Production Reactors

Temperature (°C)(b)	Reaction Rate(c) (g/cm^2-day)	Carbon-14 Release Rate (Ci/y per reactor)(d)
200	8.17×10^{-9}	926
182.2	4.80×10^{-9}	544
164.4	2.70×10^{-9}	306
146.6	1.44×10^{-9}	163
128.8	7.32×10^{-10}	83
111.0	3.48×10^{-10}	39
93.2	1.95×10^{-10}	22
75.4	6.20×10^{-11}	7
57.6	2.32×10^{-11}	2.6
39.8	7.65×10^{-12}	0.87
22.0	2.21×10^{-12}	0.24
16.0	1.40×10^{-12}	0.16

(a) Release date data (Ci/y) are used to determine the annual releases of carbon-14 to the atmosphere during surplus production reactor operational periods, during reactor cool down, during cocooning, and following burial on the 200 Area plateau. B Reactor is assumed to remain on the surface in the 100 Area.

(b) Temperatures simulate reactor operations (200°C at the core external surface), during reactor cool down (200°C to 22°C over a period of ten years linearly), and buried (16°C) on the 200 Area plateau.

(c) Reaction rate is for the conversion of carbon-14 graphite to carbon dioxide ($C + O_2 \rightarrow CO_2$) (DOE 1989, p. D.1). The reaction rate can be calculated for any temperature using the following equation:

$$k = Ae^{-E/RT}$$

where $A = 6.7 \times 10^{-3}$ g/cm^2/day,
$E = 12{,}800$ cal/mol, and
$R = 1.9873$ cal/mol-deg
T = Reactor core temperature in degrees Kelvin (°K).

(d) Assume a volume of 2,761.82 m^3 for all reactor blocks (DOE 1989, p. 3.14). A graphite density of 2.25 g/cm^3 and a graphite surface area of 1 m^2/g (DOE 1989, Appendix D, page D-2) along with the volume gives a surface area of the reactor block of 6.21×10^{13} cm^2. A specific activity of 5×10^{-6} Ci/g was used (DOE 1989, p. D.4) along with the surface area to calculate annual release rates listed in column 3 of Table 1. An example release rate calculation for KW reactor for 22°C is as follows:

$$\text{Release rate} = 2.21 \times 10^{-12}\ \text{g/cm}^2\text{-day} \times 6.21 \times 10^{13}\ \text{cm}^2 \times 5 \times 10^{-6}\ \text{Ci/g} \times 365\ \text{days/y} = 0.24\ \text{Ci/y}.$$

Table 5.16. Parameter Values for Simulating Analyte Release from Buried Waste to the Atmosphere

Coefficient	C-14 as Carbon Dioxide	Iodine-129
Distribution Coefficient (K_d) mL/g	0	0.2
Henry's Law Constant (dimensionless)(a)	4.13×10^{5}	4.17×10^{-2}
Diffusion (cm^2/sec)(b)	0.01	0.01

(a) See Appendix D for calculations.
(b) Diffusion coefficient for low atomic number gases moving through soil (Wood et al. 1995).

assume upward migration by carbon-14 (as CO_2) and iodine-129 to occur in the gas phase only. Partition coefficient values for carbon-14 (as CO_2) and iodine-129 are assumed to be 0 and 0.2, respectively. Henry's law constants for iodine-129 and carbon-14 (as CO_2) were calculated based on their vapor pressures and their solubility in water at 25°C. A diffusion rate for small gaseous molecules moving through soil (Wood et al. 1995) was used for both carbon-14 (as CO_2) and iodine-129.

6.0 Parameter Uncertainties, Data Gaps, Technical Issues, and Recommendations

The term uncertainty in simulation modeling expresses known and unknown quantities and variability in inputs and predictions due to lack of knowledge. Sources of uncertainty in the Release Module include lack of precise knowledge about inventories, site characteristics, and physical and chemical processes relating to release rates.

For the 2004 Composite Analysis, data used for the various release model parameters will be assigned the statistical treatments listed in Table 6.1. The impact of these settings on results varies by waste type. For example, all the variability in reactor core release simulations comes from whatever variability is inputted to the reactor core inventory. The same is true for cement releases that are given constant diffusion coefficients with the exception of technetium-99. In all cases, the waste site dimensions (area, height, volume) will be treated as constants over all realizations. Infiltration rate time-profiles will vary over realizations for the 2004 Composite Analysis. In particular, periods representing ground cover will be the same over all realization, but the infiltration rate for a given ground cover period will vary stochastically from realization to realization. Consequently, the variability in release flux time-profile results was probably underestimated in the SAC initial assessment. Imparting more variability to infiltration rates might be expected to result in more accurate estimate of uncertainty in the 2004 Composite Analysis.

Table 6.1. Stochastic Treatment of Release Model Parameters Expected to be Implemented in the Composite Analysis. In all cases, the waste site dimensions (cross-sectional area, height, volume, surface area) are treated as constants.

Model	Variable Parameters	Fixed Parameters	Remarks
Liquid		Fractional release rate	Release rate set at 1
Soil-Debris	Soil moisture content Soil bulk density Infiltration rate	Solubility K_d (desorption coefficient)	Tritium K_d set to 0 to express maximum mobility
Soil-Debris	K_d (desorption coefficient) Soil moisture content Soil bulk density Recharge rate	Solubility	All analytes except tritium
Cement	Diffusion coefficient		Technetium-99
Cement		Diffusion coefficient	All analytes except technetium-99
Reactor Core		Fractional release	All analytes
Saltcake	ρ (saltcake density) Recharge rate	Salt solubility	All analytes
Glass	Recharge rate		All analytes

At the present time, there is insufficient data to support improvements in models critical to simulation of contaminant release from single-shell tank residuals. To close the gap, a project titled *Geochemical Testing and Model Development-Residual Tank Waste* is underway to support the Accelerated Tank Closure Demonstration Project. In the project, a number of different types of laboratory experiments are to be performed including some to discern between three different hypothesized release processes: release from soluble salts, release from less soluble minerals, and release from insoluble solids (kinetically controlled release).

7.0 Consistency Discussion

This data package is an extension of the SAC Initial Assessment release data package (Riley and Lo Presti 2001). Areas addressed in this data package that are absent in the initial SAC data package include 1) an improved conceptualization of the structure of the Release Module of SAC, 2) a conceptual model of contaminant release from engineered waste systems, 3) an implementation model of contaminant release from engineered waste systems, 4) a description of the numerical model for simulating analyte release from glassified waste, 5) improved documentation of model parameter data sets, and 6) modeling analyte release to the atmospheric pathway.

8.0 Conclusions and Recommendations

This document contains the data package for the Release Module (VADER Revision 1) of SAC for conduct of the 2004 Composite Analysis. The document includes a description of the Release Module and associated links to the other SAC modules, a conceptual model for contaminant release from engineered waste systems represented by the Release Module, an implementation model that describes key input parameters and outputs of the numerical models comprising the Release Module, and descriptions of the numerical models used to simulate contaminant release from specific waste sources. Sources of data for numerical model input parameters are described and the data to be used in the 2004 Composite Analysis are summarized in parameter specific tables. Parameter uncertainty is addressed along with technical issues needing resolution to continue to improve Release Module capability.

A number of improvements have been made to the System Assessment Capability (SAC) Release Module capability since it was first used to conduct the SAC Initial Assessment (Bryce et al. 2002). Improvements include 1) addition of an empirical model to VADER based on release outputs of the Subsurface Transport Over Reactive Multiphases (STORM) code that allows simulation of contaminant release from ILAW waste, 2) numerical models that account for the effects of different types of waste containment (e.g., concrete containers and metal liners), and 3) the consideration of the atmospheric pathway for release of selected contaminants from buried waste. Two of these new capabilities (i.e., modeling of contaminant release from ILAW waste and buried waste to the atmosphere) are to be implemented in the 2004 Composite Analysis.

The cement model, rather than the saltcake model will be used to simulate contaminant release from tank high-level waste residuals in the 2004 Composite Analysis. This decision was made recognizing that residuals remaining after tank sluicing likely have a composition more similar to sludge and hard heel than saltcake. It is expected that this change will result in less conservative (slower release) estimates of contaminant release from tank residuals than were observed in the results of the SAC Initial Assessment. This simulation approach is viewed as the best option at this time pending the development of new models for simulating contaminant release from tank residuals based on the results of Hanford research to be completed in the near future. The approach also allows for some basis of comparison with release modeling associated with ongoing Tank Farm Closure Assessments.

The extent of documentation of parameter data has improved with the publication of this data package. This includes the traceability of the data to the updated version of the release data catalog that provides a direct link to published sources of raw data. As a result, this report serves as a technical document that will support the findings of the 2004 Composite Analysis in a scientifically defensible fashion.

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Appendix A

Technical Justification for Exclusion of the Naval Reactor Compartments as Sources of Contaminant Release in 2004 Composite Analysis

Appendix A

Technical Justification for Exclusion of the Naval Reactor Compartments as Sources of Contaminant Release in 2004 Composite Analysis

The composite analysis for the Hanford Site is a radiological assessment to estimate doses to hypothetical future members of the public from radionuclides from low-level waste disposal and all other sources of radioactive contamination at the Hanford Site. This analysis is required under U.S. Department of Energy (DOE) Order 435.1. Results of the first composite analysis were reported in 1998 (Kincaid et al. 1998) and an update of the composite analysis is underway this fiscal year (Hildebrand et al. 2003). The update of the composite analysis will simulate radionuclide release from all Hanford sources over a period beginning in 1944 and continuing through 10,000 years post-closure.

Since 1986, decommissioned Naval reactor compartments have been emplaced in trench 94 of solid waste burial ground 218-E-12B, located on the Central Plateau at DOE's Hanford Site in southeastern Washington State. Plans call for continued emplacement through 2020 when it is estimated that 220 reactor compartments will be located in the trench.

In the initial composite analysis assessment, radionuclide inventories associated with the emplaced reactor compartments were excluded from inventories associated with the 218-E-12B burial ground because they consist of activation products within corrosion-resistant metals (Kincaid et al. 1998, Appendix A, page A.6), and the analysis was for a relatively short 1,000-year post-closure period. The modeling capability to be applied in the update of the 2004 Composite Analysis is more sophisticated and allows consideration of the impact of reactor compartment inventories as an independent source term, and the analysis is now for a 10,000-year post-closure period. The new capability to examine individual sources or types of sources, and the longer time period of analysis require a re-evaluation of the Naval reactor compartments as a potential composite analysis source term.

The long-lived radionuclide inventory is contained in the reactor vessel internal structure, housed within each reactor compartment (DOE 1996, Appendix D, p. D-6). Release of radionuclide inventories from the reactor compartments requires breaching of a minimum of approximately 0.152 meter of steel containment (DOE 1996, Appendix B, p. B-4). The length of time before access to the internal structure can occur is governed by both the uncertainty in the rate of corrosion of the steel containment and soil pressure exerted on the exterior of the reactor compartment disposal package.

The Department of the Navy has estimated, based on calculations made using the maximum and expected corrosion rates and the minimum steel containment thickness (DOE 1996, Appendix B, Table B-2, p. B-9), and taking into account the effects of soil pressure (DOE 1996, Appendix B, p. B-8), that time until access to the internal structure of the reactor vessel is 10,000 to 30,000 years. Thus, the release of radionuclide inventories from the Naval reactor compartment source term will not occur during the planned simulation time frame of the updated Composite Analysis, i.e., 10,000-years post-closure. Therefore, further consideration of inclusion of this source term in the updated Composite Analysis assessment is deemed unnecessary.

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Appendix B

Justification for Exclusion from Consideration of Chlorine-36 as a Subsurface Source of Release to the Atmosphere in the 2004 Composite Analysis

Appendix B

Justification for Exclusion from Consideration of Chlorine-36 as a Subsurface Source of Release to the Atmosphere in the 2004 Composite Analysis

The surplus production reactor environmental impact statement (EIS) states that "the major pathway for transport of radionuclides and chemicals to the effected environment is groundwater" (DOE 1989, Appendix G, page G.1). Of the radionuclides modeled, only carbon-14 is considered in the atmospheric pathway (DOE 1989, Appendix G, page G.27). While chlorine-36 is considered a constituent for assessment in the groundwater pathway (DOE 1989, Appendix C, page C.2; Appendix D, page D.4), no where in the draft EIS report (DOE 1989) or in its supplement (DOE 1992) is mention made of chlorine-36 as a source of atmospheric release. Release of chlorine-36 from surplus production reactors by way of the atmospheric pathway was not considered in the past composite analysis (Kincaid et al. 1998, page 4.33) or in other Hanford assessments where the atmospheric pathway is addressed (WDOE/WDOH 2000; DOE 1996a, 1996b, 2004; Jacobs 1996; Kincaid et al. 1995; Lockheed Martin Hanford, Inc. 1995; Mann et al. 2001; Wood et al. 1995a, 1995b, 1996). Therefore, it can be concluded from the above, and while not directly addressed, that chlorine-36 was not identified as an important atmospheric pathway constituent in assessment of radionuclide contaminant release from surplus production reactors.

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Appendix C

Approach to Post-Operational Release of Carbon-14 to the Atmosphere from Above-Ground Surplus Production Reactor Sources for the 2004 Composite Analysis

Appendix C

Approach to Post-Operational Release of Carbon-14 to the Atmosphere from Above-Ground Surplus Production Reactor Sources for the 2004 Composite Analysis

Following shutdown, eight of the nine plutonium production reactors (graphite stacks) are being surface stabilized (cocooned) at their locations in the 100 Areas so that radioactivity within them can decay to safe limits. After 75 years of interim surface storage, these reactors are to be transported to a location in the 200 West Area and disposed in a burial ground (DOE 1989; BHI 1998; Romano and Miller, 1995). B Reactor is to remain above ground and un-stabilized with the intent that it may become a national landmark in the future.

Carbon-14 will be released to the atmosphere over 75 years from the interim stored reactors as part of the 10,000-year 2004 Composite Analysis simulations. For B Reactor, carbon-14 release to the atmosphere will occur post shutdown to the end of the 10,000-year simulation.

Key to the mechanism by which carbon-14 release from the graphite reactors occurs is the physical stability of the graphite cores. Ingress of air and water vapor into the core has been shown to result in conversion of carbon-14 to CO_2 (Gray 1982). Therefore, release of carbon-14 to the atmosphere can be tied to the rate at which this reaction occurs during reactor cool down and during longer periods of time where the reactors remain on the ground surface under ambient Hanford conditions (i.e., 22°C). A possible deviation to this mechanism is if graphite undergoes significant corrosion during the 10,000-year time frame and release of carbon-14 to the atmosphere occurs more rapidly because of ingress of air and water vapor contacting a higher surface area of exposure.

Graphite is extremely resistant to corrosion by the most aggressive of chemical reagents (e.g., acids and alkalies) and, therefore, would not be expected to corrode to any significant extent under Hanford surface conditions over a 10,000-year timeframe. Extreme stability is also demonstrated by the high compressive strength and hardness characteristics associated with the graphite constituting the reactor cores (Paasch 1985). Compressive strength of the graphite is equal to or greater than that of concrete proposed for use in Hanford site high integrity containers with a calculated best estimate number of years to degradation of 7,620 years(a) (Pihlajavaara 1994). Graphite is non-porous relative to concrete. This suggests that reactor graphite cores can be considered physically stable over the course of the 10,000-year 2004 Composite Analysis simulation.

(a) Personal communication between S Phillips (AG Engineering and Development Company) and RG Riley (Pacific Northwest National Laboratory, Richland, Washington), 2003.

Based on these facts, carbon-14 release to the atmosphere from reactor cores located on the ground surface is assumed to be governed by its rate of conversion to carbon dioxide as a result of reaction with chronic ingress of air and moisture into the graphite matrix. The effects of cocooning on carbon-14 releases to the atmosphere were not taken into consideration.

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Appendix D

Henry’s Law Constants for Carbon-14 (as carbon dioxide) and Iodine-129

Appendix D

Henry's Law Constants for Carbon-14 (as carbon dioxide) and Iodine-129

Calculation of Henry's Law constant for carbon dioxide.

K_h = vapor pressure of CO_2 at room temperature divided by the solubility of CO_2 in water at room temperature.

K_h = 60 atm (CRC, p. D-118) ÷ 0.5916 mol/m^3 (Dean 1999) = 1.01×10^2 atm-m^3/mol

$K_{dimensionless} = K_h \div R \bullet K$ = 1.02 atm-m^3/mol ÷ [8.20575×10^{-5} atm-m^3/mol-°K • 298°K] = 4.13×10^5

Calculation of Henry's Law constant for iodine-129.

Data on the vapor pressure of iodine as a function of temperature was obtained from the CRC handbook (CRC, p. D-115) and plotted (Figure D.1). A best-fit equation was determined. The equation was used to determine the vapor pressure of iodine at room temperature.

$[25 - 28.248] \div 49.501 = \text{Log } X$

$X = 10^{-3.248/49.501} = 10^{-0.0656} = 0.8958$ mm Hg

Vapor pressure of iodine in atmospheres = 0.8958 mm Hg • 1 atm/760 mm Hg = 0.0012 atm.

Gas/liquid partition coefficient = 0.0012 atm ÷ 1.18 mol/m^3 (CRC, p. B-182) = 1.02×10^{-3} atm-m^3/mol

Dimensionless gas/liquid partition coefficient =
[1.02×10^{-3} atm-m^3/mol] ÷ [8.20575×10^{-5} atm-m^3/mol-°K • 298°K] = 4.17×10^{-2}

D.1 References

CRC Handbook of Chemistry and Physics, 48th Edition. Chemical Rubber Company, Cleveland, Ohio.

Dean JH (ed.). 1999. *Lange's Handbook of Chemistry,* Fifteenth Edition. McGraw-Hill, Inc., New York.

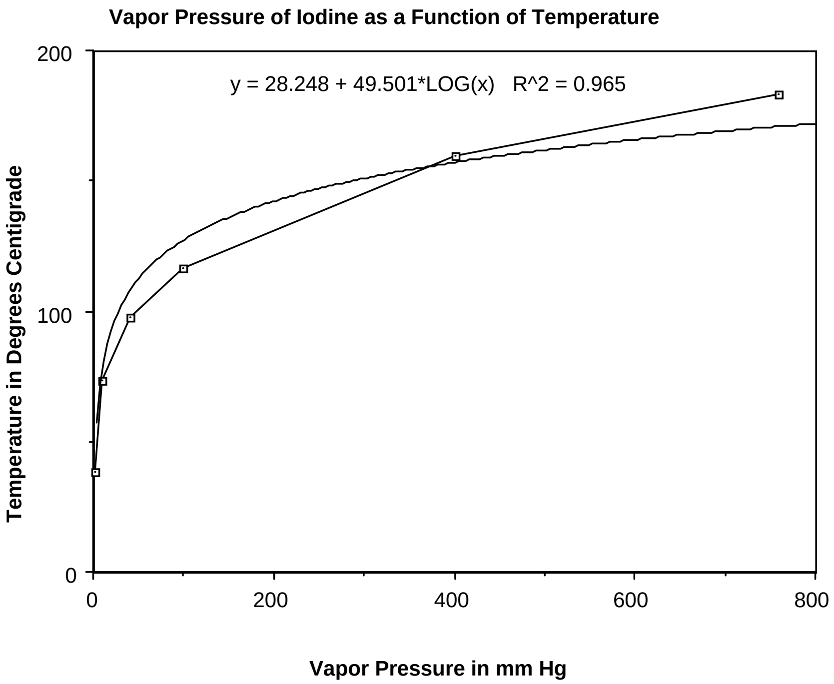

Figure D.1. Data on Vapor Pressure of Iodine as a Function of Temperature

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