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SEP 14 2011

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PPPO-02-1246584-11

Mr. Edward Winner, FFA Manager
Kentucky Department for Environmental Protection
Division of Waste Management
200 Fair Oaks Lane, 2nd Floor
Frankfort, Kentucky 40601

Dear Mr. Ballard and Mr. Winner:

APPENDIX C OF THE WASTE DISPOSAL ALTERNATIVES EVALUATION REMEDIAL INVESTIGATION/FEASIBILITY STUDY WORK PLAN AT THE PADUCAH GASEOUS DIFFUSION PLANT, PADUCAH, KENTUCKY (DOE/LX/07-0099&D2/R1)

Appendix C of the Waste Disposal Alternatives Evaluation Remedial Investigation/Feasibility Study Work Plan, DOE/LX/07-0099&D2/R1, has been revised to address comments received by Kentucky Department for Environmental Protection (KDEP) on July 6, 2011, and to address comments discussed with KDEP and the U.S. Environmental Protection Agency on September 1, 2011.

Once Appendix C is approved, a copy of the entire document will be submitted for your files and the Administrative Record. If you have any questions or require additional information, please contact Rob Seifert at (270) 441-6823.

Sincerely,

Reinhard Knerr
Paducah Site Lead
Portsmouth/Paducah Project Office

Enclosures:
1. Certification Page
2. Appendix C
3. Redlined Appendix C
4. Comment Response Summary

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CERTIFICATION

Document Identification: **Appendix C of the *Waste Disposal Alternatives Evaluation Remedial Investigation/Feasibility Study Work Plan at the Paducah Gaseous Diffusion Plant, Paducah, Kentucky,* DOE/LX/07-0099&D2/R1**

I certify under penalty of law that this document and all attachments were prepared under my direction or supervision in accordance with a system designed to ensure that qualified personnel properly gather and evaluate the information submitted. Based on my inquiry of the person or persons directly responsible for gathering the information, the information submitted is, to the best of my knowledge and belief, true, accurate, and complete. I am aware that there are significant penalties for submitting false information, including the possibility of fine and imprisonment for knowing violations.

LATA Environmental Services of Kentucky, LLC

Craig S. Jones, Manager of Projects — Date Signed: 09/14/11

I certify under penalty of law that this document and all attachments were prepared under my direction or supervision in accordance with a system designed to ensure that qualified personnel properly gather and evaluate the information submitted. Based on my inquiry of the person or persons directly responsible for gathering the information, the information submitted is to the best of my knowledge and belief, true, accurate, and complete. I am aware that there are significant penalties for submitting false information, including the possibility of fine and imprisonment for knowing violations.

U.S. Department of Energy (DOE)

Reinhard Knerr, Paducah Site Lead
Portsmouth/Paducah Project Office — Date Signed

APPENDIX C

PROPOSED GROUNDWATER MODELING METHODOLOGY

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ACRONYMS

AT123D	Analytical Transient 1-, 2-, 3-Dimensional
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
CCL	compacted clay liner
COC	contaminant of concern
COPC	chemical of potential concern
DAF	dilution attenuation factor
DOE	U.S. Department of Energy
DUSTMS	Disposal Unit Source Term-Multiple Species
ELCR	excess lifetime cancer risk
EPA	U.S. Environmental Protection Agency
FML	flexible membrane liner
HDPE	high density polyethylene
HELP	Hydrologic Evaluation of Landfill Performance
HI	hazard index
MCL	maximum contaminant level
PGDP	Paducah Gaseous Diffusion Plant
PWAC	preliminary waste acceptance criteria
RGA	Regional Gravel Aquifer
UCRS	Upper Continental Recharge System
WAC	waste acceptance criteria
WDF	waste disposal facility

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C.1. INTRODUCTION

If selected, the on-site waste disposal alternative involves the construction of a Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) waste disposal facility at the Paducah Gaseous Diffusion Plant (PGDP). This appendix presents the modeling methodology proposed for evaluating the performance of an on-site waste disposal facility, including development of preliminary waste acceptance criteria (PWAC).

C.2. PREVIOUS REPORTS AND MODELING

Several reports have been completed at PGDP for on-site waste disposal facilities. These reports include the following:

- *Operating Limit Study for the Proposed Solid Waste Landfill at Paducah Gaseous Diffusion Plant*, ORNL/TM-13008, June 1995 (ORNL 1995).

- *Remedial Investigation/Feasibility Study on Disposal Options for Comprehensive Environmental Response, Compensation, and Liability Act of 1980 (CERCLA)-Derived Waste at the Paducah Gaseous Diffusion Plant, Paducah, Kentucky*, DOE/OR/07-1935&D(-1), March (DOE 2001).

- *Risk and Performance Evaluation of the C-746-U Landfill at the Paducah Gaseous Diffusion Plant, Paducah, Kentucky*, DOE/OR/07-2041&D2R1, September (DOE 2003).

Each of these reports presents a modeling methodology similar to that proposed for evaluating the performance of an on-site waste disposal facility and serves as the basis for the development of the proposed modeling methodology presented in this appendix. This earlier work is supplemented by a review of the current technical literature related to the performance of engineered barriers. The service life of the engineered barriers established from the literature review is also proposed for use in the modeling.

The Remedial Investigation/Feasibility Study on Disposal Options for CERCLA-Derived Waste (DOE 2001) was developed under consensus of a core team; however, the report was not released for review to the regulators. The remaining reports were finalized and released to the public, but only the Risk and Performance Evaluation of the C-746-U Landfill report (DOE 2003) was approved by the regulators.

C.3. MODELING METHODOLOGY

The general modeling procedure for the development of PWAC is provided in Table C.1. This table presents the major modeling tasks and descriptions of the general task elements that are necessary within each modeling task to facilitate the determination of the PWAC.

Table C.1. General Modeling Procedure for the Development of the PWAC

MODELING TASK	GENERAL TASK ELEMENTS
Identify Waste and Indicator Chemicals Constituents	Identify constituents in waste.
	Establish chemical surrogate groups and assign contaminants to surrogate groups.
	Identify indicator chemicals for fate and transport modeling for each chemical surrogate group.
Fate and Transport Modeling	Conduct fate and transport modeling for radionuclides, metals, and indicator chemicals, and calculate dilution-attenuation factors (DAFs) for indicator chemicals.
	Calculate concentrations for chemicals within a surrogate group using the indicator chemical's DAF.
Risk Assessment	Calculate the cancer risk and hazard presented by each chemical, metal, and radionuclide using PGDP No Action screening values for the rural child resident.
PWAC Development	Derive PWAC using ratio of modeled and acceptable concentration in water and concentration in source.
Uncertainty Analysis	Perform qualitative and quantitative uncertainty analyses.

C.3.1 IDENTIFY WASTE CONSTITUENTS AND INDICATOR CHEMICALS

Chemicals to be evaluated in the model will be determined based on a combination of information from the PGDP Human Health volume of the Risk Methods Document (DOE 2011) and other available waste profile data and selected to represent the expected waste contaminants for disposal in the potential on-site disposal facility.

C.3.1.1 Identify Constituents in Waste

Appendix D presents the methods that will be used to develop an analytical profile for the wastes that are expected to be placed in the potential on-site waste disposal facility. The chemicals of potential concern (COPCs) for PGDP are provided in Table 2.1 of the Risk Methods Document (DOE 2011). Contaminants of concern (COCs) will be derived using Table 2.1, as well as other available waste profile data and will be assessed in the fate and transport modeling analyses.

C.3.1.2 Establish Surrogate Groups

In order to streamline the modeling process, each COC will be assigned to a contaminant group. The contaminant groups will represent chemicals of concern with similar chemical properties, such as

solubility, volatility, and mobility, so that each contaminant group will contain chemicals that behave similarly in the environment.

The use of indicator chemicals involves the necessity to develop a sufficient number of groups such that the groups represent the full range of potential contaminant property combinations; however, the C-746-U Landfill report (DOE 2003) states that "it was determined that transport of neither the inorganic chemicals nor the radionuclides was adequately estimated through the use of indicator chemicals." The analysis found that surrogate groups were only adequately representative for organic compounds.

Based on this conclusion, surrogates will be used to develop a PWAC for organics; however, radionuclides and metals will be assessed individually and not as surrogate groups. If the On-Site Alternative is selected, a final waste acceptance criteria (WAC) will be developed with a full analysis of potential COCs.

C.3.1.3 Identify Indicator Chemicals for Surrogate Groups

An indicator chemical will be selected to represent each organic surrogate group. The indicator chemical for each surrogate group will be a representative chemical that previously has been identified as a major COC at PGDP. Section C.3.2 provides additional discussion on the issues associated with chemical interactions affecting the fate and transport of specific chemical groups. As noted in Section C.3.1.2, metals and radionuclides will be assessed individually and not as surrogate groups.

C.3.2 FATE AND TRANSPORT MODELING

The fate and transport modeling will be performed as follows:

(1) Hydrologic Evaluation of Landfill Performance (HELP) model simulations will be used to perform three failure scenarios to estimate the water flux percolating through the waste and into the water table under each of the scenarios. As described in Section C.3.2.1.1, the failure scenarios are based on a range of estimated service lives for the engineered barriers. The model also accounts for eventual failure of the drainage layers. The various scenarios to be considered include (1) instantaneous failure, (2) gradual failure, and (3) no failure. Additional gradual failure scenarios will be analyzed as part of the uncertainty analysis described in Section C.3.5. Under the gradual and instantaneous failure scenarios, the lateral drainage layers beneath the waste will be assumed to degrade. To account for degradation, the manmade flexible membrane liner (FML) layers in both the bottom liner and cap no longer would act as barrier layers, and the two drainage layers below the waste no longer would function (i.e., they effectively become vertical percolation layers). The no failure scenario assumes that the system maintains integrity throughout the period of interest.

(2) Disposal Unit Source Term-Multiple Species (DUSTMS) modeling will be performed for each metal, radionuclide, and indicator chemical under the gradual failure scenario to predict the contaminant flux entering the aquifer over time. A unit concentration for each contaminant will be used as an initial input to DUSTMS. This unit concentration is converted to an initial contaminant mass within the landfill. The contaminant mass will be assumed to be contained in a homogenized soil. The entire landfill volume will be assumed to be filled with a single contaminant embedded in the soil waste. DUSTMS is used to calculate initial groundwater concentrations based on this initial mass/concentration. Once downgradient groundwater concentrations are obtained from the Analytical Transient, 1-, 2-, 3-Dimensional (AT123D) model and initial PWAC concentrations are calculated, DUSTMS is rerun using the initial PWAC concentrations to obtain new initial groundwater

concentrations. (DUSTMS modeling also will be performed for selected contaminants as part of an uncertainty analysis under the immediate and no failure scenarios.)

(3) MODFLOW/MODPATH modeling will be performed at Site 11 to predict the groundwater migration rate from the location where leachate enters the Regional Gravel Aquifer (RGA) groundwater flow system to the exposure point locations and the shortest transit times to each exposure point.

The sitewide groundwater model does not cover the area of interest at Site 3A. If the sitewide groundwater model cannot be expanded to include Site 3A, existing hydrogeologic data for Site 3A will be used to determine the appropriate hydrogeological parameters for Site 3A in the DUSTMS and AT123D models.

(4) AT123D modeling will be performed to predict concentrations of each indicator chemical, metal, and radionuclide at established exposure points over time due to lateral transport. The contaminant flux from the DUSTMS model will be used as input to the AT123D model.

Maximum concentrations and the time, up to 10,000 years, to attain the maximum concentrations at the exposure points will be predicted, and dilution attenuation factors (DAFs) associated with source-to-exposure point transport of the indicator chemical will be calculated.

Proposed modeling parameters are included in Attachment C.1.

C.3.2.1 Selected Models and Their Application

Several models will be required for the evaluation of the performance of an on-site waste disposal facility. The following discussion presents the models selected for use in the analysis of the groundwater transport pathway. The selection of the models was based on the modeling matrix presented in the Risk Methods Document (DOE 2001). Figure C.1 provides an illustration of the model application in the assessment. Figures C.2 and C.3 provide an illustration of how the HELP layers and DUSTMS material layers interrelate for Sites 11 and 3A, respectively.

C.3.2.1.1 HELP Model

The HELP model (Schroeder et al. 1994) will be used to determine the rate of water infiltration through the engineered cap that can be released from the bottom of the landfill. The HELP computer program is a quasi-two-dimensional hydrologic model of water movement across, into, through, and out of landfills. The model considers weather, soil, and design data and uses solution techniques that account for the effects of surface storage, snowmelt, runoff, infiltration, evapotranspiration, vegetative growth, soil moisture storage, lateral subsurface drainage, leachate recirculation, unsaturated vertical drainage, and leakage through soil, geomembrane, or composite liners. The program was developed to conduct water balance analysis of landfills, cover systems, and solid waste disposal and containment facilities. As such, the model facilitates rapid estimation of the amounts of runoff, evapotranspiration, drainage, leachate collection, and liner leakage that may be expected to result from the operation of a wide variety of landfill designs.

The HELP model will be used to determine the water balance of the facility based on preliminary facility/cap design. The modeling will account for the operational period, institutional control period, and the post-institutional control period, which are described below.

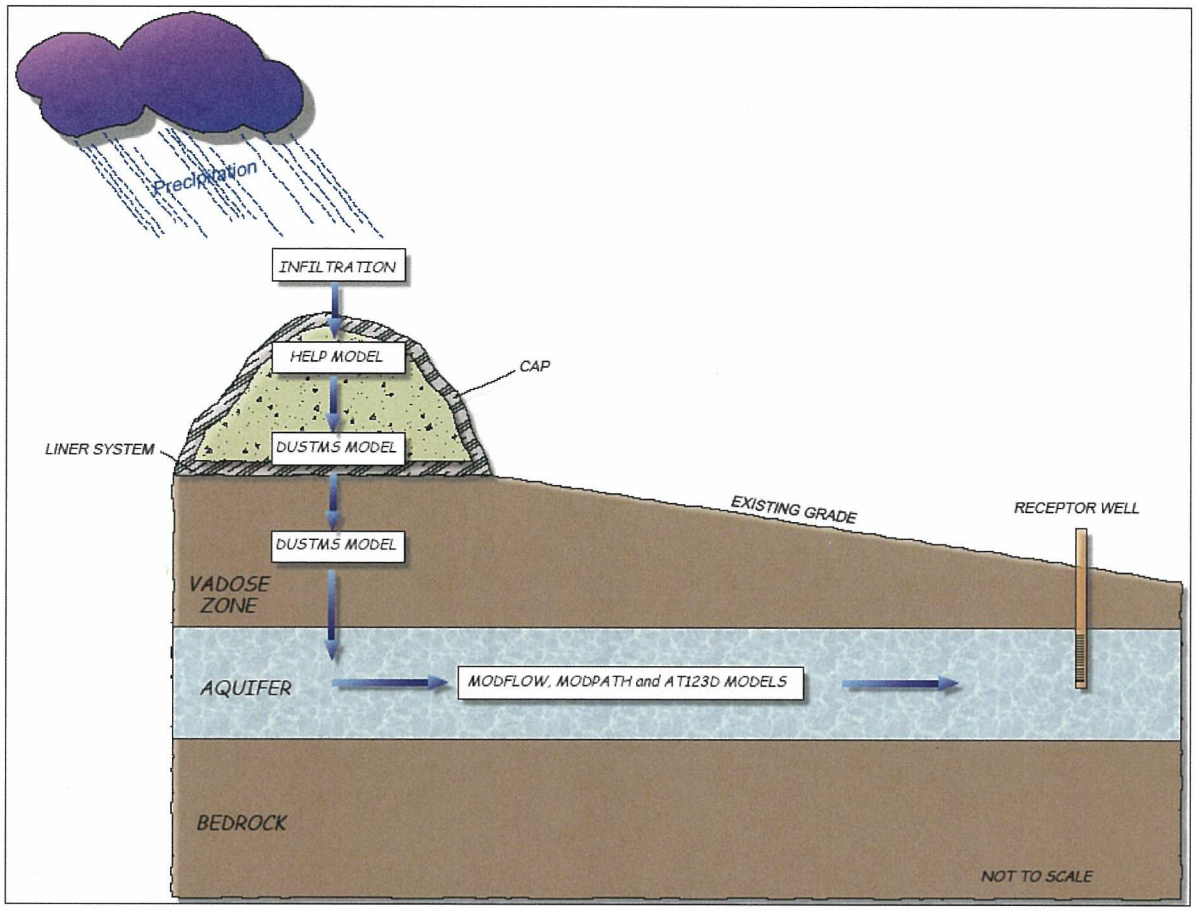

Figure C.1. Generalized Conceptual Model for an On-Site Waste Disposal Facility

Site 11 - Conceptual Model 30+ years

HELP, DUST-MS, AT123D

DUST-MS Material	HELP Soil Layers	DUST-MS Number of Computational Nodes	Thickness (ft)	DUST-MS Bulk Density	DUST-MS Initial (t = 30 yrs) Volumetric Moisture Content	HELP Initial (t = 30 yrs) Volumetric Moisture Content
1	Soil Matirx	10	5	1.34	0.3098	0.3098
2	Filter Sand	2	1	1.4	0.0452	0.0843
	Cobble/ Gravel Sand	6	3			0.0451
	Drainage Sand	2	1			0.032
3	FML (HDPE) Liner Clay	6	3	1.8	0.4251	0.4251
4	Waste Form	170	85	3.1	0.3588	0.3588
3	Clay (compacted)	2	1	1.8	0.4112	0.4112
2	Drainage Sand	2	1	1.4	0.1123	0.1123
FML (HDPE) Liner	Geocomposite		0.02			
3	Clay Barrier FML (HDPE) Liner	6	3	1.8	0.427	0.427
1	Geologic Buffer (clay)	20	10	1.34	0.342	0.342
5	Loess Deposit (Unsaturated UCRS) Bottom of HELP Model	44	22	1.43	0.393	0.393
6	Silt to Clay (Saturated Upper Continental Deposits) Bottom of DUST-MS Model	28	14	1.43	0.445	
AT123D Lateral Flow Layer	RGA		35.5	1.67	Saturated Horizontal Flow	
	McNairy Formation					

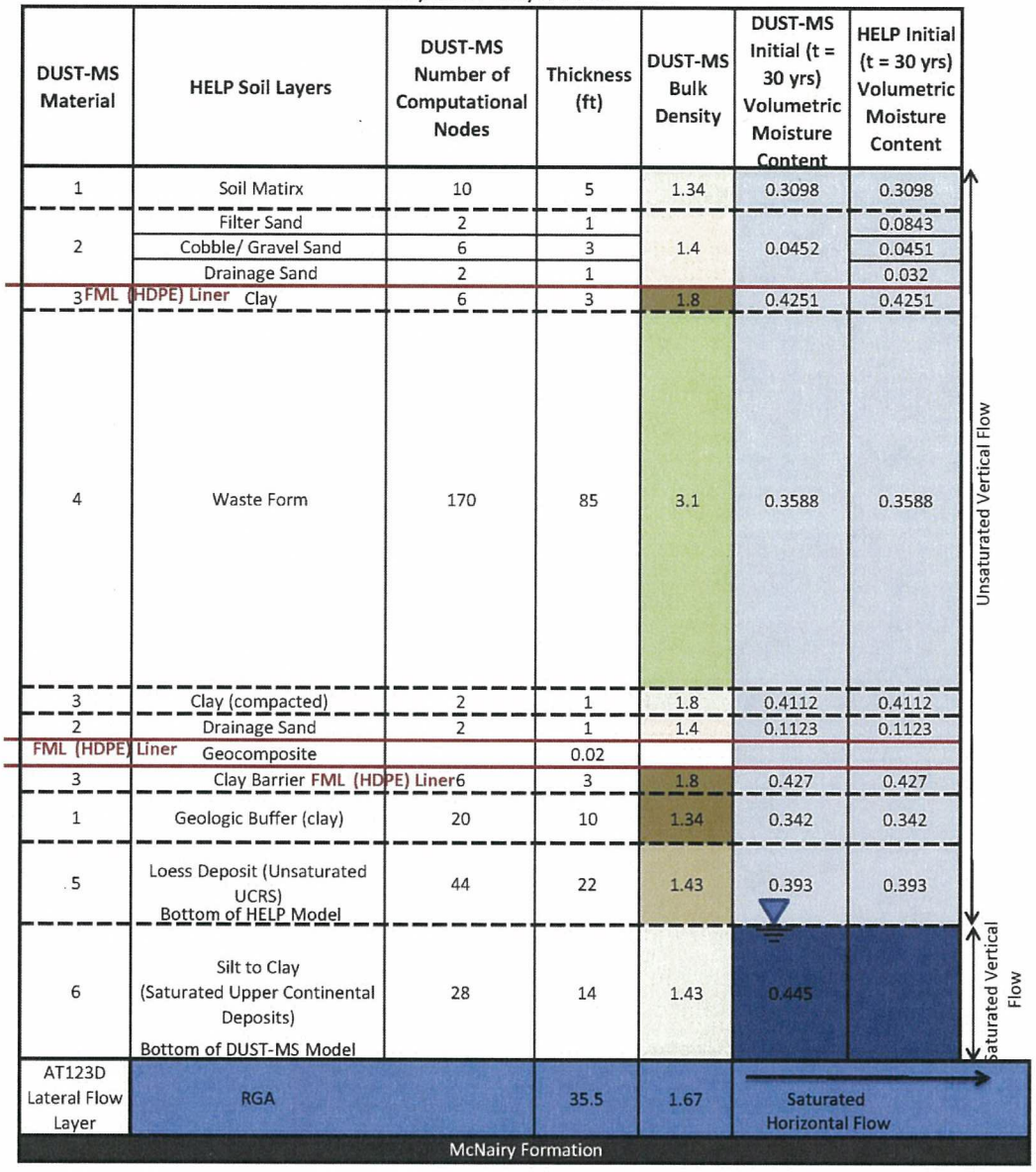

Figure C.2. DUSTMS Model Layers and Select Parameters, Site 11

Site 3A - Conceptual Model 30+ years

HELP, DUST-MS, AT123D

DUST-MS Material	HELP Soil Layers	DUST-MS Number of Computational Nodes	Thickness (ft)	DUST-MS Bulk Density	DUST-MS Initial (t = 30 yrs) Volumetric Moisture Content	HELP Initial (t = 30 yrs) Volumetric Moisture Content
1	Soil Matirx	10	5	1.34	0.3098	0.3098
2	Filter Sand	2	1	1.4	0.0452	0.0843
	Cobble/ Gravel Sand	6	3			0.0451
	Drainage Sand	2	1			0.032
3	FML (HDPE) Liner Clay	6	3	1.8	0.4251	0.4251
4	Waste Form	170	85	3.1	0.3588	0.3588
3	Clay (compacted)	2	1	1.5	0.4112	0.4112
2	Drainage Sand	2	1	1.4	0.1123	0.1123
	FML (HDPE) Liner Geocomposite		0.02			
3	FML (HDPE) Liner Clay Barrier	6	3	1.8	0.427	0.427
1	Geologic Buffer	20	10	1.34	0.342	0.393
5	Terrace Gravel (Lower Continental Deposit)	40	20	1.41	0.302	0.302
	Bottom of HELP and DUST-MS Model					
AT123D Lateral Flow Layer	Terrace Gravel (Lower Continental Deposit)		15	1.56	Saturated Horizontal Flow	
	Porter's Creek Clay		70			
	McNairy Formation					

Unsaturated Vertical Flow

Figure C.3. DUSTMS Model Layers and Select Parameters, Site 3A

During the operational period (0–30 years), landfill components that would be in place include the leachate collection system with a barrier liner beneath the waste. This is a multi component system where each component functions independently and has different failure times and rates. During this period, it is assumed that a cover system is not in place. During this period, contaminant mass removed via the leachate collection system is assumed to be collected and removed from the landfill; however, the mass removed by the leachate collection system will not be taken into account during calculation of the PWAC.

For the gradual failure scenarios, all components of the waste disposal facility would be in place (both cover and liner components, drainage layers, and low-permeability clay layers) and functioning until at least year 130. At year 130 (the end of the institutional control period), the leachate collection system is assumed to cease to function. However, very little, if any, infiltration, is expected as long as the high density polyethylene (HDPE) geomembrane in the cap is intact (Bonaparte et al. 2008). HDPE geomembrane degradation is assumed to begin at year 200. For this reason, there will be little if any impact if the leachate collection system is modeled to cease functioning at 130 years or 200 years. For simplicity in modeling, the lateral drainage layers are assumed to cease functioning at 200 years.

During the institutional control period (30–130 years and generally considered to commence after facility closure and to last for 100 years) and for 70 years beyond the postinstitutional control period, all components of the waste disposal facility would be in place (both cover and liner components, drainage layers, and low-permeability clay layers) and functioning. The basis for this time period is outlined subsequently. These conditions apply to the instantaneous, gradual, and no failure scenarios. The HELP model will be used to evaluate the flux through the facility based on initial properties of the cover and liner system.

For the no failure scenario, all components of the waste disposal cell are assumed to be in place from year 200 to 10,000.

For the instantaneous failure scenario, all components of the waste disposal cell are assumed to fail at year 200. The "end state" or complete failure of certain landfill components is assumed to mean that the leachate collection system no longer is functioning, the liners have degraded to the point that they are no longer functioning as barriers to water transmission (either in or out of the landfill), and the clay liners have increased in hydraulic conductivity by one order of magnitude; the clay liners (upper and lower), as well as the other cap system components (e.g., soil cover and biointrusion layer) are assumed to still be in place and functioning as intended.

For the gradual failure scenario, at 200 years the HDPE geomembrane components of the cap and liner system would commence to degrade (i.e., all antioxidants are depleted and the induction time for the start of degradation is completed). Degradation of the HDPE geomembrane is assumed to be completed at 600 years. Beyond 600 years, the compacted clay liners (CCLs) controls infiltration into the cap and out of the liner system. It is recognized that a longer service life and degradation period for HDPE geomembranes are supported by the technical literature (Rowe 2010). For the base case, a longer service life and degradation period are bound by the no failure scenario. Other service lives and degradation periods may be addressed as part of the uncertainty analyses described in Section C.3.5.

The rate of degradation between 200 and 600 years will be modeled, based on prior work conducted at the site, and the following equation will be used (Lee et al. 1995):

$$F(t) = \frac{f_2 \; x \; f_3}{f_2 + \left(f_3 - f_2\right) x \, e^{-a\left(t - t1\right)}}$$

where

F(t) = gradual failure function providing the groundwater recharge at any time t (cm/year)
f_2 = average groundwater recharge in the institutional control period (cm/year)
f_3 = final groundwater recharge for the post-institutional control period after cover and liner failure (cm/year)
t = time (years) at which F(t) is measure
t_1 = time (years) at the end of the institutional control period
α = decay constant (0.064 $year^{-1}$)

The decay constant, α, was set at 0.064 $year^{-1}$, which results in failure of the engineered barrier system at 600 years postclosure.

In the instantaneous and gradual failure cases, the CCL in both the base liner system and final cover system are assumed to undergo a one order of magnitude increase in hydraulic conductivity from 1×10^{-7} cm/s to 1×10^{-6} cm/s at 600 years. The degradation of the clay layer is modeled assuming a step change in hydraulic conductivity. Under this scenario, f_2 is established using an intact geomembrane over a CCL with a hydraulic conductivity of 1×10^{-7} cm/s (in both the final cover system and base liner system), and f_3 is established using only a CCL with a hydraulic conductivity of 1×10^{-6} cm/s.

The possible effects of the development of microchannels from "weathering" processes and the possible effects of chlorinated solvents upon clay liner hydraulic conductivity will be considered as an uncertainty, and the potential impacts on the PWAC will be discussed in the Remedial Investigation/Feasibility Study report.

C.3.2.1.2 DUSTMS Model

The DUSTMS model will be used to evaluate the release and migration of contaminants in the vadose zone (Sullivan 2006). The DUSTMS computer code is designed to model water flow, container degradation, release of contaminants from the waste to the contacting solution, and transport through the subsurface media. Water flow through the facility over time is modeled using tabular input. Container degradation models include three types of failure rates: instantaneous (all containers fail at once); uniformly distributed failures (containers fail at a linear rate between a specified starting and ending time); and gaussian failure rates (containers fail at a rate determined by a mean failure time, standard deviation, and gaussian distribution). As the waste is not expected to be containerized during waste placement, and because it is assumed for the purposes of modeling that the contaminants are readily available for transport and not packaged or treated to decrease leachability, containers will not be simulated. Also, according to Sullivan (2001), use of the waste containers provides an opportunity to overpredict chemical retardation if both waste-to-water and soil-to-water partitioning coefficients are assigned. Initial mass emplacement is simulated by specifying initial concentrations.

Wasteform release models include four release mechanisms: (1) rinse with partitioning [inventory is released instantly upon container failure subject to equilibrium partitioning (sorption) with the waste]; (2) diffusion release (release from either a cylindrical, spherical, or rectangular wasteform); (3) dissolution release (uniform release over time due to dissolution of the wasteform surface); and (4) the aforementioned wasteform release models with solubility limited release. The predicted wasteform releases are corrected for radioactive decay and ingrowth. Chemical transformations also can be evaluated as a rate constant, similar to radioactive decay.

A unique set of container failure and wasteform release parameters can be specified for each control volume with a container. Contaminant transport is modeled through a finite-difference solution of the advective transport equation with sources (wasteform release and ingrowth) and radioactive decay.

Although DUSTMS simulates one-dimensional transport, it can be used to simulate migration down to an aquifer and then transport in the aquifer by running the code twice; however, AT123D will be used to simulate contaminant fate and transport in the RGA and Terrace Gravel formations.

The DUSTMS model will be used to determine contaminant release rates from unit source concentrations (i.e., 1 mg/kg) in the disposal unit to the RGA water table, using water infiltration rates determined from the HELP model. DUSTMS is a one-dimensional model that allows for simplification of the disposal system while still accounting for the most important physical processes and parameters influencing contaminant releases.

Certain areas of the Upper Continental Recharge System (UCRS) have been found to be saturated above the RGA. The CERCLA waste disposal facility would be constructed above ground surface and, as such, contaminant releases initially will migrate through an unsaturated zone. DUSTMS, an unsaturated flow and transport model, will be used to model the flow and transport of contaminants from the waste disposal facility through this unsaturated zone and downward to the RGA. It is recognized, that while migrating vertically through the UCRS to the RGA, different moisture conditions, including saturated conditions, possibly will be encountered. Conservation of mass dictates that the DUSTMS predicted steady-state unsaturated mass flux (g/yr) would be the same throughout the vertical transport profile whether that profile is saturated or unsaturated or combinations of both. If portions of the UCRS are saturated, the specified moisture content will be adjusted accordingly. AT123D, will be used to simulate RGA contaminant migration, and uses the DUSTMS model-predicted mass flux as input.

C.3.2.1.3 MODFLOW and MODPATH

A sitewide flow model (DOE 1997) has been developed for PGDP using MODFLOW. MODFLOW (McDonald and Harbaugh 1988) and MODPATH (Pollack 1994) will be used to estimate hydraulic gradients, flow distances, and hydraulic conductivities along site-to-receptor flow paths. This information subsequently is used to develop input parameters for the AT123D saturated zone flow and transport model. MODFLOW is a three-dimensional, finite difference model capable of simulating both steady-state and transient head distribution for a saturated groundwater flow field. MODPATH is a three-dimensional, particle-tracking model capable of using the steady-state, head distribution generated by MODFLOW to track flow paths of particles released in the groundwater flow field modeled in MODFLOW. Figure C.4 presents an example of the flow path analysis using MODFLOW and MODPATH.

The MODFLOW model was used in the development of the sitewide groundwater flow model at PGDP (DOE 1997). This model covers most of the U.S. Department of Energy (DOE) Reservation except that portion above the Porters Creek Clay Terrace (southern geologic setting). The model was endorsed by both the PGDP Modeling Steering Committee and the Risk Assessment Working Group. The sitewide groundwater flow model has been updated in consultation with Kentucky and U.S. Environmental Protection Agency (EPA) using more recent groundwater monitoring data (DOE 2010). The revised sitewide groundwater model will be used in the development of an on-site waste disposal facility modeling effort. If the sitewide groundwater model cannot be expanded to include Site 3A, existing hydrogeologic data for Site 3A will be used to determine the appropriate hydrogeological parameters for Site 3A in the DUSTMS and AT123D models.

The MODPATH model will be used to track flowpaths of particles released from the disposal unit based on the steady-state flow from MODFLOW. The hydraulic gradient along the fastest flowpath to the exposure points of interest then will be estimated to ensure the transit time is conservatively estimated. The heads along the flowpath of interest will be determined, and the hydraulic gradient estimated as the head difference between the release point and exposure point of interest, divided by the distance from the

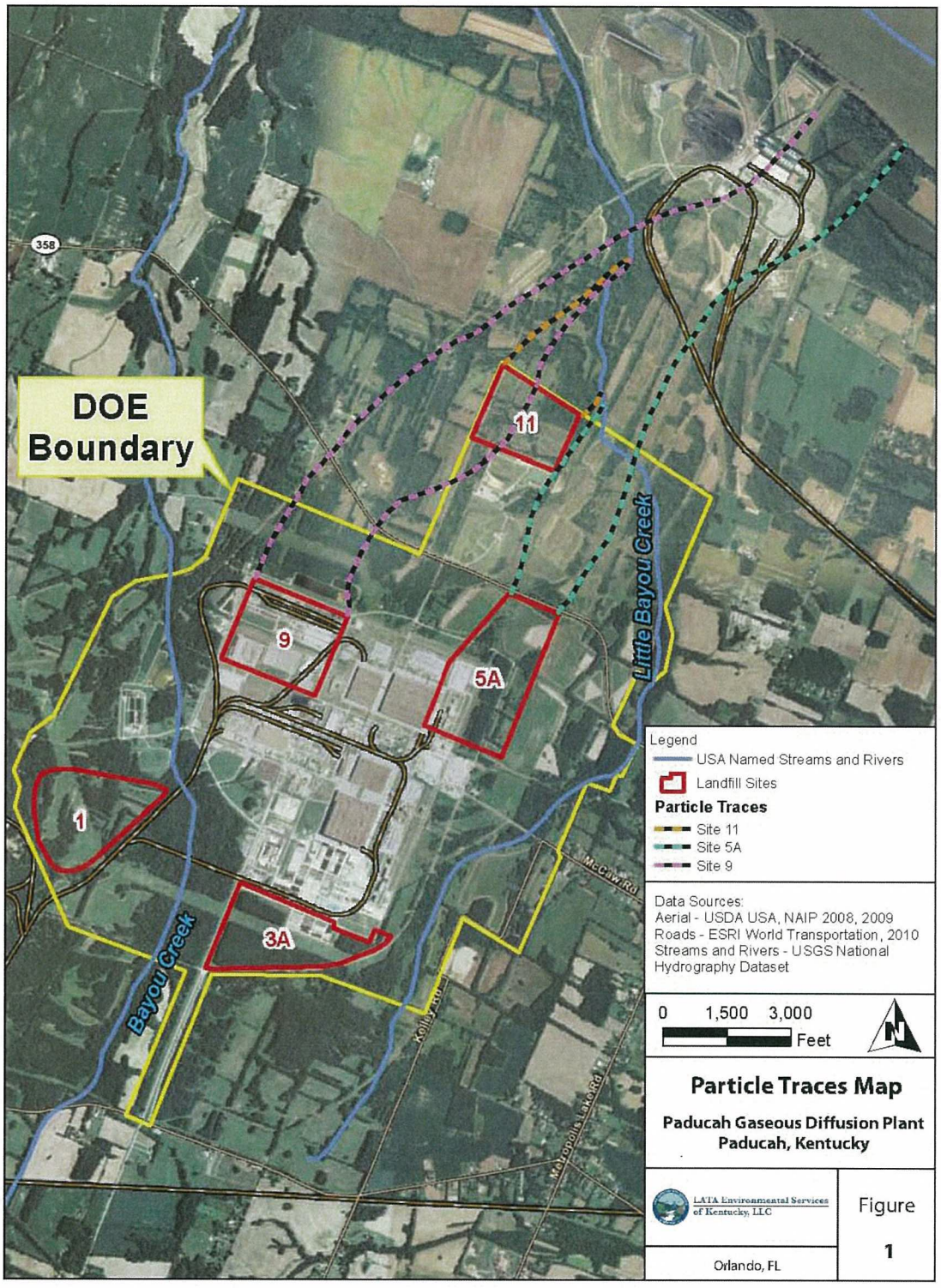

Figure C.4. Example Flow Paths from the Sitewide Groundwater Model

release point to the exposure point of interest. The hydraulic conductivity, along the fastest flowpath of interest, also will be estimated. The maximum hydraulic conductivity along the flowpath of interest will be selected for use in the AT123D model to ensure the transit time is not underestimated.

C.3.2.1.4 AT123D Model

The AT123D model will be used to model the lateral transport of contaminants in the groundwater to the exposure points (Yeh et al. 1987). AT123D is based on an analytical solution for transient one-, two-, or three-dimensional transport of a dissolved chemical or radionuclide in a homogeneous aquifer with uniform, stationary regional flow. The program assumes a stationary flow field parallel to the X-axis and allows for retardation (based on reversible instantaneous linear equilibrium sorption isotherm) and first-order decay. Longitudinal, horizontal, and vertical transverse dispersion can be input independently. The program calculates the concentration distribution in space and time in mg/L, parts per million, or pCi/L. AT123D models transport caused by a single source starting release of solute at time T = 0. It can accommodate various source configurations and boundary conditions. It also simulates a point source; a line source parallel to the X-, Y-, or Z-axis; an area (patch) source in the X-Y, X-Z, or Y-Z direction; and a volume source. The source release may be instantaneous, continuous, or finite step duration (up to 15 steps) and is assumed to be distributed equally over the source area.

Predicted contaminant concentrations for each organic indicator chemical in groundwater developed by AT123D will be used to develop the DAFs for use in estimating the remaining chemical groundwater concentrations within each surrogate group. As discussed previously, metals and radionuclides will be assessed individually and not as surrogate groups.

AT123D cannot model decay chains associated with radionuclide COPCs or chemical transformations from one species to another. Three methods are proposed for the assessment of these issues. The DUSTMS computer model could be used to evaluate the decay and transformation reaction uncertainty in the aquifer in a 1-D type analysis. Secondly, the groundwater concentration results from the AT123D model, for each contaminant run individually in AT123D, can be evaluated against decay chain and chemical transformation calculations conducted in DUSTMS to determine the uncertainty for these reactions. Third, an evaluation can be performed by comparing transit times to half-lives. If the half-lives are longer than the transit times to the points of exposure, then progeny formation during lateral migration in the aquifers likely is not a concern.

C.3.2.1.5 Dilution Attenuation Factors

To determine the transport times to and concentrations at the point of exposure for contaminants within each of the surrogate groups, the DAF for the indicator chemicals assigned to each surrogate group will be determined. The DAFs will then be applied to the other chemical's concentration within the surrogate group in the disposal unit to provide the resulting groundwater concentration at the receptor location of interest.

The determination of the DAF for an indicator chemical is represented graphically in Figure C.5. The DAF for the source-to-water table path is

$$DAF_{1,indicator} = \frac{\left(C_{s,indicator} / K_{d,indicator}\right)}{C_{L,indicator}}$$

where

DAF_1 = Dilution attenuation factor for the source-to-water table path (unitless)

C_s = Contaminant concentration in the disposal unit (mg/kg or pCi/g)
K_d = Contaminant distribution coefficient (L/kg)
C_L = Contaminant leachate concentration at the water table (mg/L or pCi/L)

The indicator chemical DAF for the water table-to-exposure point of interest is

$$DAF_{2,indicator} = \frac{C_{L,indicator}}{C_{w,indicator}}$$

where

DAF_2 = Dilution attenuation factor for the water table-to-exposure point path (unitless)
C_w = Contaminant concentration in groundwater at the exposure point of interest (mg/L or pCi/L)

Therefore, the DAF for the source-to-exposure point path for the indicator chemical is defined as

$$DAF = DAF_{1,indicator} \; x \; DAF_{2,indicator} = \frac{\left(C_{s,indicator} / K_{d,indicator}\right)}{C_{w,indicator}}$$

where

DAF = Dilution attenuation factor for the source-to-exposure point path (unitless)

The DAF then will be used to calculate the groundwater concentration for each chemical in the surrogate group by

$$C_{w,consituent} = \frac{\left(C_{s,consituent} / K_{d,consituent}\right)}{DAF_{indicator}}$$

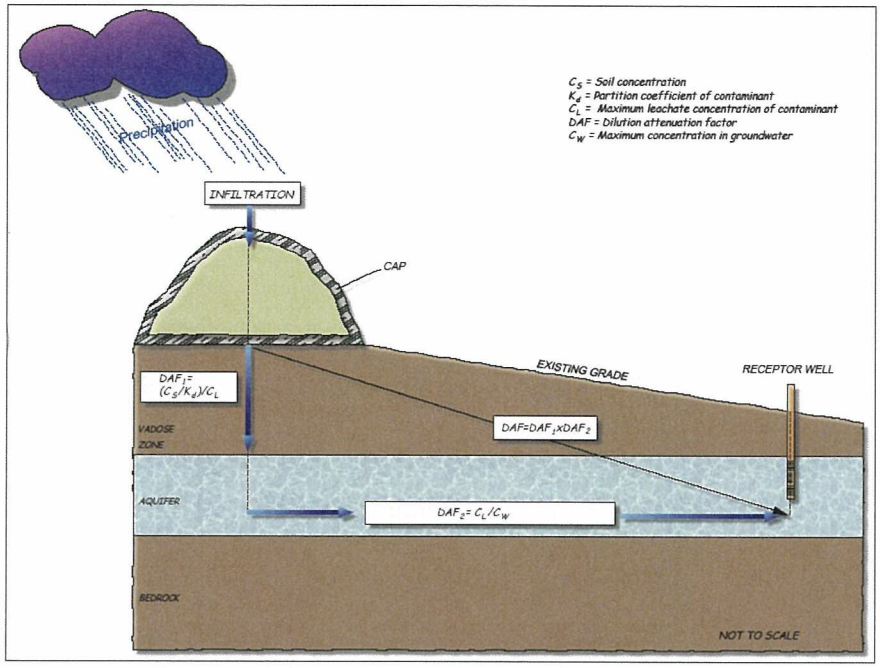

Figure C.5. Determination of the Dilution Attenuation Factor

C.3.3 RISK AND DOSE ASSESSMENT

The concentrations of COCs in groundwater at the exposure points will be used to calculate the cancer risk and non-cancer hazard [i.e., hazard index (HI)] for the chemicals, metals, and radionuclides resulting from exposure to the groundwater. The Risk Methods Document will be the basis of these calculations.

The analyses for exposure to constituents potentially released to groundwater will utilize the following risk and hazard target values at three points of exposure [i.e., at the edge of the waste unit, at the waste disposal facility (WDF) boundary, and at the DOE property line] and two time periods (i.e., 0 to 1,600 years and beyond 1,600 years). The edge of the waste unit is at the toe of containment berm that forms the WDF, which from a practical perspective is considered the edge of the waste mass. The WDF boundary is the site on which the WDF and associated infrastructure is located. For the purposes of the PWAC, this boundary is considered to 100 m from the edge of waste. Note, the final location will depend on site geometry and site layout and will be at least 100 m from the edge of waste (DOE Order 435.1). These points are depicted conceptually in Figure C.6.

(i) *At the edge of the waste unit (both time periods)*:

(1) The target concentrations will be the chemical-specific primary maximum contaminant levels (MCLs), if this value is greater than the constituent's background concentration. If the background concentration for the constituent is greater than the MCL, then the background concentration will be selected.

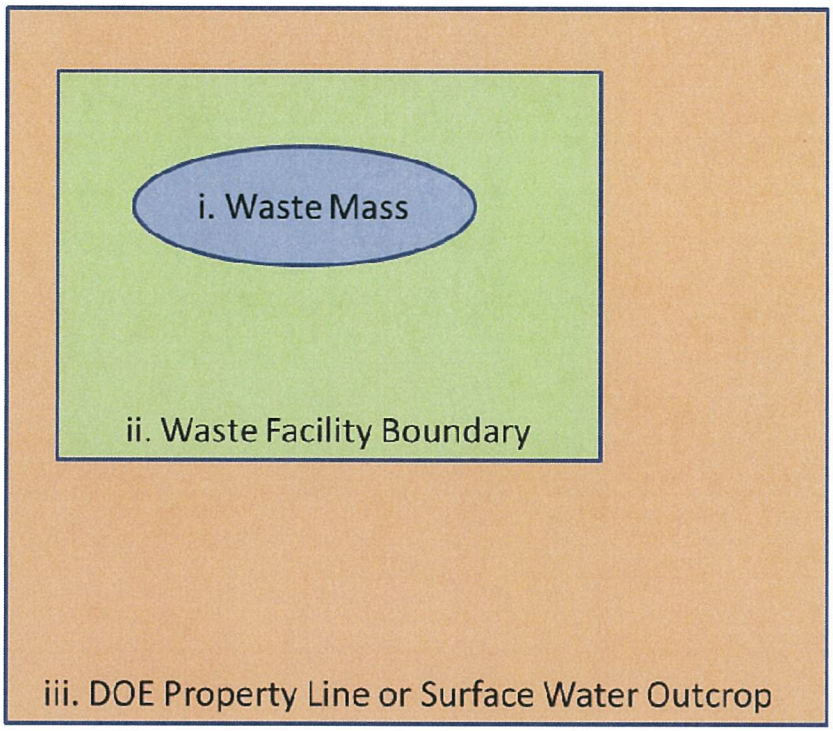

Figure C.6. Locations Where Target Values Need To Be Established

(2) If chemical-specific primary MCLs are not available, then chemical-specific risk- and hazard-based targets based on residential use of groundwater will be used to derive the constituent's target concentration in groundwater. The chemical-specific risk-based target will be 1E-06 and the chemical-specific hazard-based target will be 1. If both a risk-based concentration and hazard-based concentration can be derived for a constituent, then the lower of the two concentrations will be selected. If, however, the selected value is less than the background concentration, then the background concentration will be used.

(ii) *At the boundary of the WDF*:

(1) 0 to 1,600 years:

(a) The risk-based target will be a cumulative excess lifetime cancer risk (ELCR) of 1E-04.
(b) The hazard-based target will be a cumulative HI of 1.

(2) Beyond 1,600 years:

(a) The risk-based target will be a cumulative ELCR of 1E-04.
(b) The hazard-based target will be a cumulative HI of 3.

(Consistent with COPC selection in the Risk Methods Document, the calculation of cumulative ELCR and cumulative HI at the boundary of the WDF will exclude any constituents that use the constituent's background concentration as the chemical-specific target at the edge of the waste unit.)

(iii) *At the DOE property line or nearer surface water outcrop:*

(1) 0 to 1,600 years:

(a) The risk-based target will be a cumulative ELCR of 1E-06.
(b) The hazard-based target will be a cumulative HI of 1.

(2) Beyond 1,600 years:

(a) The risk-based target will be a cumulative ELCR of 1E-05.
(b) The hazard-based target will be a cumulative HI of 3.

(Consistent with COPC selection in the Risk Methods Document, the calculation of cumulative ELCR and cumulative HI at the DOE property line will exclude any constituents that use the constituent's background concentration as the chemical-specific target at the edge of the waste unit. Additionally, to target the more important risk and hazard contributors, only constituents with a chemical-specific contribution to cumulative ELCR and/or HI at the boundary of the WDF greater than 1E-07 or 0.05, respectively, will be included in the calculation of cumulative ELCR and HI at the DOE property line.)

The increased cumulative ELCR and/or HI targets of 1E-05 and 3, respectively, are used beyond 1,600 years at the boundary of the WDF and DOE property line to address the uncertainties in exposure (e.g., receptor location relative to ground water flow) and constituent release and migration.

The target concentrations at the edge of the waste unit are used to establish an initial PWAC. This PWAC is then used to calculate the contaminant concentrations in water at the boundary of the WDF. If these calculated contaminant concentrations exceed the risk-based and hazard-based targets established for the boundary of the WDF, then the initial PWAC is adjusted until these target risks are met. This iterative approach is then repeated for the property boundary.

The equations used to calculate the chemical-specific risk and non-cancer hazard estimates are as follows:

$$Chemical - Specific\ Risk\ Value = \frac{C_{w\,Chemical}\ x\ Target\ Risk\ Value}{C_{w\,No\ Action}}$$

where

Chemical-Specific Risk Value	= cancer risk and non-cancer hazard from groundwater exposure
$C_{w\ Chemical}$	= chemical concentration in groundwater (mg/L or pCi/L)
Target Risk Value	= target cancer risk, hazard level, or MCL to maintain
$C_{w\ No\ Action}$	= cancer risk/hazard no-action screening value or MCL as appropriate (mg/L or pCi/L)

C.3.4 PRELIMINARY WAC DEVELOPMENT

A PWAC will be developed for an on-site waste disposal facility. The PWAC is an estimate of the average contaminant concentrations allowed in the total waste volume. Individual loads could be higher or lower. Additionally, the PWAC is the total contaminant amount, such as maximum curies permitted in the cell or the single contaminant mass limit (in grams or kilograms) per COPC.

The PWAC will be useful in evaluating the viability of an on-site disposal facility only. If selected as the preferred alternative, the PWAC values for an on-site disposal facility would require modification after the design for the disposal facility is finalized. As used here, the PWAC for a contaminant is defined as

the maximum allowable concentration of a contaminant in disposed material that will not result in (1) releases to receiving media that exceed regulatory or risk-based criteria or (2) direct exposure risks or doses that exceed acceptable cancer risk-based and non-cancer hazard-based levels. This definition is consistent with, but goes beyond that presented in Attachment 2 of DOE Order 435.1 (*Radioactive Waste Management Manual*). In that attachment, PWAC are defined as technical and administrative requirements that a waste must meet in order for it to be accepted at a storage, treatment, or disposal facility. Generally, PWAC as defined here are dependent on five primary characteristics. These are the following:

- Facility design, including liner and cover, integrity, and institutional controls;
- Mobility of contaminants from or retention of contaminants within a waste (e.g., soil, stabilized soils, concrete, metals, etc.);
- Exposure point characteristics, including type of receptor (e.g., human or ecological), location, and exposure media;
- Target cancer risk, target hazard level, MCLs, and period of compliance; or
- Potential engineered barrier failure.

The method used to calculate the PWAC is presented in the following equations.

$$\frac{PWAC}{C_{s\ \ chemical}} = \frac{C_{w\ \ target}}{C_{w\ \ chemical}}$$

or

$$PWAC = \frac{C_{w\ \ target}\ x\ C_{s\ \ chemical}}{C_{w\ \ chemical}}$$

where

PWAC = preliminary WAC (mg/kg or pCi/g)
$C_{w\ target}$ = target concentrations for groundwater (i.e., back calculation value)
$C_{s\ chemical}$ = constituent concentration in source used in the modeling (mg/kg or pCi/g)
$C_{w\ chemical}$ = constituent concentration in groundwater from modeling results (mg/L or pCi/L)

The PWAC for the total mass or activity allowed in an on-site waste disposal facility will be calculated from the waste volume of the WDF and the PWAC concentration values as follows:

$$PWAC\ (kg\ or\ Ci) = PWAC\ (mg/kg\ or\ pCi/g) \times r_b \times V \times CF$$

where

ρ_b = bulk density (3.1 g/cm^3)
V = facility volume (4.1mcy or 3.13 x 10^{12} cm^3)
CF = conversion factors as necessary for unit conversion

The PWAC methodology, as presented in this work plan, is based on the assumption that the entire landfill would be filled with a single waste, assumed to be soil with a single contaminant. The contaminant is assumed to be immediately available for transport, thus maximizing release rates (i.e., many waste types will be solid materials for which associated contaminants would not be readily available for release). The cumulative risk from all contaminants will be evaluated during development of a final WAC, if the on-site disposal is chosen as the preferred remedial option. The PWAC will be calculated using the peak concentration between 0 and 1,600 years and 1,600 and 10,000 years. In the event the peak concentration in groundwater of a constituent has not been reached at 1,600 years, the model will be run until the peak concentration is reached, or until 10,000 years. The model will not be run beyond 10,000 years.

C.3.5 UNCERTAINTY ANALYSIS

The proposed modeling for an on-site waste disposal facility will consist of evaluating the COCs in a "forward" calculation based on unit inventory concentrations. The forward calculation provides the predicted groundwater contaminant concentrations released from the waste disposal facility into the aquifer at PGDP. These concentrations then are used in a "backward" calculation to determine the PWAC for the waste disposal facility. The term "backward" calculation is used in the sense that the analyst is using the forward calculation results to back calculate an acceptable waste concentration and total mass (or activity) of a given contaminant.

The use of this methodology does not provide a means to determine if the solubility limits for COCs may be reached in the disposal unit pore water; therefore, the PWAC values will be compared to solubility limit concentrations in terms of the disposal pore water concentrations. If the PWAC values result in concentrations exceeding the solubility limits, then the disposal mass of the COPC is no longer limited.

Another issue of potential importance to a disposal facility environment pertains to the facilitated transport of PCBs through cosolvent effects (EPA 1989). A modeling study was completed for the C-746-U Landfill at PGDP to evaluate the cosolvency impact at this landfill (BJC 2003). A similar analysis may need to be conducted for the waste disposal unit. The evaluation should be based on expected disposal concentrations of PCBs and potential solvents; therefore, the cosolvent issue will be evaluated if the On-Site Disposal Alternative is selected and the final WAC is to be developed.

An additional issue relates to facilitated transport possibly caused by the inclusion of nonhazardous solid waste/organic materials in the waste mix disposed of in the waste disposal facility. The phenomenon of such facilitated transport will be considered in the development of PWAC. Also, because some radionuclide contaminants (and decay products from ingrowth) will not reach their peak concentration prior to 10,000 years, an uncertainty analysis examining ingrowth and risk beyond 10,000 years will be completed for uranium-238 (U-238) (parent compound) and thorium-230 (Th-230) (progeny). This analysis will use a forward run of the transport model for the gradual failure scenario to the peak concentrations for U-238 and Th-230 and the selected initial PWAC for U-238 and Th-230 as the source term concentration. Due to modeling software constraints, the time step used in this analysis will be larger than that used for development of the PWAC. Another consideration in the development of the PWAC involves the potential impacts to inadvertent intruders. The preliminary disposal facility design provides 16 ft of cover over the waste. This cover thickness should prevent an inadvertent intruder from reaching the waste through excavation of a typical basement. Nonetheless, the inadvertent intruder scenario will be considered qualitatively in the development of the PWAC as an uncertainty.

The fate and transport modeling will have associated uncertainties due to abstraction of the physical and chemical processes of the real system into a model system. In addition, uncertainties in the waste inventories, model parameterization, and conceptual model uncertainties will need to be addressed.

Several iterations of the modeling will be necessary to evaluate and quantify the sensitivity and uncertainty in the results. In general, the sensitivity and uncertainty will be addressed by assessing parameter variations in the models. This may include such parameters as the following:

- Clay barrier degradation
- Geomembrane service life
- Geomembrane rate of degradation
- Sorption coefficients variations
- Solubility variations
- Hydraulic conductivity variations
- Off-centerline groundwater concentration evaluations
- Ingrowth of radionuclide progeny
- Degradation of organic COPCs
- Ingrowth of organic COPCs
- Potential for facilitated transport

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ATTACHMENT C1

PROPOSED MODELING PARAMETERS

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Table C1.1. Proposed Landfill/Soil Profile - Post-Closure Period (30 to 200 years)

			HELP Parameters/Characteristics											
Layer #	Material Type	Layer Type	Layer Thickness (inches)	Soil Texture Type	Total Porosity (vol/vol)	Field Capacity (vol/vol)	Wilting Point (vol/vol)	Saturated Hydraulic Conductivity (cm/sec)	Initial Moisture Content	Drainage Length (ft)	Drain Slope (%)	FML Pinhole Density	FML Installation Defects	FML Placement Quality
1	Native Soil (vegetative)	1	18	12	0.45 *	0.342	0.21	2.32E-06 *	0.2347 ***					
2	Native Soil	1	42	12	0.45 *	0.342	0.21	5.00E-07 *	0.3420 ***					
3	Filter sand	1	12	3	0.457	0.083	0.033	3.10E-03	0.0843 ***					
4	Geotextile	1	0.0625	20	0.85	0.01	0.005	1.00E+01	0.0501 ***					
5	Cobble/gravel/ sand	1	36	21	0.397	0.032	0.013	3.00E-01	0.0321 ***					
6	Drainage sand	2	12	1	0.417	0.045	0.018	1.00E-02	0.0452 ***	380	2			
7	Geotextile	2	0.125	20	0.85	0.01	0.005	1.00E+01	0.0100 ***	380	2			
8	FML (HDPE)	4	0.04	35				2.00E-13	0.0000 ***			0	0.5	2 (Excellent)
9	Clay barrier/ contour layer	3	36	16	0.427	0.418	0.367	1.00E-07 *	0.4270 ***					
10	Waste	1	1020	22	0.419	0.307	0.18	1.90E-05	0.3588					
11	Contour layer	1	12	26	0.445	0.393	0.277	1.90E-06	0.4112					
12	Geotextile	1	0.125	20	0.85	0.01	0.005	1.00E+01	0.1103					
13	Drainage sand	2	12	1	0.417	0.045	0.018	1.00E-02	0.1158	364	5			
14	Geotextile	2	0.125	20	0.85	0.01	0.005	1.00E+01	0.0766	364	5			
15	FML (HDPE)	4	0.06	35				2.00E-13	0.0000			0	0.5	2 (Excellent)
16	Bonded Geotextile	2	0.236	34	0.85	0.01	0.005	3.30E+01	0.0100	364	5			
17	FML (HDPE)	4	0.06	35				2.00E-13	0.0000			0	0.5	2 (Excellent)
18	Clay barrier **	3	36	16	0.427	0.418	0.367	1.00E-07 *	0.4270					
19	Geo-buffer layer	1	120	12	0.45 *	0.342	0.21	5.00E-07 *	0.3420					
20	Existing Silty Clay	1	264 (Site 11) 240 (Site 3A)	26	0.400 * (Site 3A) 0.445 (Site 11)	0.393	0.277	3.67E-06 * (Site 3A) 3.80E-07 * (Site 11)	0.3930					

Notes:

- FML = flexible membrane lining.
- FML Pinhole Density in units of number of holes per acre. Diameter of defect is equal to geomembrane thickness.
- FML installation defects are in units of defects per acre. A defect is estimated using an area of 1 cm^2.
- The cover system design curve number is 87.6 (slope 2%, slope length 380 ft, fair stand of grass (3), with soil texture type 12).
- Soil layering and properties are based upon the June 2010 PGDP Public Fact Sheet, Waste Disposal Options.
- HDPE = high density polyethylene.
- No recirculation of leachate is assumed.

* - Signifies value is not the default value associated with the specified HELP Soil Texture Type.

** - Signifies location where HELP Percolation/Leakage rate is used as DUST-MS water velocity.

*** - Initial soil moisture content was calculated by HELP (Schroeder et al. 1994). Remaining moisture contents were assigned using the final moisture content of the Operational Period HELP scenario.

- Moisture content values are in units of pore water volume per total volume soil and void space.
- "Native Soil", "Geo-buffer layer", and "Existing Silty Clay" soil porosities and hydraulic conductivities are from Site 3A Seismic Investigation Report, Assessment of the Adequacy of Data Report, and GB-02D lithologic log.

Table C1.2. Proposed Landfill Design Profile and Soil Characteristics - Long Term Monitoring Period (600+ years)

Layer #	Material Type	HELP Layer Type	Layer Thickness (inches)	HELP Soil Texture Type	Total Porosity (vol/vol)	Field Capacity (vol/vol)	Wilting Point (vol/vol)	Saturated Hydraulic Conductivity (cm/sec)	Initial Moisture Content (vol. water/total vol.)
1	Native Soil (vegetative)	1	18	12	0.45 *	0.342	0.21	2.32E-06 *	0.3071
2	Native Soil	1	42	12	0.45 *	0.342	0.21	5.00E-07 *	0.3491
3	Filter sand	1	12	3	0.457	0.083	0.033	3.10E-03	0.1118
4	Cobble/gravel/sand	1	36	21	0.397	0.032	0.013	3.00E-01	0.0364
5	Drainage sand	1	12	1	0.417	0.045	0.018	1.00E-02	0.0547
6	Clay barrier	1	36	16	0.427	0.418	0.367	1.00E-06*	0.4270
7	Waste	1	1020	22	0.419	0.307	0.18	1.90E-05	0.3070
8	Silty clay	1	12	26	0.445	0.393	0.277	1.90E-06	0.3930
9	Drainage sand	1	12	1	0.417	0.045	0.018	1.00E-02	0.0450
10	Clay barrier	1	36	16	0.427	0.418	0.367	1.00E-06 *	0.4270
11	Geo-buffer layer **	1	120	12	0.45 *	0.342	0.21	5.00E-07 *	0.3420
12	Existing Silty Clay	1	264 (Site 11) 240 (Site 3A)	26	0.400 * (Site 3A) 0.445 (Site 11)	0.393	0.277	3.67E-06* (Site 3A) 3.80E-07* (Site 11)	0.3930

Notes:

* - Signifies value is not the default value associated with the specified HELP Soil Texture Type.

** - Signifies location where HELP Percolation/Leakage rate is used as DUST-MS water velocity.

- Moisture content values are in units of pore water volume per total volume soil and void space.

- The cover system design curve number is 87.6 (slope 2%, slope length 380 ft, fair stand of grass (3), with soil texture type 12).

- "Native Soil", "Geo-buffer layer", and "Existing Silty Clay" soil porosities and hydraulic conductivities are from Site 3A Seismic Investigation Report, Assessment of the Adequacy of Data Report, and GB-02D lithologic log.

Table C1.3. Chemical Specific Parameters

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Vinyl Chloride (VC) - Atomic Weight 62.5 g/mol								
Half Life (years)	7.90E+00	Howard et al., 1991, Page 138	--[1]	--	7.90E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	62.5	--	62.5	--	62.5	EPA (1996)	--	--
Solubility Limit (gm/cc)	2.76E-03	EPA (1996), Table 36, Pages 134 to 136	2.76E-03	EPA (1996), Table 36, Pages 134 to 136.	2.76E-03	EPA (1996), Table 36, Pages 134 to 136	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd[4] (cc/gm)	1.49E-02	Koc[5] referenced from EPA (1996), Table 39, Pages 143 to 145. foc[6] referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (1.86E+01 l/kg) by foc (8.01E-4 unitless).	1.49E-02	Sheppard and Thibault (1990) (Not Verified)	1.49E-02	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	6.51E-03	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (1.86E+01 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	1.23E-06	EPA (1996), Table 37, Pages 137 to 139	1.23E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.23E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
Trichloroethylene (TCE) - Atomic Weight 131.4 g/mol								
Half Life (years)	4.50E+00	Howard et al., 1991, Page 190	2.50E+01	--	4.50E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	131.4	--	131.4	--	131	EPA (1996)	--	--
Solubility Limit (gm/cc)	1.10E-03	EPA (1996), Table 36, Pages 134 to 136	1.10E-03	EPA (1996), Table 36, Pages 134 to 136	1.10E-03	EPA (1996), Table 36, Pages 134 to 136	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	7.55E-02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (9.43E+01 l/kg) by foc (8.01E-4 unitless).	7.52E-02	Sheppard and Thibault (1990) (Not Verified)	7.52E-02	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	3.30E-02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (9.43E+01 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	9.10E-06	EPA (1996), Table 37, Pages 137 to 139	9.10E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	9.10E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
2-Butanone (Methyl Ethyl Ketone) - Atomic Weight 72.1 g/mol								
Half Life (years)	3.80E-02	Howard et al., 1991, Page 186	--	--	1.97E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	72.1	--	72.1	--	72.1	EPA (1996)	--	--
Solubility Limit (gm/cc)	7.40E-02	EPA (1996), Table 36, Pages 134 to 136	2.75E-01	EPA (1996), number not found in table	2.75E-01	EPA (1996), number not found in table	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	5.54E-03	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (6.92E+00 l/kg) by foc (8.01E-4 unitless).	9.20E-04	Sheppard and Thibault (1990) (Not Verified)	9.20E-04	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	2.42E-03	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (6.92E+00 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	9.30E-06	EPA (1996), Table 37, Pages 137 to 139	1.02E-05	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.02E-05	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
Chlorobenzene - Atomic Weight 112.6 g/mol								
Half Life (years)	1.64E+00	Howard et al., 1991, Page 412	--	--	1.64E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	112.6		112.6		112.6	EPA (1996)	--	--
Solubility Limit (gm/cc)	4.72E-04	EPA (1996), Table 36, Pages 134 to 136	4.72E-04	EPA (1996), Table 36, Pages 134 to 136	4.72E-04	EPA (1996), Table 36, Pages 134 to 136	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	1.79E-01	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (2.24E+02 l/kg) by foc (8.01E-4 unitless).	1.79E-01	Sheppard and Thibault (1990) (Not Verified)	1.79E-01	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	7.84E-02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (2.24E+02 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	8.70E-06	EPA (1996), Table 37, Pages 137 to 139	8.70E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	8.70E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Benzene - Atomic Weight 78.1 g/mol								
Half Life (years)	2.00E+00	Howard et al., 1991, Page 111	--	--	1.97E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	78.1	--	78.1	--	78.1	EPA (1996)	--	--
Solubility Limit (gm/cc)	1.75E-03	EPA (1996), Table 36, Pages 134 to 136	1.75E-03	EPA (1996), Table 36, Pages 134 to 136	1.75E-03	EPA (1996), Table 36, Pages 134 to 136	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	4.94E-02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (6.17E+01 l/kg) by foc (8.01E-4 unitless).	4.96E-02	Sheppard and Thibault (1990) (Not Verified)	4.96E-02	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	2.16E-02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (6.17E+01 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	9.80E-06	EPA (1996), Table 37, Pages 137 to 139	9.80E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	9.80E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
2-Methylphenol (o-Cresol) - Atomic Weight 108 g/mol								
Half Life (years)	7.70E-02	Howard et al., 1991, Page 294	--	--	1.97E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	108	--	108	--	108	EPA (1996)	--	--
Solubility Limit (gm/cc)	2.60E-02	EPA (1996), Table 36, Pages 134 to 136	2.00E-02	EPA (1996), Table 36, Pages 134 to 136	2.00E-02	EPA (1996), Table 36, Pages 134 to 136	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	7.31E-02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (9.12E+01 l/kg) by foc (8.01E-4 unitless).	1.60E-02	Sheppard and Thibault (1990) (Not Verified)	1.60E-02	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	3.19E-02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (9.12E+01 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	8.30E-06	EPA (1996), Table 37, Pages 137 to 139	8.30E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	8.30E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Pentachlorophenol - Atomic Weight 266.3 g/mol								
Half Life (years)	4.20E+00	Howard et al., 1991, Page 242	--	--	4.20E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	266.3		266.3		266.3	EPA (1996)	--	--
Solubility Limit (gm/cc)	1.95E-03	EPA (1996), Table 36, Pages 134 to 136	1.95E-03	EPA (1996), Table 36, Pages 134 to 136	1.95E-03	EPA (1996), Table 36, Pages 134 to 136	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	4.74E-01	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (5.92E+02 l/kg) by foc (8.01E-4 unitless).	4.74E-01	Sheppard and Thibault (1990) (Not Verified)	4.74E-01	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	2.07E-01	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (5.92E+02 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	6.10E-06	EPA (1996), Table 37, Pages 137 to 139	6.10E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	6.10E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
Benzo(a)pyrene - Atomic Weight 252.3 g/mol								
Half Life (years)	5.80E+00	Howard et al., 1991, Page 12	--	--	5.80E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	252.3		252.3		252.3	EPA (1996)	--	--
Solubility Limit (gm/cc)	1.62E-09	EPA (1996), Table 36, Pages 134 to 136	1.62E-03	EPA (1996), appears that the units are not correct	1.62E-03	EPA (1996), appears that the units are not correct	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	7.76E+02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (9.69E+05 l/kg) by foc (8.01E-4 unitless).	7.75E+02	Sheppard and Thibault (1990) (Not Verified)	7.75E+02	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	3.39E+02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (9.69E+05 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	9.00E-06	EPA (1996), Table 37, Pages 137 to 139	9.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	9.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
PCB (Aroclor 1254) - Atomic Weight 375.7 g/mol								
Half Life (years)	1.00E+02	U-Landfill Report, (DOE 2003)	--	--	1.00E+02	Howard et al., 1991	--	--
Atomic Weight (g/mol)	375.7		375.7		375.7	EPA (1996)	--	--
Solubility Limit (gm/cc)	7.00E-07	EPA (2004), Page A-295	8.00E-08	EPA (1996)	8.00E-08	EPA (1996)	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	2.48E+02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (3.09E+05 l/kg) by foc (8.01E-4 unitless).	2.47E+02	Sheppard and Thibault (1990) (Not Verified)	2.47E+02	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	1.08E+02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (3.09E+05 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	U-Landfill Report (DOE 2003)	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
gamma-Chlordane (Chlordane) - Atomic Weight 409.8 g/mol								
Half Life (years)	7.60E+00	Howard et al., 1991, Page 48	--	--	7.60E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	409.8		409.8		409.8	EPA (1996)		
Solubility Limit (gm/cc)	5.60E-08	EPA (1996), Table 36, Pages 134 to 136	5.60E-08	EPA (1996), Table 36, Pages 134 to 136	5.60E-08	EPA (1996), Table 36, Pages 134 to 136	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	4.11E+01	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (5.13E+04 l/kg) by foc (8.01E-4 unitless).	4.71E+01	Sheppard and Thibault (1990) (Not Verified)	4.71E+01	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	1.80E+01	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (5.13E+04 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	4.37E-06	EPA (1996), Table 37, Pages 137 to 139	4.37E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	4.37E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Antimony - Atomic Weight 121.7 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	121.7		121.7		--	--	--	--
Solubility Limit (gm/cc)	1.70E-01	EPA (2004), Page A-25.	1.00E+01	EPA (1996)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	45 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	45 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	--	--
	250 (clay)		250 (clay)		--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--
Arsenic - Atomic Weight 74.9 g/mol								
Half Life (years)	--	--	--	--	1.00E+05	Disposal Unit Source Term (DUST) default library	--	--
Atomic Weight (g/mol)	74.9		74.9		75	EPA (1996)	--	--
Solubility Limit (gm/cc)	1.20E-01	EPA (2004), Page A-29.	1.00E+01	EPA (1996)	1.00E+01	EPA (1996)	--	--
Kd (cc/gm)	2.90E+01	EPA (1996), Table 46, Page 158.	200 (sand)	Sheppard and Thibault (1990) (Not Verified)	200 (sand)	Sheppard and Thibault (1990) (Not Verified)	--	--
			200 (clay)		200 (clay)		--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	U-Landfill Report (DOE 2003)	1.00E-06	No reference given, from DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
Barium - Atomic Weight 137.3 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	137.3		137.3		--	--	--	--
Solubility Limit (gm/cc)	2.80E-03	EPA (2004), Page A-33.	1.00E+01	EPA (1996)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	4.10E+01	EPA (1996), Table 46, Page 158.	5 (sand)	Sheppard and Thibault (1990) (Not Verified)	--	--	--	--
			50 (clay)		--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Beryllium - Atomic Weight 9.01 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	9.01		9.01		--	--	--	--
Solubility Limit (gm/cc)	8.40E-02	EPA (2004), Page A-49.	1.00E+01	EPA (1996) (Not Verified)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	250 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	250 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	--	--
	1,300 (clay)		1,300 (clay)		--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--
Cadmium - Atomic Weight 112.4 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	112.4		112.4		--	--	--	--
Solubility Limit (gm/cc)	1.70E-03	EPA (2004), Page A-59.	1.00E+01	EPA (1996) (Not Verified)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	80 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	80 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	--	--
	560 (clay)		560 (clay)		--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--
Chromium - Atomic Weight 51.9 g/mol								
Half Life (years)	--	--	--	--	1.00E+05	Disposal Unit Source Term (DUST) default library	--	--
Atomic Weight (g/mol)	51.9		51.9		52	EPA (1996)	--	--
Solubility Limit (gm/cc)	6.00E-01	EPA (2004), Page A-83.	1.00E+01	EPA (1996) (Not Verified)	1.00E+01	EPA (1996) (Not Verified)	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal	3.21E+01	DOE (2002a), Min: 17.4 Max: 56.8 Mean: 32.1	19 (sand)	Sheppard and Thibault (1990), different than what was seen in the table (70 sand, 1500 clay).	19 (sand)	Sheppard and Thibault (1990), different than what was seen in the table.	--	--
			30 (clay)		30 (clay)		--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Copper - Atomic Weight 63.6 g/mol								
Half Life (years)	--	--	--	--	1.00E+05	Disposal Unit Source Term (DUST) default library	--	--
Atomic Weight (g/mol)	63.6		63.6		63.5	EPA (1996)	--	--
Solubility Limit (gm/cc)	5.70E-04	EPA (2004), Page A-97.	1.00E+01	EPA (1996) (Not Verified)	1.00E+01	EPA (1996) (Not Verified)	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	3.1	Dragun (1988), (Range 1.4 to 333 ml/g)	35 (sand) 35 (clay)	Sheppard and Thibault (1990), not found in document	35 (sand) 35 (clay)	Sheppard and Thibault (1990), not found in document	-- --	-- --
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
Lead - Atomic Weight 207.2 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	207.2	--	207.2	--	--	--	--	--
Solubility Limit (gm/cc)	8.70E-04	EPA (2004), Page A-223.	1.00E+01	EPA (1996)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	270 (sand and all other materials) 550 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	270 (sand) 550 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	-- --	-- --	-- --	-- --
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--
Manganese - Atomic Weight 54.9 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	54.9		54.9		--	--	--	--
Solubility Limit (gm/cc)	1.10E-03	EPA (2004), Page A-231.	1.00E+01	EPA (1996)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	50 (sand and all other materials) 180 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	50 (sand) 180 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	-- --	-- --	-- --	-- --
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Mercury - Atomic Weight 200.6 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	200.6		200.6		--	--	--	--
Solubility Limit (gm/cc)	4.50E-04	EPA (2004), Page A-235.	1.00E+01	EPA (1996) (Not Verified)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	5.20E+01	EPA (1996), Table 46, Page 158.	10 (sand) 100 (clay)	Sheppard and Thibault (1990), not found in document	--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--
Nickel - Atomic Weight 58.7 g/mol								
Half Life (years)	--	--	--	--	1.00E+05	Disposal Unit Source Term (DUST) default library	--	--
Atomic Weight (g/mol)	58.7		58.7		58.7	EPA (1996)	--	--
Solubility Limit (gm/cc)	1.50E-03	EPA (2004), Page A-255.	1.00E+01	EPA (1996)	1.00E+01	EPA (1996)	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	1.079E+02	DOE (2002a), Min: 20.3 Max: 163 Mean: 107.9	400 (sand) 650 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	400 (sand) 650 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	-- --	-- --
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
Selenium - Atomic Weight 78.9 g/mol								
Half Life (years)	--	--	--	--	1.00E+05	Disposal Unit Source Term (DUST) default library	--	--
Atomic Weight (g/mol)	78.9		78.9		78.9	EPA (1996)	--	--
Solubility Limit (gm/cc)	2.60E+00	EPA (2004), Page A-309.	1.00E+01	EPA (1996) (Not Verified)	1.00E+01	EPA (1996) (Not Verified)	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	150 (sand and all other materials) 740 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	150 (sand) 740 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	150 (sand) 740 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	-- --	-- --
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Silver - Atomic Weight 107.9 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	107.9		107.9		--	--	--	--
Solubility Limit (gm/cc)	2.50E-04	EPA (2004), Page A-311.	1.00E+01	EPA (1996) (Not Verified)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	90 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	90 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	--	--
	180 (clay)		180 (clay)		--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--
Thallium - Atomic Weight 204.4 g/mol								
Half Life (years)	--	--	--	--	1.00E+05	Disposal Unit Source Term (DUST) default library	--	--
Atomic Weight (g/mol)	204.4		204.4		204.4	EPA (1996)	--	--
Solubility Limit (gm/cc)	8.60E-03	EPA (2004), Page A-337.	1.00E+01	EPA (1996) (Not Verified)	1.00E+01	EPA (1996) (Not Verified)	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	7.10E+01	EPA (1996), Table 46, Page 158.	71 (sand)	Sheppard and Thibault (1990), not found in table	71 (sand)	Sheppard and Thibault (1990), not found in table	--	--
			1500 (clay)		1500 (clay)		--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
Vanadium - Atomic Weight 50.9 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	50.9		50.9		--	--	--	--
Solubility Limit (gm/cc)	7.00E-04	EPA (2004), Page A-391.	1.00E+01	EPA (1996) (Not Verified)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	1.00E+03	EPA (1996), Table 46, Page 158.	100 (sand)	Sheppard and Thibault (1990), not found in table	--	--	--	--
			1000 (clay)		--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Zinc - Atomic Weight 65.4 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	65.4		65.4		--	--	--	--
Solubility Limit (gm/cc)	1.40E-03	EPA (2004), Page A-405.	1.00E+01	EPA (1996)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	200 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	200 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	--	--
	2,400 (clay)		2,400 (clay)		--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--
Cs-137 - Atomic Weight 137 g/mol								
Half Life (years)	3.02E+01	Disposal Unit Source Term (DUST) default library	3.02E+01	--	--	--	None Specified	--
Atomic Weight (g/mol)	137		137		--	--	None Specified	
Solubility Limit (gm/cc)	3.40E-01	EPA (2004), Page A-71.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	280 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	280 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	280 (sand) 280 (waste) 1900 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	1,900 (clay)		1,900 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Tc-99 - Atomic Weight 99 g/mol								
Half Life (years)	2.13E+05	Disposal Unit Source Term (DUST) default library	2.13E+05	--	2.13E+05	Disposal Unit Source Term (DUST) default library	None Specified	--
Atomic Weight (g/mol)	99	--	99	--	99	EPA (1996)	None Specified	--
Solubility limit (gm/cc)	7.18E-03	Derived from geochemical database prepared by Lawrence Livermore National Laboratory and converted to PHREEQC format.	1.00E+01	EPA (1996) (Not Verified)	1.00E+01	EPA (1996) (Not Verified)	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	2.82E-01	DOE (2002a), Min: 5.27E-10 Max: 0.848 Mean: 0.282	0.2 (sand) 20 (clay)	Sheppard and Thibault (1990), not found table (sand - 0.1, clay - 1)	0.2 (sand) 1.0 (waste) 20 (clay)	Sheppard and Thibault (1990), not found table DOE 1997 and DOE (2002b)	0.2 (sand) 1.0 (waste) 20 (clay)	The distribution coefficients for Tc-99 are available in Table C.3.1. Chemical and physical properties of different classes of chemicals identified as COPCs for the C-746-U Landfill of DOE 2003b, page C3-301. Table 4.5 DUST model input parameters, page 4-12, has Kds for Tc-99. Table 4.5 references Sheppard and Thibault (1990).
Diffusion coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	None Specified	--
Ac-227 - Atomic Weight 227 g/mol								
Half Life (years)	22	ANL (2005)	21.8	--	--	--	None Specified	--
Atomic Weight (g/mol)	227		227		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E+01	No value found. Assume 10 gm/cc to prevent solubility from limiting migration.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	450 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	450 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	450 (sand) 450 (waste) 2400 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	2,400 (clay)		2,400 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Am-241 - Atomic Weight 241 g/mol								
Half Life (years)	4.32E+02	--	4.32E+02	--	--	--	None Specified	--
Atomic Weight (g/mol)	241		241		--	--	None Specified	
Solubility Limit (gm/cc)	8.00E-03	Derived from geochemical database prepared by Lawrence Livermore National Laboratory and converted to PHREEQC format.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	1900 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	1900 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	1900 (sand) 1900 (waste) 8400 (clay)	DOE 2003b, page C3-313 and Table Att. 1. Distribution coefficient of radionuclides and their daughter products in different zones, page C3-314.
	8400 (clay)		8400 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
Np-237 - Atomic Weight 237 g/mol								
Half Life (years)	2.14E+06	Disposal Unit Source Term (DUST) default library	2.14E+06	--	2.14E+06	Disposal Unit Source Term (DUST) default library	None Specified	--
Atomic Weight (g/mol)	237		237		237	EPA (1996)	None Specified	
Solubility Limit (gm/cc)	1.00E+01	No value found. Assume 10 gm/cc to prevent solubility from limiting migration.	1.00E+01	EPA (1996) (Not Verified)	1.00E+01	EPA (1996) (Not Verified)	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	5 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	5 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	70 (sand)	Sheppard and Thibault (1990), conflict with numbers in the table	70 (sand) 70 (waste) 144 (clay)	DOE 2003b, page C3-313 and Table Att. 1. Distribution coefficient of radionuclides and their daughter products in different zones, page C3-314. No Kd values for NP-237 reported in table.
	55 (clay)		55 (clay)		144 (clay)	DOE (1997) and DOE (2002b)		
Diffusion Coefficient (cm^2/sec)	1.00E-06	DOE (2003) (U-Landfill Report)	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Pa-231 - Atomic Weight 231 g/mol								
Half Life (years)	3.30E+04	ANL (2005)	3.28E+04	--	--	--	None Specified	--
Atomic Weight (g/mol)	231		231		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E+01	No value found. Assume 10 gm/cc to prevent solubility from limiting migration.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	550 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	550 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	550 (sand) 550 (waste) 2700 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	2,700 (clay)		2,700 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
Pb-210 - Atomic Weight 210 g/mol								
Half Life (years)	2.20E+01	ANL (2005)	2.20E+01	--	--	--	None Specified	--
Atomic Weight (g/mol)	210		210		--	--	None Specified	
Solubility Limit (gm/cc)	8.70E-04	EPA (2004), Page A-225	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	270 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	270 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	270 (sand) 270 (waste) 550 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	550 (clay)		550 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Pu-238 - Atomic Weight 238 g/mol								
Half Life (years)	8.78E+01	Disposal Unit Source Term (DUST) default library	8.78E+01	--	--	--	None Specified	--
Atomic Weight (g/mol)	238		238		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E+01	No value found. Assume 10 gm/cc to prevent solubility from limiting migration.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	550 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	550 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	550 (sand) 550 (waste) 5100 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	5100 (clay)		5100 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
Pu-239 - Atomic Weight 239 g/mol								
Half Life (years)	2.41E+04	Disposal Unit Source Term (DUST) default library	2.41E+04	--	--	--	None Specified	--
Atomic Weight (g/mol)	239		239		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E+01	No value found. Assume 10 gm/cc to prevent solubility from limiting migration.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	550 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	550 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	550 (sand) 550 (waste) 5100 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	5100 (clay)		5100 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Pu-240 - Atomic Weight 240 g/mol								
Half Life (years)	6.54E+03	Disposal Unit Source Term (DUST) default library	6.57E+03	--	--	--	None Specified	--
Atomic Weight (g/mol)	240		240		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E+01	No value found. Assume 10 gm/cc to prevent solubility from limiting migration.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	550 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	550 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	550 (sand) 550 (waste) 5100 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	5100 (clay)		5100 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
Ra-226 - Atomic Weight 226 g/mol								
Half Life (years)	1.60E+03	Disposal Unit Source Term (DUST) default library	1.60E+03	--	--	--	None Specified	--
Atomic Weight (g/mol)	226		226		--	--	None Specified	
Solubility Limit (gm/cc)	3.10E-01	EPA (2004), Page A-301	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	500 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	500 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	500 (sand) 500 (waste) 9100 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	9,100 (clay)		9,100 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Ra-228 - Atomic Weight 228 g/mol								
Half Life (years)	5.80E+00	Disposal Unit Source Term (DUST) default library	5.75E+00	--	--	--	None Specified	--
Atomic Weight (g/mol)	228		228		--	--	None Specified	
Solubility Limit (gm/cc)	3.10E-01	EPA (2004), Page A-303	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	500 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	500 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	500 (sand) 500 (waste) 9100 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	9,100 (clay)		9,100 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
Th-228 - Atomic Weight 228 g/mol								
Half Life (years)	1.90E+00	ANL (2005)	1.90E+00	--	--	--	None Specified	--
Atomic Weight (g/mol)	228		228		--	--	None Specified	
Solubility Limit (gm/cc)	2.80E-01	EPA (2004), Page A-343	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	3200 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	3200 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	3200 (sand) 3200 (waste) 5800 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	5800 (clay)		5800 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Th-229 - Atomic Weight 229 g/mol								
Half Life (years)	7.34E+03	Disposal Unit Source Term (DUST) default library	7.34E+03	--	--	--	None Specified	--
Atomic Weight (g/mol)	229		229		--	--	None Specified	
Solubility Limit (gm/cc)	2.80E-01	EPA (2004), Page A-345.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	3200 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	3200 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	3200 (sand) 3200 (waste) 5800 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	5800 (clay)		5800 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
Th-230 - Atomic Weight 230 g/mol								
Half Life (years)	7.70E+04	ANL (2005)	7.70E+04	--	--	--	None Specified	--
Atomic Weight (g/mol)	230		230		--	--	None Specified	
Solubility Limit (gm/cc)	2.80E-01	EPA (2004), Page A-347	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	3200 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	3200 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	3200 (sand) 3200 (waste) 5800 (clay)	DOE 2003b, page C3-313 and Table Att. 1. Distribution coefficient of radionuclides and their daughter products in different zones, page C3-314.
	5800 (clay)		5800 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Th-232 - Atomic Weight 232 g/mol								
Half Life (years)	1.40E+10	ANL (2005)	1.40E+10	--	--	--	None Specified	--
Atomic Weight (g/mol)	232		232		--	--	None Specified	
Solubility Limit (gm/cc)	2.80E-01	EPA (2004), Page A-351	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	3200 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	3200 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	3200 (sand) 3200 (waste) 5800 (clay)	DOE 2003b, page C3-313 and Table Att. 1. Distribution coefficient of radionuclides and their daughter products in different zones, page C3-314.
	5800 (clay)		5800 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
U-233 - Atomic Weight 233 g/mol								
Half Life (years)	1.59E+05	Disposal Unit Source Term (DUST) default library	1.59E+05	--	--	--	None Specified	--
Atomic Weight (g/mol)	233		233		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E-04	EPA (2004), Page A-381	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	35 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	66.8 (sand)	Sheppard and Thibault (1990), does not match number in table	--	--	66.8 (sand) 410 (waste) 3640 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	1600 (clay)		3640 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
U-234 - Atomic Weight 234 g/mol								
Half Life (years)	2.40E+05	ANL (2005)	2.44E+05	--	--	--	None Specified	--
Atomic Weight (g/mol)	234		234		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E-04	EPA (2004), Page A-383	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	35 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	66.8 (sand)	Sheppard and Thibault (1990), does not match number in table	--	--	66.8 (sand) 410 (waste) 3640 (clay)	DOE 2003b, page C3-313 and Table Att. 1. Distribution coefficient of radionuclides and their daughter products in different zones, page C3-314.
	1600 (clay)		3640 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
U-235 - Atomic Weight 235 g/mol								
Half Life (years)	7.00E+08	ANL (2005)	7.04E+08	--	--	--	None Specified	--
Atomic Weight (g/mol)	235		235		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E-04	EPA (2004), Page A-385	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	35 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	66.8 (sand)	Sheppard and Thibault (1990), does not match number in table	--	--	66.8 (sand) 410 (waste) 3640 (clay)	DOE 2003b, page C3-313 and Table Att. 1. Distribution coefficient of radionuclides and their daughter products in different zones, page C3-314.
	1600 (clay)		3640 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
U-236 - Atomic Weight 236 g/mol								
Half Life (years)	2.34E+07	Disposal Unit Source Term (DUST) default library	2.34E+07	--	--	--	None Specified	--
Atomic Weight (g/mol)	236		236		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E-04	EPA (2004), Page A-387	1.00E+01	EPA (1996)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	35 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	66.8 (sand)	Sheppard and Thibault (1990), does not match number in table	--	--	66.8 (sand) 410 (waste) 3640 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	1600 (clay)		3640 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
U-238 - Atomic Weight 238 g/mol								
Half Life (years)	4.50E+09	ANL (2005)	4.47E+09	--	4.47E+09	Disposal Unit Source Term (DUST) default library	None Specified	--
Atomic Weight (g/mol)	238		238		238	EPA (1996)	None Specified	
Solubility Limit (gm/cc)	1.00E-04	EPA (2004), Page A-389	1.00E+01	EPA (1996)	1.00E+01	EPA (1996)	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	35 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	66.8 (sand)	Sheppard and Thibault (1990), does not match number in table	66.8 (sand) 410 (organic) 3640 (clay)	Sheppard and Thibault (1990), does not match number in table DOE (1997) and DOE (2002b)	66.8 (sand) 410 (waste) 3640 (clay)	DOE 2003b, page C3-313 and Table Att. 1. Distribution coefficient of radionuclides and their daughter products in different zones, page C3-314. Table does not give references or justification for Kd values presented
	1600 (clay)		3640 (clay)					
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)

Notes

1. -- Denotes information not available.
2. ORISE RESRAD Model Value information provided by personal communication (John Volpe email - 04/24/2011).
3. User's Manual for RESRAD Version 6. "The default value is assigned; however, it is not used by the code. This parameter is one of the options in RESRAD to derive distribution coefficients (Kds) when site-specific data is not available. In this case site-specific Kds are available and are used by the code; therefore, there was no need to use this option to derive them."
4. Kd - chemical specific distribution coefficient.
5. Koc - chemical specific octanol/water partition coefficient.
6. foc - fraction organic carbon.

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Table C1.4. HELP Model Input Parameters

Parameter	Units	Deterministic Value
Fraction of area allowing runoff	%	100% (18.94 acres)
Evaporative zone depth	inches	8 inches for Operational Period (low end of silts) 18 inches for Postclosure and Long-Term Modeling Periods (high end of silts)
Start of growing season	day	96th Julian Day
End of growing season	day	300th Julian Day
Average annual wind speed	mph	8.2
Average 1st quarter relative humidity	%	70
Average 2nd quarter relative humidity	%	67
Average 3rd quarter relative humidity	%	72
Average 4th quarter relative humidity	%	54
Normal mean monthly precipitation (Jan)	inches	3.27
Normal mean monthly precipitation (Feb)	inches	3.9
Normal mean monthly precipitation (Mar)	inches	4.92
Normal mean monthly precipitation (April)	inches	5.01
Normal mean monthly precipitation (May)	inches	4.94
Normal mean monthly precipitation (June)	inches	4.05
Normal mean monthly precipitation (July)	inches	4.19
Normal mean monthly precipitation (Aug)	inches	3.34
Normal mean monthly precipitation (Sept)	inches	3.69
Normal mean monthly precipitation (Oct)	inches	3
Normal mean monthly precipitation (Nov)	inches	4.32
Normal mean monthly precipitation (Dec)	inches	4.65
Normal mean monthly temperature (Jan)	^{o}F	32.6
Normal mean monthly temperature (Feb)	^{o}F	36.9
Normal mean monthly temperature (Mar)	^{o}F	47.5
Normal mean monthly temperature (April)	^{o}F	57.9
Normal mean monthly temperature (May)	^{o}F	66.7
Normal mean monthly temperature (June)	^{o}F	75.2
Normal mean monthly temperature (July)	^{o}F	78.8
Normal mean monthly temperature (Aug)	^{o}F	76.8
Normal mean monthly temperature (Sept)	^{o}F	70.2
Normal mean monthly temperature (Oct)	^{o}F	58.7
Normal mean monthly temperature (Nov)	^{o}F	47.9
Normal mean monthly temperature (Dec)	^{o}F	37.3
Solar Radiation Data Station Latitude	Decimal Degrees	37.1 N

Table C1.5. DUST-MS Model Input Parameters

Parameter	Units	Deterministic Value
Title and General Problem Definition		
Number of Nodes	n/a	298 (Site 11) 266 (Site 3A)
Number of Isotopes	n/a	Varies
Mass Units	grams	grams
Decay Chains	n/a	Varies
Time Parameters		
Number of Time Steps	n/a	10000
Initial Time Interval (yrs)	years	1.6 0.16 0.08
Fractional Change in Time Interval	n/a	0
Maximum Time Interval	years	1.6 0.16 0.08
Maximum Simulation Time	years	16000 1600 800
Number of Time Step Resets	n/a	0
Material Parameters		
Number of Materials	n/a	6 (Site 11) 5 (Site 3A)
Number of Material Changes	n/a	298 (Site 11) 266 (Site 3A)
K-d (Distribution Coefficient)	cc/gm	Chemical Specific
Density	gm/cc	Material - Density 1 - 1.34 2- 1.4 3 - 1.8 4 - 3.1 5 - 1.43 (Site 11) 5 - 1.41 (Site 3A) 6 - 1.43 (Site 11)
Dispersion Coefficient	cm	415 (Site 11) 366 (Site 3A)
Diffusion Coefficient	cm^2/s	Chemical Specific
Changes to Node Material Types	n/a	First Node to Last Node = Material 1 to 10 = 1 11 to 20 = 2 21 to 26 = 3 27 to 196 = 4 197 to 198 = 3 199 to 200 = 2 201 to 206 = 3 207 to 226 = 1 227 to 270 = 5 (Site 11) 227 to 266 = 5 (Site 3A) 271 to 298 = 6 (Site 11)
Change in Node Number	n/a	1

Table C1.5. DUST-MS Model Input Parameters (Continued)

Parameter	Units	Deterministic Value
Change in Material Type	n/a	0
Output Parameters		
Output for Time Steps	n/a	Print Concentrations at time step = 1 and every 999 time steps
Number of Concentration Traces	n/a	5 (Site 11) 4 (Site 3A)
Node Locations for Concentration Traces	n/a	1, 26, 206, 270, 298 (Site 11) 1, 26, 206, 266 (Site 3A)
Number of Flux Traces	n/a	5 (Site 11) 4 (Site 3A)
Node Locations for Flux Traces	n/a	1, 26, 206, 270, 298 (Site 11) 1, 26, 206, 266 (Site 3A)
Facility Dimensions		
Area of Facility	cm^2	7.67E+08
Node Coordinates		
First Node	n/a	1
Last Node	n/a	298 (Site 11) 266 (Site 3A)
Change in Node Number	n/a	1
Starting Location	cm	0
Change in Delta X	cm	15.24
Incremental Change in Delta X	n/a	0

Table C1.5. DUST-MS Model Input Parameters (Continued)

Parameter	Units	Deterministic Value
Initial Conditions		
First, Last Node, and Initial Concentration	g/cc	First Node to Last Node = Initial Concentration 1 to 26 = 0 27 to 196 = Chemical Specific 197 to 266 (Site 3A) or 298 (Site 11) = 0
Change in Node Number	n/a	1
Fractional Change in Concentration	n/a	0
Boundary Conditions		
Upper Boundary	$g/cm^2/s$	Total Flux = 0
Lower Boundary	g/cc	Concentration = 0
Number of Data Points	n/a	2
Use BC File	n/a	No - All
Water Velocity Parameters		
Number of Data Points	n/a	10 - Gradual Failure (BL) Scenario 4 - Instantaneous Failure (IF) Scenario 2 - No Failure (NF) Scenario
Time and Water Velocity Parameters	years and cm/s	Time - Water Velocity 0 - 2.458E-14 (BL, IF, NF) 170 - 2.458E-14 (BL, IF, NF) 195 - 1.217E-13 (BL) 220 - 6.030E-13 (BL) 320 - 3.626E-10 (BL) 395 - 3.962E-08 (BL) 470 - 3.636E-07 (BL) 520 - 3.889E-07 (BL) 570 - 3.901E-07 (BL, IF) 16000 - 3.907E-07 (BL, IF)

Table C1.5. DUST-MS Model Input Parameters (Continued)

Parameter	Units	Deterministic Value
Moisture Content		
First and Last Node - Initial Moisture Content	n/a	First Node to Last Node = Material 1 to 10 = 0.3098 11 to 20 = 0.0452 21 to 26 = 0.4251 27 to 196 = 0.3588 197 to 198 = 0.4112 199 to 200 = 0.1123 201 to 206 = 0.427 207 to 226 = 0.342 227 to 270 = 0.393 (Site 11) 227 to 266 = 0.3025 (Site 3A) 271 t0 298 = 0.445 (Site 11)
Change in Node Number	n/a	1
Incremental Change in Moisture Content	n/a	0
Container Failure Times		
Number of Containers	n/a	0
Number of Failure Types	n/a	none
Failure Times for Containers	n/a	none
Waste Forms		
Not used	n/a	Not used
Sources		
Number of Source/Sink Nodes	n/a	0

Table C1.6. AT123D Model Input Parameters

Parameter	Units	Deterministic Value
Aquifer Tab		
Hydraulic Conductivity	m/hr	35.6 (Site 11) 1.18 (Site 3A)
Hydraulic Gradient	m/m	0.00066 (Site 11) 0.0032 (Site 3A)
Effective Porosity	n/a	0.3
Soil Bulk Density	kg/m^3	1670 (Site 11) 1560 (Site 3A)
Longitudinal Dispersivity	m	15
Transverse Dispersivity	m	1.5
Vertical Dispersivity	m	0.15
Aquifer Width	m	Infinite
Aquifer Depth	m	10.8 (Site 11) 4.572 (Site 3A)
Number of Eigenvalues	n/a	500
Steady-State Error Tolerance	n/a	0.01
Input Tab		
Release Coordinates	m	Site 11 X - Start = -113.1, End = 113.1 Y - Start = -169.6, End = 169.6 Z - Start = 0, End = 0 Site 3A X - Start = -124.8, End = 124.8 Y - Start = -153.6, End = 153.6 Z - Start = 0, End = 0
Soil organic carbon content	%	0
Koc - Organic carbon adsorption coefficient	(ug/g)/ (ug/ml)	0
Kd - Distribution Coefficient	m^3/kg	Chemical Specific
Water Diffusion Coefficient	m^2/hr	Chemical Specific
First-Order Decay Coefficient	1/hr	Chemical Specific

Table C1.6. AT123D Model Input Parameters (Continued)

Parameter	Units	Deterministic Value
Output Tab		
Starting Time Step		1
Ending Time Step		10001
Time Step		1
X-Axis Coordinates	m	Site 11 - 113.1, 213.1, 225.9, 1356.3, 3907.6 Site 3A - 124.8, 224.8, 242.6, 625.7, 1000
Y-Axis Coordinates	m	0
Z-Axis Coordinates	m	0
Load Tab		
Initial Concentration	mg/L	0
Single Mass Load	kg	not used
Model Time Step	hrs	14025.6 1402.56 701.28
Continuous = 0, >1 Varying	n/a	10000
Water Density	kg/m^3	1000
Release Type	n/a	Continuous Release
Load Release Rate	kg/hr	Varies by Chemical

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APPENDIX C

PROPOSED GROUNDWATER MODELING METHODOLOGY

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ACRONYMS

AT123D	Analytical Transient 1-, 2-, 3-Dimensional
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
CCL	compacted clay liner
COC	contaminant of concern
COPC	chemical of potential concern
DAF	dilution attenuation factor
DOE	U.S. Department of Energy
DUSTMS	Disposal Unit Source Term-Multiple Species
ELCR	excess lifetime cancer risk
EPA	U.S. Environmental Protection Agency
FML	flexible membrane liner
HDPE	high density polyethylene
HELP	Hydrologic Evaluation of Landfill Performance
HI	hazard index
MCL	maximum contaminant level
PGDP	Paducah Gaseous Diffusion Plant
PWAC	preliminary waste acceptance criteria
RGA	Regional Gravel Aquifer
UCRS	Upper Continental Recharge System
WAC	waste acceptance criteria
WDF	waste disposal facility

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C.1. INTRODUCTION

If selected, the on-site waste disposal alternative involves the construction of a Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) waste disposal facility at the Paducah Gaseous Diffusion Plant (PGDP). This appendix presents the modeling methodology proposed for evaluating the performance of an on-site waste disposal facility, including development of preliminary waste acceptance criteria (PWAC).

C.2. PREVIOUS REPORTS AND MODELING

Several reports have been completed at PGDP for on-site waste disposal facilities. These reports include the following:

- *Operating Limit Study for the Proposed Solid Waste Landfill at Paducah Gaseous Diffusion Plant*, ORNL/TM-13008, June 1995 (ORNL 1995).
- *Remedial Investigation/Feasibility Study on Disposal Options for Comprehensive Environmental Response, Compensation, and Liability Act of 1980 (CERCLA)-Derived Waste at the Paducah Gaseous Diffusion Plant, Paducah, Kentucky*, DOE/OR/07-1935&D(-1), March (DOE 2001).
- *Risk and Performance Evaluation of the C-746-U Landfill at the Paducah Gaseous Diffusion Plant, Paducah, Kentucky*, DOE/OR/07-2041&D2R1, September (DOE 2003).

Each of these reports presents a modeling methodology similar to that proposed for evaluating the performance of an on-site waste disposal facility and serves as the basis for the development of the proposed modeling methodology presented in this appendix. This earlier work is supplemented by a review of the current technical literature related to the performance of engineered barriers. The service life of the engineered barriers established from the literature review is also proposed for use in the modeling.

The Remedial Investigation/Feasibility Study on Disposal Options for CERCLA-Derived Waste (DOE 2001) was developed under consensus of a core team; however, the report was not released for review to the regulators. The remaining reports were finalized and released to the public, but only the Risk and Performance Evaluation of the C-746-U Landfill report (DOE 2003) was approved by the regulators.

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C.3. MODELING METHODOLOGY

The general modeling procedure for the development of PWAC is provided in Table C.1. This table presents the major modeling tasks and descriptions of the general task elements that are necessary within each modeling task to facilitate the determination of the PWAC.

Table C.1. General Modeling Procedure for the Development of the PWAC

MODELING TASK	GENERAL TASK ELEMENTS
Identify Waste and Indicator Chemicals Constituents	Identify constituents in waste.
	Establish chemical surrogate groups and assign contaminants to surrogate groups.
	Identify indicator chemicals for fate and transport modeling for each chemical surrogate group.
Fate and Transport Modeling	Conduct fate and transport modeling for radionuclides, metals, and indicator chemicals, and calculate dilution-attenuation factors (DAFs) for indicator chemicals.
	Calculate concentrations for chemicals within a surrogate group using the indicator chemical's DAF.
Risk Assessment	Calculate the cancer risk and hazard presented by each chemical, metal, and radionuclide using PGDP No Action screening values for the rural child resident.
PWAC Development	Derive PWAC using ratio of modeled and acceptable concentration in water and concentration in source.
Uncertainty Analysis	Perform qualitative and quantitative uncertainty analyses.

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C.3.1 IDENTIFY WASTE CONSTITUENTS AND INDICATOR CHEMICALS

Chemicals to be evaluated in the model will be determined based on a combination of information from the PGDP Human Health volume of the Risk Methods Document (DOE 2011) and other available waste profile data and selected to represent the expected waste contaminants for disposal in the potential on-site disposal facility.

C.3.1.1 Identify Constituents in Waste

Appendix D presents the methods that will be used to develop an analytical profile for the wastes that are expected to be placed in the potential on-site waste disposal facility. The chemicals of potential concern (COPCs) for PGDP are provided in Table 2.1 of the Risk Methods Document (DOE 2011). Contaminants of concern (COCs) will be derived using Table 2.1, as well as other available waste profile data and will be assessed in the fate and transport modeling analyses.

C.3.1.2 Establish Surrogate Groups

In order to streamline the modeling process, each COC will be assigned to a contaminant group. The contaminant groups will represent chemicals of concern with similar chemical properties, such as

solubility, volatility, and mobility, so that each contaminant group will contain chemicals that behave similarly in the environment.

The use of indicator chemicals involves the necessity to develop a sufficient number of groups such that the groups represent the full range of potential contaminant property combinations; however, the C-746-U Landfill report (DOE 2003) states that "it was determined that transport of neither the inorganic chemicals nor the radionuclides was adequately estimated through the use of indicator chemicals." The analysis found that surrogate groups were only adequately representative for organic compounds.

Based on this conclusion, surrogates will be used to develop a PWAC for organics; however, radionuclides and metals will be assessed individually and not as surrogate groups. If the On-Site Alternative is selected, a final waste acceptance criteria (WAC) will be developed with a full analysis of potential COCs.

C.3.1.3 Identify Indicator Chemicals for Surrogate Groups

An indicator chemical will be selected to represent each organic surrogate group. The indicator chemical for each surrogate group will be a representative chemical that previously has been identified as a major COC at PGDP. Section C.3.2 provides additional discussion on the issues associated with chemical interactions affecting the fate and transport of specific chemical groups. As noted in Section C.3.1.2, metals and radionuclides will be assessed individually and not as surrogate groups.

C.3.2 FATE AND TRANSPORT MODELING

The fate and transport modeling will be performed as follows:

(1) Hydrologic Evaluation of Landfill Performance (HELP) model simulations will be used to perform three failure scenarios to estimate the water flux percolating through the waste and into the water table under each of the scenarios. As described in Section C.3.2.1.1, the failure scenarios are based on a range of estimated service lives for the engineered barriers. The model also accounts for eventual failure of the drainage layers. The various scenarios to be considered include (1) instantaneous failure, (2) gradual failure, and (3) no failure. Additional gradual failure scenarios will be analyzed as part of the uncertainty analysis described in Section C.3.5. Under the gradual and instantaneous failure scenarios, the lateral drainage layers beneath the waste will be assumed to degrade. To account for degradation, the manmade flexible membrane liner (FML) layers in both the bottom liner and cap no longer would act as barrier layers, and the two drainage layers below the waste no longer would function (i.e., they effectively become vertical percolation layers). The no failure scenario assumes that the system maintains integrity throughout the period of interest.

(2) Disposal Unit Source Term-Multiple Species (DUSTMS) modeling will be performed for each metal, radionuclide, and indicator chemical under the gradual failure scenario to predict the contaminant flux entering the aquifer over time. A unit concentration for each contaminant will be used as an initial input to DUSTMS. This unit concentration is converted to an initial contaminant mass within the landfill. The contaminant mass will be assumed to be contained in a homogenized soil. The entire landfill volume will be assumed to be filled with a single contaminant embedded in the soil waste. DUSTMS is used to calculate initial groundwater concentrations based on this initial mass/concentration. Once downgradient groundwater concentrations are obtained from the Analytical Transient, 1-, 2-, 3-Dimensional (AT123D) model and initial PWAC concentrations are calculated, DUSTMS is rerun using the initial PWAC concentrations to obtain new initial groundwater

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concentrations. (DUSTMS modeling also will be performed for selected contaminants as part of an uncertainty analysis under the immediate and no failure scenarios.)

(3) MODFLOW/MODPATH modeling will be performed at Site 11 to predict the groundwater migration rate from the location where leachate enters the Regional Gravel Aquifer (RGA) groundwater flow system to the exposure point locations and the shortest transit times to each exposure point.

The sitewide groundwater model does not cover the area of interest at Site 3A. If the sitewide groundwater model cannot be expanded to include Site 3A, existing hydrogeologic data for Site 3A will be used to determine the appropriate hydrogeological parameters for Site 3A in the DUSTMS and AT123D models.

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(4) AT123D modeling will be performed to predict concentrations of each indicator chemical, metal, and radionuclide at established exposure points over time due to lateral transport. The contaminant flux from the DUSTMS model will be used as input to the AT123D model.

Maximum concentrations and the time, up to 10,000 years, to attain the maximum concentrations at the exposure points will be predicted, and dilution attenuation factors (DAFs) associated with source-to-exposure point transport of the indicator chemical will be calculated.

Proposed modeling parameters are included in Attachment C.1.

C.3.2.1 Selected Models and Their Application

Several models will be required for the evaluation of the performance of an on-site waste disposal facility. The following discussion presents the models selected for use in the analysis of the groundwater transport pathway. The selection of the models was based on the modeling matrix presented in the Risk Methods Document (DOE 2001). Figure C.1 provides an illustration of the model application in the assessment. Figures C.2 and C.3 provide an illustration of how the HELP layers and DUSTMS material layers interrelate for Sites 11 and 3A, respectively.

C.3.2.1.1 HELP Model

The HELP model (Schroeder et al. 1994) will be used to determine the rate of water infiltration through the engineered cap that can be released from the bottom of the landfill. The HELP computer program is a quasi-two-dimensional hydrologic model of water movement across, into, through, and out of landfills. The model considers weather, soil, and design data and uses solution techniques that account for the effects of surface storage, snowmelt, runoff, infiltration, evapotranspiration, vegetative growth, soil moisture storage, lateral subsurface drainage, leachate recirculation, unsaturated vertical drainage, and leakage through soil, geomembrane, or composite liners. The program was developed to conduct water balance analysis of landfills, cover systems, and solid waste disposal and containment facilities. As such, the model facilitates rapid estimation of the amounts of runoff, evapotranspiration, drainage, leachate collection, and liner leakage that may be expected to result from the operation of a wide variety of landfill designs.

The HELP model will be used to determine the water balance of the facility based on preliminary facility/cap design. The modeling will account for the operational period, institutional control period, and the post-institutional control period, which are described below.

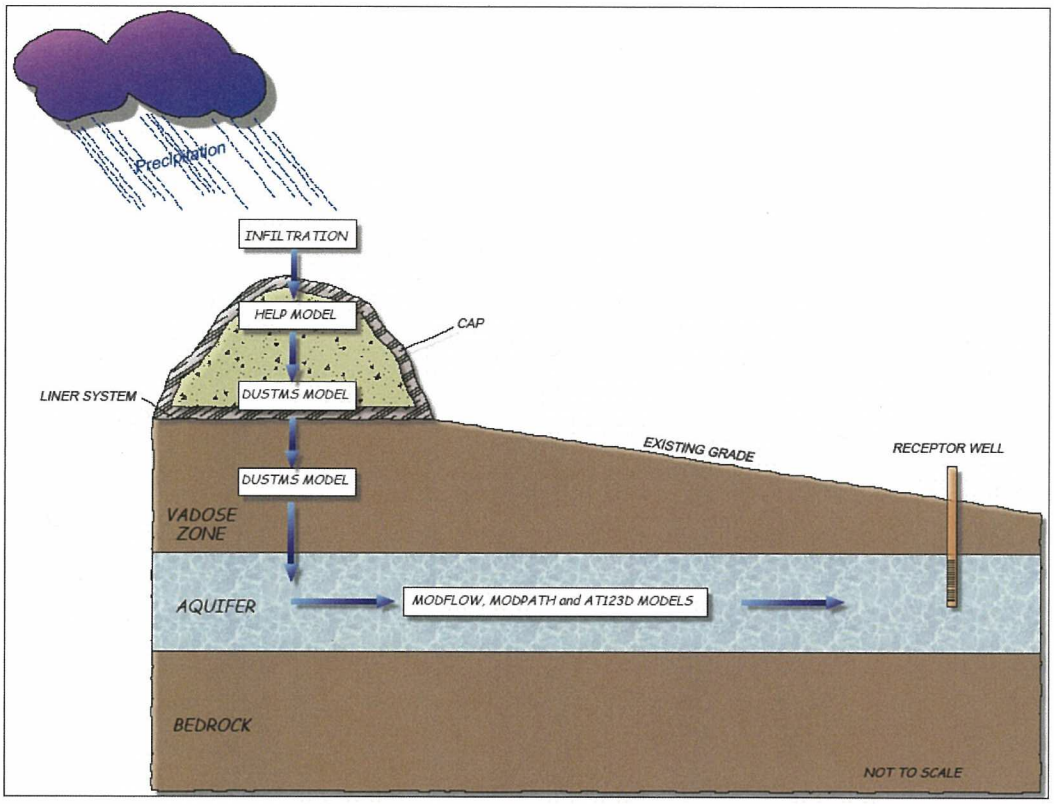

Figure C.1. Generalized Conceptual Model for an On-Site Waste Disposal Facility

Site 11 - Conceptual Model 30+ years

HELP, DUST-MS, AT123D

DUST-MS Material	HELP Soil Layers	DUST-MS Number of Computational Nodes	Thickness (ft)	DUST-MS Bulk Density	DUST-MS Initial (t = 30 yrs) Volumetric Moisture Content	HELP Initial (t = 30 yrs) Volumetric Moisture Content
1	Soil Matirx	10	5	1.34	0.3098	0.3098
2	Filter Sand	2	1	1.4	0.0452	0.0843
	Cobble/ Gravel Sand	6	3			0.0451
	Drainage Sand	2	1			0.032
3	FML (HDPE) Liner Clay	6	3	1.8	0.4251	0.4251
4	Waste Form	170	85	3.1	0.3588	0.3588
3	Clay (compacted)	2	1	1.8	0.4112	0.4112
2	Drainage Sand	2	1	1.4	0.1123	0.1123
FML (HDPE) Liner	Geocomposite		0.02			
3	Clay Barrier FML (HDPE) Liner	6	3	1.8	0.427	0.427
1	Geologic Buffer (clay)	20	10	1.34	0.342	0.342
5	Loess Deposit (Unsaturated UCRS) Bottom of HELP Model	44	22	1.43	0.393	0.393
6	Silt to Clay (Saturated Upper Continental Deposits) Bottom of DUST-MS Model	28	14	1.43	0.445	
AT123D Lateral Flow Layer	RGA		35.5	1.67	Saturated Horizontal Flow	
	McNairy Formation					

Unsaturated Vertical Flow

Saturated Vertical Flow

Figure C.2. DUSTMS Model Layers and Select Parameters, Site 11

Site 3A - Conceptual Model 30+ years

HELP, DUST-MS, AT123D

DUST-MS Material	HELP Soil Layers	DUST-MS Number of Computational Nodes	Thickness (ft)	DUST-MS Bulk Density	DUST-MS Initial (t = 30 yrs) Volumetric Moisture Content	HELP Initial (t = 30 yrs) Volumetric Moisture Content
1	Soil Matirx	10	5	1.34	0.3098	0.3098
2	Filter Sand	2	1	1.4	0.0452	0.0843
	Cobble/ Gravel Sand	6	3			0.0451
	Drainage Sand	2	1			0.032
FML (HDPE) Liner	Clay	6	3	1.8	0.4251	0.4251
4	Waste Form	170	85	3.1	0.3588	0.3588
3	Clay (compacted)	2	1	1.5	0.4112	0.4112
2	Drainage Sand	2	1	1.4	0.1123	0.1123
FML (HDPE) Liner	Geocomposite		0.02			
FML (HDPE) Liner	Clay Barrier	6	3	1.8	0.427	0.427
1	Geologic Buffer	20	10	1.34	0.342	0.393
5	Terrace Gravel (Lower Continental Deposit)	40	20	1.41	0.302	0.302
	Bottom of HELP and DUST-MS Model					
AT123D Lateral Flow Layer	Terrace Gravel (Lower Continental Deposit)		15	1.56	Saturated Horizontal Flow	
	Porter's Creek Clay		70			
	McNairy Formation					

Unsaturated Vertical Flow

Figure C.3. DUSTMS Model Layers and Select Parameters, Site 3A

During the operational period (0–30 years), landfill components that would be in place include the leachate collection system with a barrier liner beneath the waste. This is a multi component system where each component functions independently and has different failure times and rates. During this period, it is assumed that a cover system is not in place. During this period, contaminant mass removed via the leachate collection system is assumed to be collected and removed from the landfill; however, the mass removed by the leachate collection system will not be taken into account during calculation of the PWAC.

For the gradual failure scenarios, all components of the waste disposal facility would be in place (both cover and liner components, drainage layers, and low-permeability clay layers) and functioning until at least year 130. At year 130 (the end of the institutional control period), the leachate collection system is assumed to cease to function. However, very little, if any, infiltration, is expected as long as the high density polyethylene (HDPE) geomembrane in the cap is intact (Bonaparte et al. 2008). HDPE geomembrane degradation is assumed to begin at year 200. For this reason, there will be little if any impact if the leachate collection system is modeled to cease functioning at 130 years or 200 years. For simplicity in modeling, the lateral drainage layers are assumed to cease functioning at 200 years.

During the institutional control period (30–130 years and generally considered to commence after facility closure and to last for 100 years) and for 70 years beyond the postinstitutional control period, all components of the waste disposal facility would be in place (both cover and liner components, drainage layers, and low-permeability clay layers) and functioning. The basis for this time period is outlined subsequently. These conditions apply to the instantaneous, gradual, and no failure scenarios. The HELP model will be used to evaluate the flux through the facility based on initial properties of the cover and liner system.

For the no failure scenario, all components of the waste disposal cell are assumed to be in place from year 200 to 10,000.

For the instantaneous failure scenario, all components of the waste disposal cell are assumed to fail at year 200. The "end state" or complete failure of certain landfill components is assumed to mean that the leachate collection system no longer is functioning, the liners have degraded to the point that they are no longer functioning as barriers to water transmission (either in or out of the landfill), and the clay liners have increased in hydraulic conductivity by one order of magnitude; the clay liners (upper and lower), as well as the other cap system components (e.g., soil cover and biointrusion layer) are assumed to still be in place and functioning as intended.

For the gradual failure scenario, at 200 years the HDPE geomembrane components of the cap and liner system would commence to degrade (i.e., all antioxidants are depleted and the induction time for the start of degradation is completed). Degradation of the HDPE geomembrane is assumed to be completed at 600 years. Beyond 600 years, the compacted clay liners (CCLs) controls infiltration into the cap and out of the liner system. It is recognized that a longer service life and degradation period for HDPE geomembranes are supported by the technical literature (Rowe 2010). For the base case, a longer service life and degradation period are bound by the no failure scenario. Other service lives and degradation periods may be addressed as part of the uncertainty analyses described in Section C.3.5.

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The rate of degradation between 200 and 600 years will be modeled, based on prior work conducted at the site, and the following equation will be used (Lee et al. 1995):

$$F(t) = \frac{f_2 \; x \; f_3}{f_2 + (f_3 - f_2) \, x \, e^{-\alpha(t - t1)}}$$

where

F(t) = gradual failure function providing the groundwater recharge at any time t (cm/year)
f_2 = average groundwater recharge in the institutional control period (cm/year)
f_3 = final groundwater recharge for the post-institutional control period after cover and liner failure (cm/year)
t = time (years) at which F(t) is measure
t_1 = time (years) at the end of the institutional control period
α = decay constant (0.064 $year^{-1}$)

The decay constant, α, was set at 0.064 $year^{-1}$, which results in failure of the engineered barrier system at 600 years postclosure.

In the instantaneous and gradual failure cases, the CCL in both the base liner system and final cover system are assumed to undergo a one order of magnitude increase in hydraulic conductivity from 1×10^{-7} cm/s to 1×10^{-6} cm/s at 600 years. The degradation of the clay layer is modeled assuming a step change in hydraulic conductivity. Under this scenario, f_2 is established using an intact geomembrane over a CCL with a hydraulic conductivity of 1×10^{-7} cm/s (in both the final cover system and base liner system), and f_3 is established using only a CCL with a hydraulic conductivity of 1×10^{-6} cm/s.

The possible effects of the development of microchannels from "weathering" processes and the possible effects of chlorinated solvents upon clay liner hydraulic conductivity will be considered as an uncertainty, and the potential impacts on the PWAC will be discussed in the Remedial Investigation/Feasibility Study report.

C.3.2.1.2 DUSTMS Model

The DUSTMS model will be used to evaluate the release and migration of contaminants in the vadose zone (Sullivan 2006). The DUSTMS computer code is designed to model water flow, container degradation, release of contaminants from the waste to the contacting solution, and transport through the subsurface media. Water flow through the facility over time is modeled using tabular input. Container degradation models include three types of failure rates: instantaneous (all containers fail at once); uniformly distributed failures (containers fail at a linear rate between a specified starting and ending time); and gaussian failure rates (containers fail at a rate determined by a mean failure time, standard deviation, and gaussian distribution). As the waste is not expected to be containerized during waste placement, and because it is assumed for the purposes of modeling that the contaminants are readily available for transport and not packaged or treated to decrease leachability, containers will not be simulated. Also, according to Sullivan (2001), use of the waste containers provides an opportunity to overpredict chemical retardation if both waste-to-water and soil-to-water partitioning coefficients are assigned. Initial mass emplacement is simulated by specifying initial concentrations.

Wasteform release models include four release mechanisms: (1) rinse with partitioning [inventory is released instantly upon container failure subject to equilibrium partitioning (sorption) with the waste]; (2) diffusion release (release from either a cylindrical, spherical, or rectangular wasteform); (3) dissolution release (uniform release over time due to dissolution of the wasteform surface); and (4) the aforementioned wasteform release models with solubility limited release. The predicted wasteform releases are corrected for radioactive decay and ingrowth. Chemical transformations also can be evaluated as a rate constant, similar to radioactive decay.

A unique set of container failure and wasteform release parameters can be specified for each control volume with a container. Contaminant transport is modeled through a finite-difference solution of the advective transport equation with sources (wasteform release and ingrowth) and radioactive decay.

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Although DUSTMS simulates one-dimensional transport, it can be used to simulate migration down to an aquifer and then transport in the aquifer by running the code twice; however, AT123D will be used to simulate contaminant fate and transport in the RGA and Terrace Gravel formations.

The DUSTMS model will be used to determine contaminant release rates from unit source concentrations (i.e., 1 mg/kg) in the disposal unit to the RGA water table, using water infiltration rates determined from the HELP model. DUSTMS is a one-dimensional model that allows for simplification of the disposal system while still accounting for the most important physical processes and parameters influencing contaminant releases.

Certain areas of the Upper Continental Recharge System (UCRS) have been found to be saturated above the RGA. The CERCLA waste disposal facility would be constructed above ground surface and, as such, contaminant releases initially will migrate through an unsaturated zone. DUSTMS, an unsaturated flow and transport model, will be used to model the flow and transport of contaminants from the waste disposal facility through this unsaturated zone and downward to the RGA. It is recognized, that while migrating vertically through the UCRS to the RGA, different moisture conditions, including saturated conditions, possibly will be encountered. Conservation of mass dictates that the DUSTMS predicted steady-state unsaturated mass flux (g/yr) would be the same throughout the vertical transport profile whether that profile is saturated or unsaturated or combinations of both. If portions of the UCRS are saturated, the specified moisture content will be adjusted accordingly. AT123D, will be used to simulate RGA contaminant migration, and uses the DUSTMS model-predicted mass flux as input.

C.3.2.1.3 MODFLOW and MODPATH

A sitewide flow model (DOE 1997) has been developed for PGDP using MODFLOW. MODFLOW (McDonald and Harbaugh 1988) and MODPATH (Pollack 1994) will be used to estimate hydraulic gradients, flow distances, and hydraulic conductivities along site-to-receptor flow paths. This information subsequently is used to develop input parameters for the AT123D saturated zone flow and transport model. MODFLOW is a three-dimensional, finite difference model capable of simulating both steady-state and transient head distribution for a saturated groundwater flow field. MODPATH is a three-dimensional, particle-tracking model capable of using the steady-state, head distribution generated by MODFLOW to track flow paths of particles released in the groundwater flow field modeled in MODFLOW. Figure C.4 presents an example of the flow path analysis using MODFLOW and MODPATH.

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The MODFLOW model was used in the development of the sitewide groundwater flow model at PGDP (DOE 1997). This model covers most of the U.S. Department of Energy (DOE) Reservation except that portion above the Porters Creek Clay Terrace (southern geologic setting). The model was endorsed by both the PGDP Modeling Steering Committee and the Risk Assessment Working Group. The sitewide groundwater flow model has been updated in consultation with Kentucky and U.S. Environmental Protection Agency (EPA) using more recent groundwater monitoring data (DOE 2010). The revised sitewide groundwater model will be used in the development of an on-site waste disposal facility modeling effort. If the sitewide groundwater model cannot be expanded to include Site 3A, existing hydrogeologic data for Site 3A will be used to determine the appropriate hydrogeological parameters for Site 3A in the DUSTMS and AT123D models.

The MODPATH model will be used to track flowpaths of particles released from the disposal unit based on the steady-state flow from MODFLOW. The hydraulic gradient along the fastest flowpath to the exposure points of interest then will be estimated to ensure the transit time is conservatively estimated. The heads along the flowpath of interest will be determined, and the hydraulic gradient estimated as the head difference between the release point and exposure point of interest, divided by the distance from the

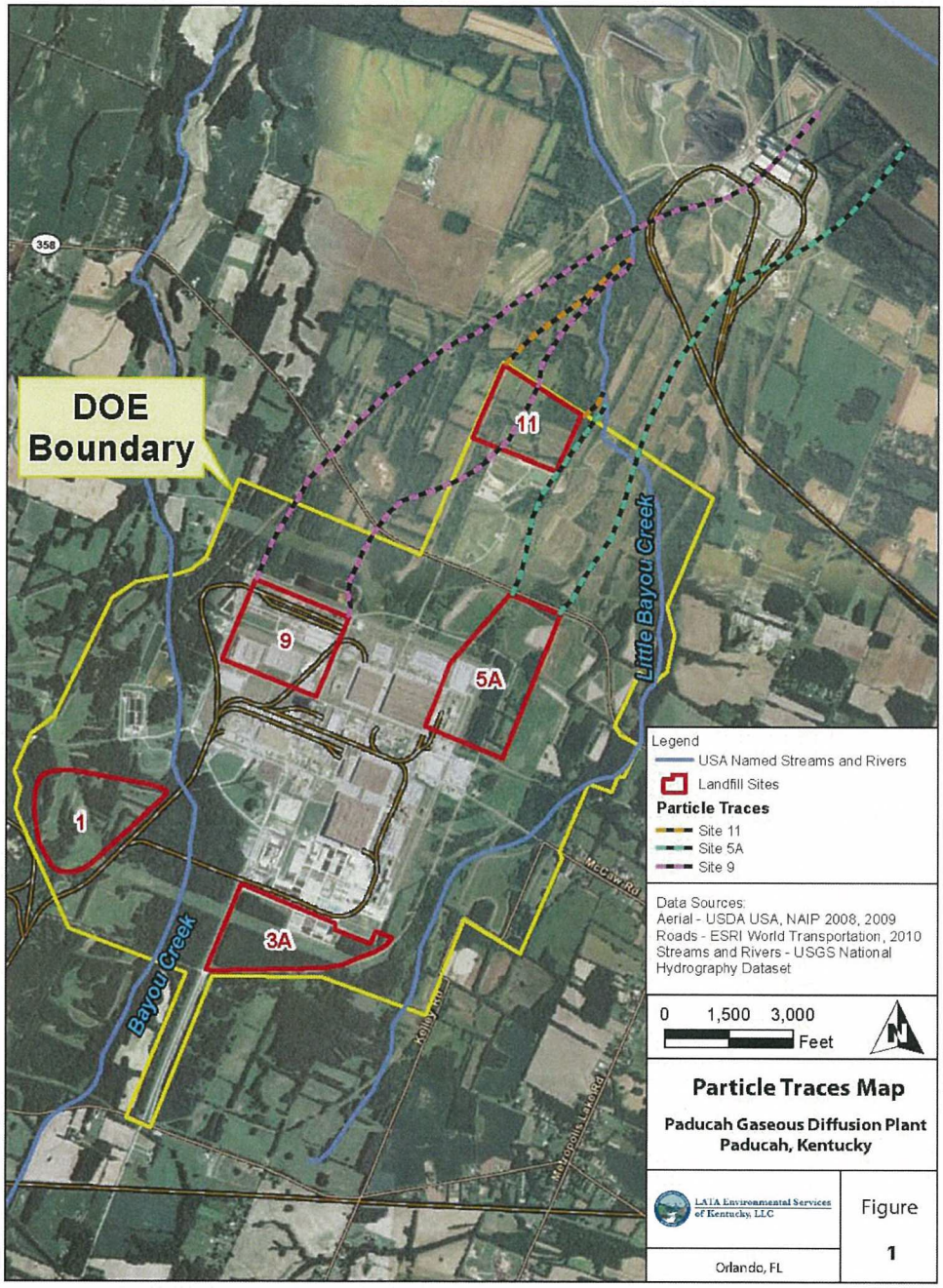

Figure C-4. Example Flow Paths from the Sitewide Groundwater Model

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release point to the exposure point of interest. The hydraulic conductivity, along the fastest flowpath of interest, also will be estimated. The maximum hydraulic conductivity along the flowpath of interest will be selected for use in the AT123D model to ensure the transit time is not underestimated.

C.3.2.1.4 AT123D Model

The AT123D model will be used to model the lateral transport of contaminants in the groundwater to the exposure points (Yeh et al. 1987). AT123D is based on an analytical solution for transient one-, two-, or three-dimensional transport of a dissolved chemical or radionuclide in a homogeneous aquifer with uniform, stationary regional flow. The program assumes a stationary flow field parallel to the X-axis and allows for retardation (based on reversible instantaneous linear equilibrium sorption isotherm) and first-order decay. Longitudinal, horizontal, and vertical transverse dispersion can be input independently. The program calculates the concentration distribution in space and time in mg/L, parts per million, or pCi/L. AT123D models transport caused by a single source starting release of solute at time T = 0. It can accommodate various source configurations and boundary conditions. It also simulates a point source; a line source parallel to the X-, Y-, or Z-axis; an area (patch) source in the X-Y, X-Z, or Y-Z direction; and a volume source. The source release may be instantaneous, continuous, or finite step duration (up to 15 steps) and is assumed to be distributed equally over the source area.

Predicted contaminant concentrations for each organic indicator chemical in groundwater developed by AT123D will be used to develop the DAFs for use in estimating the remaining chemical groundwater concentrations within each surrogate group. As discussed previously, metals and radionuclides will be assessed individually and not as surrogate groups.

AT123D cannot model decay chains associated with radionuclide COPCs or chemical transformations from one species to another. Three methods are proposed for the assessment of these issues. The DUSTMS computer model could be used to evaluate the decay and transformation reaction uncertainty in the aquifer in a 1-D type analysis. Secondly, the groundwater concentration results from the AT123D model, for each contaminant run individually in AT123D, can be evaluated against decay chain and chemical transformation calculations conducted in DUSTMS to determine the uncertainty for these reactions. Third, an evaluation can be performed by comparing transit times to half-lives. If the half-lives are longer than the transit times to the points of exposure, then progeny formation during lateral migration in the aquifers likely is not a concern.

C.3.2.1.5 Dilution Attenuation Factors

To determine the transport times to and concentrations at the point of exposure for contaminants within each of the surrogate groups, the DAF for the indicator chemicals assigned to each surrogate group will be determined. The DAFs will then be applied to the other chemical's concentration within the surrogate group in the disposal unit to provide the resulting groundwater concentration at the receptor location of interest.

The determination of the DAF for an indicator chemical is represented graphically in Figure C.5. The DAF for the source-to-water table path is

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$$DAF_{1,indicator} = \frac{\left(C_{s,indicator} / K_{d,indicator}\right)}{C_{L,indicator}}$$

where

DAF_1 = Dilution attenuation factor for the source-to-water table path (unitless)

C_s = Contaminant concentration in the disposal unit (mg/kg or pCi/g)
K_d = Contaminant distribution coefficient (L/kg)
C_L = Contaminant leachate concentration at the water table (mg/L or pCi/L)

The indicator chemical DAF for the water table-to-exposure point of interest is

$$DAF_{2,indicator} = \frac{C_{L,indicator}}{C_{w,indicator}}$$

where
DAF_2 = Dilution attenuation factor for the water table-to-exposure point path (unitless)
C_w = Contaminant concentration in groundwater at the exposure point of interest (mg/L or pCi/L)

Therefore, the DAF for the source-to-exposure point path for the indicator chemical is defined as

$$DAF = DAF_{1,indicator} \; x \; DAF_{2,indicator} = \frac{\left(C_{s,indicator} / K_{d,indicator}\right)}{C_{w,indicator}}$$

where

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DAF = Dilution attenuation factor for the source-to-exposure point path (unitless)

The DAF then will be used to calculate the groundwater concentration for each chemical in the surrogate group by

$$C_{w,consituent} = \frac{\left(C_{s,consituent} / K_{d,consituent}\right)}{DAF_{indicator}}$$

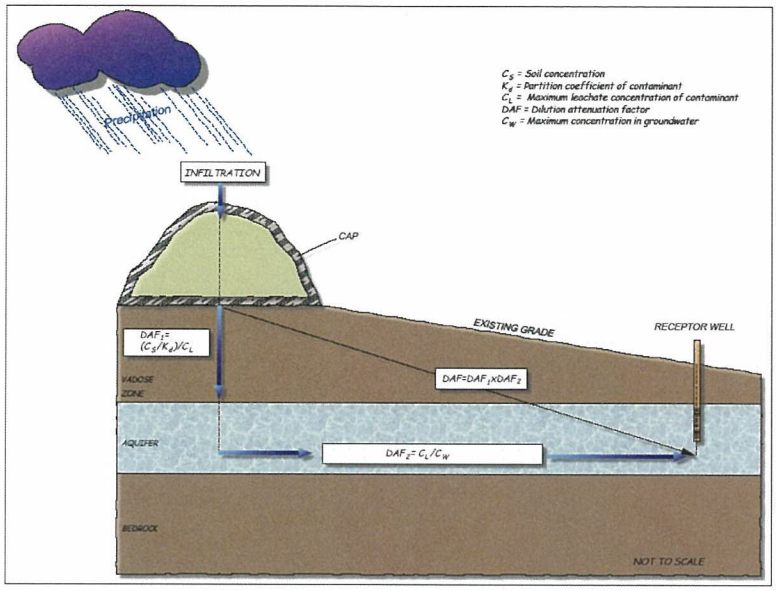

Figure C.5. Determination of the Dilution Attenuation Factor

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C.3.3 RISK AND DOSE ASSESSMENT

The concentrations of COCs in groundwater at the exposure points will be used to calculate the cancer risk and non-cancer hazard [i.e., hazard index (HI)] for the chemicals, metals, and radionuclides resulting from exposure to the groundwater. The Risk Methods Document will be the basis of these calculations.

The analyses for exposure to constituents potentially released to groundwater will utilize the following risk and hazard target values at three points of exposure [i.e., at the edge of the waste unit, at the waste disposal facility (WDF) boundary, and at the DOE property line] and two time periods (i.e., 0 to 1,600 years and beyond 1,600 years). The edge of the waste unit is at the toe of containment berm that forms the WDF, which from a practical perspective is considered the edge of the waste mass. The WDF boundary is the site on which the WDF and associated infrastructure is located. For the purposes of the PWAC, this boundary is considered to 100 m from the edge of waste. Note, the final location will depend on site geometry and site layout and will be at least 100 m from the edge of waste (DOE Order 435.1). These points are depicted conceptually in Figure C.6.

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(i) *At the edge of the waste unit (both time periods)*:

(1) The target concentrations will be the chemical-specific primary maximum contaminant levels (MCLs), if this value is greater than the constituent's background concentration. If the background concentration for the constituent is greater than the MCL, then the background concentration will be selected.

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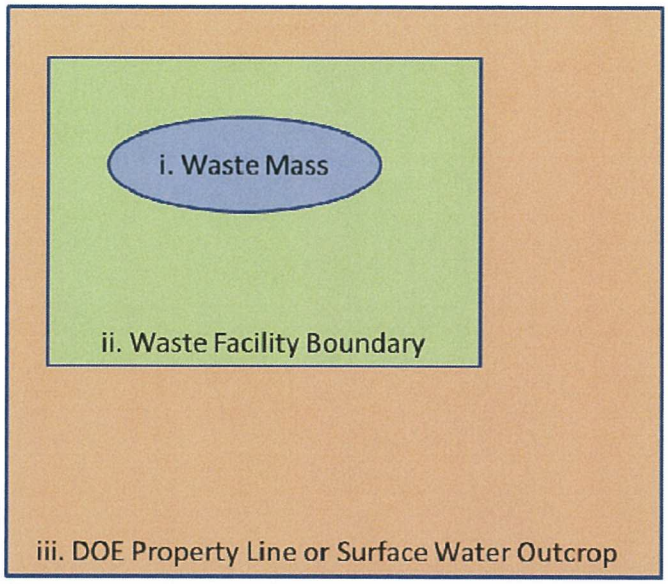

Figure C-6. Locations Where Target Values Need To Be Established

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(2) If chemical-specific primary MCLs are not available, then chemical-specific risk- and hazard-based targets based on residential use of groundwater will be used to derive the constituent's target concentration in groundwater. The chemical-specific risk-based target will be 1E-06 and the chemical-specific hazard-based target will be 1. If both a risk-based concentration and hazard-based concentration can be derived for a constituent, then the lower of the two concentrations will be selected. If, however, the selected value is less than the background concentration, then the background concentration will be used.

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(ii) *At the boundary of the WDF*:

(1) 0 to 1,600 years:

(a) The risk-based target will be a cumulative excess lifetime cancer risk (ELCR) of 1E-04.
(b) The hazard-based target will be a cumulative HI of 1.

(2) Beyond 1,600 years:

(a) The risk-based target will be a cumulative ELCR of 1E-04.
(b) The hazard-based target will be a cumulative HI of 3.

(Consistent with COPC selection in the Risk Methods Document, the calculation of cumulative ELCR and cumulative HI at the boundary of the WDF will exclude any constituents that use the constituent's background concentration as the chemical-specific target at the edge of the waste unit.)

(iii) *At the DOE property line or nearer surface water outcrop:*

(1) 0 to 1,600 years:

(a) The risk-based target will be a cumulative ELCR of 1E-06.
(b) The hazard-based target will be a cumulative HI of 1.

(2) Beyond 1,600 years:

(a) The risk-based target will be a cumulative ELCR of 1E-05.
(b) The hazard-based target will be a cumulative HI of 3.

(Consistent with COPC selection in the Risk Methods Document, the calculation of cumulative ELCR and cumulative HI at the DOE property line will exclude any constituents that use the constituent's background concentration as the chemical-specific target at the edge of the waste unit. Additionally, to target the more important risk and hazard contributors, only constituents with a chemical-specific contribution to cumulative ELCR and/or HI at the boundary of the WDF greater than 1E-07 or 0.05, respectively, will be included in the calculation of cumulative ELCR and HI at the DOE property line.)

The increased cumulative ELCR and/or HI targets of 1E-05 and 3, respectively, are used beyond 1,600 years at the boundary of the WDF and DOE property line to address the uncertainties in exposure (e.g., receptor location relative to ground water flow) and constituent release and migration.

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The target concentrations at the edge of the waste unit are used to establish an initial PWAC. This PWAC is then used to calculate the contaminant concentrations in water at the boundary of the WDF. If these calculated contaminant concentrations exceed the risk-based and hazard-based targets established for the boundary of the WDF, then the initial PWAC is adjusted until these target risks are met. This iterative approach is then repeated for the property boundary.

The equations used to calculate the chemical-specific risk and non-cancer hazard estimates are as follows:

$$Chemical - Specific\ Risk\ Value = \frac{C_{w\,Chemical}\ x\ Target\ Risk\ Value}{C_{w\,No\ Action}}$$

where

Chemical-Specific Risk Value	=	cancer risk and non-cancer hazard from groundwater exposure
$C_{w\ Chemical}$	=	chemical concentration in groundwater (mg/L or pCi/L)
Target Risk Value	=	target cancer risk, hazard level, or MCL to maintain
$C_{w\ No\ Action}$	=	cancer risk/hazard no-action screening value or MCL as appropriate (mg/L or pCi/L)

C.3.4 PRELIMINARY WAC DEVELOPMENT

A PWAC will be developed for an on-site waste disposal facility. The PWAC is an estimate of the average contaminant concentrations allowed in the total waste volume. Individual loads could be higher or lower. Additionally, the PWAC is the total contaminant amount, such as maximum curies permitted in the cell or the single contaminant mass limit (in grams or kilograms) per COPC.

The PWAC will be useful in evaluating the viability of an on-site disposal facility only. If selected as the preferred alternative, the PWAC values for an on-site disposal facility would require modification after the design for the disposal facility is finalized. As used here, the PWAC for a contaminant is defined as

the maximum allowable concentration of a contaminant in disposed material that will not result in (1) releases to receiving media that exceed regulatory or risk-based criteria or (2) direct exposure risks or doses that exceed acceptable cancer risk-based and non-cancer hazard-based levels. This definition is consistent with, but goes beyond that presented in Attachment 2 of DOE Order 435.1 (*Radioactive Waste Management Manual*). In that attachment, PWAC are defined as technical and administrative requirements that a waste must meet in order for it to be accepted at a storage, treatment, or disposal facility. Generally, PWAC as defined here are dependent on five primary characteristics. These are the following:

- Facility design, including liner and cover, integrity, and institutional controls;
- Mobility of contaminants from or retention of contaminants within a waste (e.g., soil, stabilized soils, concrete, metals, etc.);
- Exposure point characteristics, including type of receptor (e.g., human or ecological), location, and exposure media;
- Target cancer risk, target hazard level, MCLs, and period of compliance; or
- Potential engineered barrier failure.

The method used to calculate the PWAC is presented in the following equations.

$$\frac{PWAC}{C_{s\ \ chemical}} = \frac{C_{w\ \ target}}{C_{w\ \ chemical}}$$

or

$$PWAC = \frac{C_{w\ \ target}\ x\ C_{s\ \ chemical}}{C_{w\ \ chemical}}$$

where

PWAC = preliminary WAC (mg/kg or pCi/g)
$C_{w\ target}$ = target concentrations for groundwater (i.e., back calculation value)
$C_{s\ chemical}$ = constituent concentration in source used in the modeling (mg/kg or pCi/g)
$C_{w\ chemical}$ = constituent concentration in groundwater from modeling results (mg/L or pCi/L)

The PWAC for the total mass or activity allowed in an on-site waste disposal facility will be calculated from the waste volume of the WDF and the PWAC concentration values as follows:

$$PWAC\ (kg\ or\ Ci) = PWAC\ (mg/kg\ or\ pCi/g) \times \rho_b \times V \times CF$$

where

ρ_b = bulk density (3.1 g/cm^3)
V = facility volume (4.1mcy or 3.13 x 10^{12} cm^3)
CF = conversion factors as necessary for unit conversion

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The PWAC methodology, as presented in this work plan, is based on the assumption that the entire landfill would be filled with a single waste, assumed to be soil with a single contaminant. The contaminant is assumed to be immediately available for transport, thus maximizing release rates (i.e., many waste types will be solid materials for which associated contaminants would not be readily available for release). The cumulative risk from all contaminants will be evaluated during development of a final WAC, if the on-site disposal is chosen as the preferred remedial option. The PWAC will be calculated using the peak concentration between 0 and 1,600 years and 1,600 and 10,000 years. In the event the peak concentration in groundwater of a constituent has not been reached at 1,600 years, the model will be run until the peak concentration is reached, or until 10,000 years. The model will not be run beyond 10,000 years.

C.3.5 UNCERTAINTY ANALYSIS

The proposed modeling for an on-site waste disposal facility will consist of evaluating the COCs in a "forward" calculation based on unit inventory concentrations. The forward calculation provides the predicted groundwater contaminant concentrations released from the waste disposal facility into the aquifer at PGDP. These concentrations then are used in a "backward" calculation to determine the PWAC for the waste disposal facility. The term "backward" calculation is used in the sense that the analyst is using the forward calculation results to back calculate an acceptable waste concentration and total mass (or activity) of a given contaminant.

The use of this methodology does not provide a means to determine if the solubility limits for COCs may be reached in the disposal unit pore water; therefore, the PWAC values will be compared to solubility limit concentrations in terms of the disposal pore water concentrations. If the PWAC values result in concentrations exceeding the solubility limits, then the disposal mass of the COPC is no longer limited.

Another issue of potential importance to a disposal facility environment pertains to the facilitated transport of PCBs through cosolvent effects (EPA 1989). A modeling study was completed for the C-746-U Landfill at PGDP to evaluate the cosolvency impact at this landfill (BJC 2003). A similar analysis may need to be conducted for the waste disposal unit. The evaluation should be based on expected disposal concentrations of PCBs and potential solvents; therefore, the cosolvent issue will be evaluated if the On-Site Disposal Alternative is selected and the final WAC is to be developed.

An additional issue relates to facilitated transport possibly caused by the inclusion of nonhazardous solid waste/organic materials in the waste mix disposed of in the waste disposal facility. The phenomenon of such facilitated transport will be considered in the development of PWAC. Also, because some radionuclide contaminants (and decay products from ingrowth) will not reach their peak concentration prior to 10,000 years, an uncertainty analysis examining ingrowth and risk beyond 10,000 years will be completed for uranium-238 (U-238) (parent compound) and thorium-230 (Th-230) (progeny). This analysis will use a forward run of the transport model for the gradual failure scenario to the peak concentrations for U-238 and Th-230 and the selected initial PWAC for U-238 and Th-230 as the source term concentration. Due to modeling software constraints, the time step used in this analysis will be larger than that used for development of the PWAC. Another consideration in the development of the PWAC involves the potential impacts to inadvertent intruders. The preliminary disposal facility design provides 16 ft of cover over the waste. This cover thickness should prevent an inadvertent intruder from reaching the waste through excavation of a typical basement. Nonetheless, the inadvertent intruder scenario will be considered qualitatively in the development of the PWAC as an uncertainty.

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Deleted: Also, it is acknowledged that some radionuclide contaminants (and possibly their daughter products) will not reach their peak concentrations at the point of compliance during the 10,000-year period of interest; however, simulations will be performed only for a maximum 10,000 years in accordance with the performance evaluation period.

The fate and transport modeling will have associated uncertainties due to abstraction of the physical and chemical processes of the real system into a model system. In addition, uncertainties in the waste inventories, model parameterization, and conceptual model uncertainties will need to be addressed.

Several iterations of the modeling will be necessary to evaluate and quantify the sensitivity and uncertainty in the results. In general, the sensitivity and uncertainty will be addressed by assessing parameter variations in the models. This may include such parameters as the following:

- Clay barrier degradation
- Geomembrane service life
- Geomembrane rate of degradation
- Sorption coefficients variations
- Solubility variations
- Hydraulic conductivity variations
- Off-centerline groundwater concentration evaluations
- Ingrowth of radionuclide progeny
- Degradation of organic COPCs
- Ingrowth of organic COPCs
- Potential for facilitated transport

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ATTACHMENT C1

PROPOSED MODELING PARAMETERS

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Table C1.1. Proposed Landfill/Soil Profile - Post-Closure Period (30 to 200 years)

			HELP Parameters/Characteristics											
Layer #	Material Type	Layer Type	Layer Thickness (inches)	Soil Texture Type	Total Porosity (vol/vol)	Field Capacity (vol/vol)	Wilting Point (vol/vol)	Saturated Hydraulic Conductivity (cm/sec)	Initial Moisture Content	Drainage Length (ft)	Drain Slope (%)	FML Pinhole Density	FML Installation Defects	FML Placement Quality
1	Native Soil (vegetative)	1	18	12	0.45 *	0.342	0.21	2.32E-06 *	0.2347 ***					
2	Native Soil	1	42	12	0.45 *	0.342	0.21	5.00E-07 *	0.3420 ***					
3	Filter sand	1	12	3	0.457	0.083	0.033	3.10E-03	0.0843 ***					
4	Geotextile	1	0.0625	20	0.85	0.01	0.005	1.00E+01	0.0501 ***					
5	Cobble/gravel/ sand	1	36	21	0.397	0.032	0.013	3.00E-01	0.0321 ***					
6	Drainage sand	2	12	1	0.417	0.045	0.018	1.00E-02	0.0452 ***	380	2			
7	Geotextile	2	0.125	20	0.85	0.01	0.005	1.00E+01	0.0100 ***	380	2			
8	FML (HDPE)	4	0.04	35				2.00E-13	0.0000 ***			0	0.5	2 (Excellent)
9	Clay barrier/ contour layer	3	36	16	0.427	0.418	0.367	1.00E-07 *	0.4270 ***					
10	Waste	1	1020	22	0.419	0.307	0.18	1.90E-05	0.3588					
11	Contour layer	1	12	26	0.445	0.393	0.277	1.90E-06	0.4112					
12	Geotextile	1	0.125	20	0.85	0.01	0.005	1.00E+01	0.1103					
13	Drainage sand	2	12	1	0.417	0.045	0.018	1.00E-02	0.1158	364	5			
14	Geotextile	2	0.125	20	0.85	0.01	0.005	1.00E+01	0.0766	364	5			
15	FML (HDPE)	4	0.06	35				2.00E-13	0.0000			0	0.5	2 (Excellent)
16	Bonded Geotextile	2	0.236	34	0.85	0.01	0.005	3.30E+01	0.0100	364	5			
17	FML (HDPE)	4	0.06	35				2.00E-13	0.0000			0	0.5	2 (Excellent)
18	Clay barrier **	3	36	16	0.427	0.418	0.367	1.00E-07 *	0.4270					
19	Geo-buffer layer	1	120	12	0.45 *	0.342	0.21	5.00E-07 *	0.3420					
20	Existing Silty Clay	1	264 (Site 11) 240 (Site 3A)	26	0.400 * (Site 3A) 0.445 (Site 11)	0.393	0.277	3.67E-06 * (Site 3A) 3.80E-07 * (Site 11)	0.3930					

Notes:

- FML = flexible membrane lining.
- FML Pinhole Density in units of number of holes per acre. Diameter of defect is equal to geomembrane thickness.
- FML installation defects are in units of defects per acre. A defect is estimated using an area of 1 cm^2.
- The cover system design curve number is 87.6 (slope 2%, slope length 380 ft, fair stand of grass (3), with soil texture type 12).
- Soil layering and properties are based upon the June 2010 PGDP Public Fact Sheet, Waste Disposal Options.
- HDPE = high density polyethylene.
- No recirculation of leachate is assumed.

* - Signifies value is not the default value associated with the specified HELP Soil Texture Type.

** - Signifies location where HELP Percolation/Leakage rate is used as DUST-MS water velocity.

*** - Initial soil moisture content was calculated by HELP (Schroeder et al. 1994). Remaining moisture contents were assigned using the final moisture content of the Operational Period HELP scenario.

- Moisture content values are in units of pore water volume per total volume soil and void space.
- "Native Soil", "Geo-buffer layer", and "Existing Silty Clay" soil porosities and hydraulic conductivities are from Site 3A Seismic Investigation Report, Assessment of the Adequacy of Data Report, and GB-02D lithologic log.

Table C1.2. Proposed Landfill Design Profile and Soil Characteristics - Long Term Monitoring Period (600+ years)

Layer #	Material Type	HELP Layer Type	Layer Thickness (inches)	HELP Soil Texture Type	Total Porosity (vol/vol)	Field Capacity (vol/vol)	Wilting Point (vol/vol)	Saturated Hydraulic Conductivity (cm/sec)	Initial Moisture Content (vol. water/total vol.)
1	Native Soil (vegetative)	1	18	12	0.45 *	0.342	0.21	2.32E-06 *	0.3071
2	Native Soil	1	42	12	0.45 *	0.342	0.21	5.00E-07 *	0.3491
3	Filter sand	1	12	3	0.457	0.083	0.033	3.10E-03	0.1118
4	Cobble/gravel/sand	1	36	21	0.397	0.032	0.013	3.00E-01	0.0364
5	Drainage sand	1	12	1	0.417	0.045	0.018	1.00E-02	0.0547
6	Clay barrier	1	36	16	0.427	0.418	0.367	1.00E-06*	0.4270
7	Waste	1	1020	22	0.419	0.307	0.18	1.90E-05	0.3070
8	Silty clay	1	12	26	0.445	0.393	0.277	1.90E-06	0.3930
9	Drainage sand	1	12	1	0.417	0.045	0.018	1.00E-02	0.0450
10	Clay barrier	1	36	16	0.427	0.418	0.367	1.00E-06 *	0.4270
11	Geo-buffer layer **	1	120	12	0.45 *	0.342	0.21	5.00E-07 *	0.3420
12	Existing Silty Clay	1	264 (Site 11) 240 (Site 3A)	26	0.400 * (Site 3A) 0.445 (Site 11)	0.393	0.277	3.67E-06* (Site 3A) 3.80E-07* (Site 11)	0.3930

Notes:

* - Signifies value is not the default value associated with the specified HELP Soil Texture Type.

** - Signifies location where HELP Percolation/Leakage rate is used as DUST-MS water velocity.

- Moisture content values are in units of pore water volume per total volume soil and void space.

- The cover system design curve number is 87.6 (slope 2%, slope length 380 ft, fair stand of grass (3), with soil texture type 12).

- "Native Soil", "Geo-buffer layer", and "Existing Silty Clay" soil porosities and hydraulic conductivities are from Site 3A Seismic Investigation Report, Assessment of the Adequacy of Data Report, and GB-02D lithologic log.

Table C1.3. Chemical Specific Parameters

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Vinyl Chloride (VC) - Atomic Weight 62.5 g/mol								
Half Life (years)	7.90E+00	Howard et al., 1991, Page 138	--[1]	--	7.90E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	62.5	--	62.5	--	62.5	EPA (1996)	--	--
Solubility Limit (gm/cc)	2.76E-03	EPA (1996), Table 36, Pages 134 to 136	2.76E-03	EPA (1996), Table 36, Pages 134 to 136.	2.76E-03	EPA (1996), Table 36, Pages 134 to 136	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd[4] (cc/gm)	1.49E-02	Koc[5] referenced from EPA (1996), Table 39, Pages 143 to 145. foc[6] referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (1.86E+01 l/kg) by foc (8.01E-4 unitless).	1.49E-02	Sheppard and Thibault (1990) (Not Verified)	1.49E-02	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	6.51E-03	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (1.86E+01 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	1.23E-06	EPA (1996), Table 37, Pages 137 to 139	1.23E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.23E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
Trichloroethylene (TCE) - Atomic Weight 131.4 g/mol								
Half Life (years)	4.50E+00	Howard et al., 1991, Page 190	2.50E+01	--	4.50E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	131.4	--	131.4	--	131	EPA (1996)	--	--
Solubility Limit (gm/cc)	1.10E-03	EPA (1996), Table 36, Pages 134 to 136	1.10E-03	EPA (1996), Table 36, Pages 134 to 136	1.10E-03	EPA (1996), Table 36, Pages 134 to 136	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	7.55E-02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (9.43E+01 l/kg) by foc (8.01E-4 unitless).	7.52E-02	Sheppard and Thibault (1990) (Not Verified)	7.52E-02	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	3.30E-02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (9.43E+01 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	9.10E-06	EPA (1996), Table 37, Pages 137 to 139	9.10E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	9.10E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
2-Butanone (Methyl Ethyl Ketone) - Atomic Weight 72.1 g/mol								
Half Life (years)	3.80E-02	Howard et al., 1991, Page 186	--	--	1.97E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	72.1	--	72.1	--	72.1	EPA (1996)	--	--
Solubility Limit (gm/cc)	7.40E-02	EPA (1996), Table 36, Pages 134 to 136	2.75E-01	EPA (1996), number not found in table	2.75E-01	EPA (1996), number not found in table	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	5.54E-03	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (6.92E+00 l/kg) by foc (8.01E-4 unitless).	9.20E-04	Sheppard and Thibault (1990) (Not Verified)	9.20E-04	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	2.42E-03	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (6.92E+00 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	9.30E-06	EPA (1996), Table 37, Pages 137 to 139	1.02E-05	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.02E-05	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
Chlorobenzene - Atomic Weight 112.6 g/mol								
Half Life (years)	1.64E+00	Howard et al., 1991, Page 412	--	--	1.64E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	112.6		112.6		112.6	EPA (1996)	--	--
Solubility Limit (gm/cc)	4.72E-04	EPA (1996), Table 36, Pages 134 to 136	4.72E-04	EPA (1996), Table 36, Pages 134 to 136	4.72E-04	EPA (1996), Table 36, Pages 134 to 136	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	1.79E-01	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (2.24E+02 l/kg) by foc (8.01E-4 unitless).	1.79E-01	Sheppard and Thibault (1990) (Not Verified)	1.79E-01	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	7.84E-02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (2.24E+02 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	8.70E-06	EPA (1996), Table 37, Pages 137 to 139	8.70E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	8.70E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Benzene - Atomic Weight 78.1 g/mol								
Half Life (years)	2.00E+00	Howard et al., 1991, Page 111	--	--	1.97E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	78.1	--	78.1	--	78.1	EPA (1996)	--	--
Solubility Limit (gm/cc)	1.75E-03	EPA (1996), Table 36, Pages 134 to 136	1.75E-03	EPA (1996), Table 36, Pages 134 to 136	1.75E-03	EPA (1996), Table 36, Pages 134 to 136	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	4.94E-02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (6.17E+01 l/kg) by foc (8.01E-4 unitless).	4.96E-02	Sheppard and Thibault (1990) (Not Verified)	4.96E-02	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	2.16E-02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (6.17E+01 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	9.80E-06	EPA (1996), Table 37, Pages 137 to 139	9.80E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	9.80E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
2-Methylphenol (o-Cresol) - Atomic Weight 108 g/mol								
Half Life (years)	7.70E-02	Howard et al., 1991, Page 294	--	--	1.97E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	108	--	108	--	108	EPA (1996)	--	--
Solubility Limit (gm/cc)	2.60E-02	EPA (1996), Table 36, Pages 134 to 136	2.00E-02	EPA (1996), Table 36, Pages 134 to 136	2.00E-02	EPA (1996), Table 36, Pages 134 to 136	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	7.31E-02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (9.12E+01 l/kg) by foc (8.01E-4 unitless).	1.60E-02	Sheppard and Thibault (1990) (Not Verified)	1.60E-02	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	3.19E-02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (9.12E+01 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	8.30E-06	EPA (1996), Table 37, Pages 137 to 139	8.30E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	8.30E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Pentachlorophenol - Atomic Weight 266.3 g/mol								
Half Life (years)	4.20E+00	Howard et al., 1991, Page 242	--	--	4.20E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	266.3		266.3		266.3	EPA (1996)	--	--
Solubility Limit (gm/cc)	1.95E-03	EPA (1996), Table 36, Pages 134 to 136	1.95E-03	EPA (1996), Table 36, Pages 134 to 136	1.95E-03	EPA (1996), Table 36, Pages 134 to 136	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	4.74E-01	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (5.92E+02 l/kg) by foc (8.01E-4 unitless).	4.74E-01	Sheppard and Thibault (1990) (Not Verified)	4.74E-01	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	2.07E-01	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (5.92E+02 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	6.10E-06	EPA (1996), Table 37, Pages 137 to 139	6.10E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	6.10E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
Benzo(a)pyrene - Atomic Weight 252.3 g/mol								
Half Life (years)	5.80E+00	Howard et al., 1991, Page 12	--	--	5.80E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	252.3		252.3		252.3	EPA (1996)	--	--
Solubility Limit (gm/cc)	1.62E-09	EPA (1996), Table 36, Pages 134 to 136	1.62E-03	EPA (1996), appears that the units are not correct	1.62E-03	EPA (1996), appears that the units are not correct	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	7.76E+02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (9.69E+05 l/kg) by foc (8.01E-4 unitless).	7.75E+02	Sheppard and Thibault (1990) (Not Verified)	7.75E+02	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	3.39E+02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (9.69E+05 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	9.00E-06	EPA (1996), Table 37, Pages 137 to 139	9.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	9.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
PCB (Aroclor 1254) - Atomic Weight 375.7 g/mol								
Half Life (years)	1.00E+02	U-Landfill Report, (DOE 2003)	--	--	1.00E+02	Howard et al., 1991	--	--
Atomic Weight (g/mol)	375.7		375.7		375.7	EPA (1996)	--	--
Solubility Limit (gm/cc)	7.00E-07	EPA (2004), Page A-295	8.00E-08	EPA (1996)	8.00E-08	EPA (1996)	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	2.48E+02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (3.09E+05 l/kg) by foc (8.01E-4 unitless).	2.47E+02	Sheppard and Thibault (1990) (Not Verified)	2.47E+02	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	1.08E+02	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (3.09E+05 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	U-Landfill Report (DOE 2003)	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
gamma-Chlordane (Chlordane) - Atomic Weight 409.8 g/mol								
Half Life (years)	7.60E+00	Howard et al., 1991, Page 48	--	--	7.60E+00	Howard et al., 1991	--	--
Atomic Weight (g/mol)	409.8		409.8		409.8	EPA (1996)		
Solubility Limit (gm/cc)	5.60E-08	EPA (1996), Table 36, Pages 134 to 136	5.60E-08	EPA (1996), Table 36, Pages 134 to 136	5.60E-08	EPA (1996), Table 36, Pages 134 to 136	--	--
Unsaturated Soils, Waste, and Saturated Vertical Flow Kd (cc/gm)	4.11E+01	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.3 "Likeliest" value. Kd calculated by multiplying Koc (5.13E+04 l/kg) by foc (8.01E-4 unitless).	4.71E+01	Sheppard and Thibault (1990) (Not Verified)	4.71E+01	Sheppard and Thibault (1990) (Not Verified)	--	--
Saturated Horizontal Flow Kd (cc/gm)	1.80E+01	Koc referenced from EPA (1996), Table 39, Pages 143 to 145. foc referenced from DOE (2007), Table F.2.8 "Likeliest" value. Kd calculated by multiplying Koc (5.13E+04 l/kg) by foc (3.5E-4 unitless).					--	--
Diffusion Coefficient (cm^2/sec)	4.37E-06	EPA (1996), Table 37, Pages 137 to 139	4.37E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	4.37E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Antimony - Atomic Weight 121.7 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	121.7		121.7		--	--	--	--
Solubility Limit (gm/cc)	1.70E-01	EPA (2004), Page A-25.	1.00E+01	EPA (1996)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	45 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	45 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	--	--
	250 (clay)		250 (clay)		--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--
Arsenic - Atomic Weight 74.9 g/mol								
Half Life (years)	--	--	--	--	1.00E+05	Disposal Unit Source Term (DUST) default library	--	--
Atomic Weight (g/mol)	74.9		74.9		75	EPA (1996)	--	--
Solubility Limit (gm/cc)	1.20E-01	EPA (2004), Page A-29.	1.00E+01	EPA (1996)	1.00E+01	EPA (1996)	--	--
Kd (cc/gm)	2.90E+01	EPA (1996), Table 46, Page 158.	200 (sand)	Sheppard and Thibault (1990) (Not Verified)	200 (sand)	Sheppard and Thibault (1990) (Not Verified)	--	--
			200 (clay)		200 (clay)		--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	U-Landfill Report (DOE 2003)	1.00E-06	No reference given, from DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
Barium - Atomic Weight 137.3 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	137.3		137.3		--	--	--	--
Solubility Limit (gm/cc)	2.80E-03	EPA (2004), Page A-33.	1.00E+01	EPA (1996)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	4.10E+01	EPA (1996), Table 46, Page 158.	5 (sand)	Sheppard and Thibault (1990) (Not Verified)	--	--	--	--
			50 (clay)		--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Beryllium - Atomic Weight 9.01 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	9.01		9.01		--	--	--	--
Solubility Limit (gm/cc)	8.40E-02	EPA (2004), Page A-49.	1.00E+01	EPA (1996) (Not Verified)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	250 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	250 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	--	--
	1,300 (clay)		1,300 (clay)		--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--
Cadmium - Atomic Weight 112.4 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	112.4		112.4		--	--	--	--
Solubility Limit (gm/cc)	1.70E-03	EPA (2004), Page A-59.	1.00E+01	EPA (1996) (Not Verified)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	80 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	80 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	--	--
	560 (clay)		560 (clay)		--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--
Chromium - Atomic Weight 51.9 g/mol								
Half Life (years)	--	--	--	--	1.00E+05	Disposal Unit Source Term (DUST) default library	--	--
Atomic Weight (g/mol)	51.9		51.9		52	EPA (1996)	--	--
Solubility Limit (gm/cc)	6.00E-01	EPA (2004), Page A-83.	1.00E+01	EPA (1996) (Not Verified)	1.00E+01	EPA (1996) (Not Verified)	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal	3.21E+01	DOE (2002a), Min: 17.4 Max: 56.8 Mean: 32.1	19 (sand)	Sheppard and Thibault (1990), different than what was seen in the table (70 sand, 1500 clay).	19 (sand)	Sheppard and Thibault (1990), different than what was seen in the table.	--	--
			30 (clay)		30 (clay)		--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Copper - Atomic Weight 63.6 g/mol								
Half Life (years)	--	--	--	--	1.00E+05	Disposal Unit Source Term (DUST) default library	--	--
Atomic Weight (g/mol)	63.6		63.6		63.5	EPA (1996)	--	--
Solubility Limit (gm/cc)	5.70E-04	EPA (2004), Page A-97.	1.00E+01	EPA (1996) (Not Verified)	1.00E+01	EPA (1996) (Not Verified)	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	3.1	Dragun (1988), (Range 1.4 to 333 ml/g)	35 (sand) 35 (clay)	Sheppard and Thibault (1990), not found in document	35 (sand) 35 (clay)	Sheppard and Thibault (1990), not found in document	-- --	-- --
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
Lead - Atomic Weight 207.2 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	207.2	--	207.2	--	--	--	--	--
Solubility Limit (gm/cc)	8.70E-04	EPA (2004), Page A-223.	1.00E+01	EPA (1996)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	270 (sand and all other materials) 550 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	270 (sand) 550 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	-- --	-- --	-- --	-- --
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--
Manganese - Atomic Weight 54.9 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	54.9		54.9		--	--	--	--
Solubility Limit (gm/cc)	1.10E-03	EPA (2004), Page A-231.	1.00E+01	EPA (1996)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	50 (sand and all other materials) 180 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	50 (sand) 180 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	-- --	-- --	-- --	-- --
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Mercury - Atomic Weight 200.6 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	200.6		200.6		--	--	--	--
Solubility Limit (gm/cc)	4.50E-04	EPA (2004), Page A-235.	1.00E+01	EPA (1996) (Not Verified)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	5.20E+01	EPA (1996), Table 46, Page 158.	10 (sand) 100 (clay)	Sheppard and Thibault (1990), not found in document	--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--
Nickel - Atomic Weight 58.7 g/mol								
Half Life (years)	--	--	--	--	1.00E+05	Disposal Unit Source Term (DUST) default library	--	--
Atomic Weight (g/mol)	58.7		58.7		58.7	EPA (1996)	--	--
Solubility Limit (gm/cc)	1.50E-03	EPA (2004), Page A-255.	1.00E+01	EPA (1996)	1.00E+01	EPA (1996)	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	1.079E+02	DOE (2002a), Min: 20.3 Max: 163 Mean: 107.9	400 (sand) 650 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	400 (sand) 650 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	-- --	-- --
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
Selenium - Atomic Weight 78.9 g/mol								
Half Life (years)	--	--	--	--	1.00E+05	Disposal Unit Source Term (DUST) default library	--	--
Atomic Weight (g/mol)	78.9		78.9		78.9	EPA (1996)	--	--
Solubility Limit (gm/cc)	2.60E+00	EPA (2004), Page A-309.	1.00E+01	EPA (1996) (Not Verified)	1.00E+01	EPA (1996) (Not Verified)	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	150 (sand and all other materials) 740 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	150 (sand) 740 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	150 (sand) 740 (clay)	Sheppard and Thibault (1990), Table 1, Page 472	-- --	-- --
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Silver - Atomic Weight 107.9 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	107.9		107.9		--	--	--	--
Solubility Limit (gm/cc)	2.50E-04	EPA (2004), Page A-311.	1.00E+01	EPA (1996) (Not Verified)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	90 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	90 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	--	--
	180 (clay)		180 (clay)		--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--
Thallium - Atomic Weight 204.4 g/mol								
Half Life (years)	--	--	--	--	1.00E+05	Disposal Unit Source Term (DUST) default library	--	--
Atomic Weight (g/mol)	204.4		204.4		204.4	EPA (1996)	--	--
Solubility Limit (gm/cc)	8.60E-03	EPA (2004), Page A-337.	1.00E+01	EPA (1996) (Not Verified)	1.00E+01	EPA (1996) (Not Verified)	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	7.10E+01	EPA (1996), Table 46, Page 158.	71 (sand)	Sheppard and Thibault (1990), not found in table	71 (sand)	Sheppard and Thibault (1990), not found in table	--	--
			1500 (clay)		1500 (clay)		--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--
Vanadium - Atomic Weight 50.9 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	50.9		50.9		--	--	--	--
Solubility Limit (gm/cc)	7.00E-04	EPA (2004), Page A-391.	1.00E+01	EPA (1996) (Not Verified)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	1.00E+03	EPA (1996), Table 46, Page 158.	100 (sand)	Sheppard and Thibault (1990), not found in table	--	--	--	--
			1000 (clay)		--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Zinc - Atomic Weight 65.4 g/mol								
Half Life (years)	--	--	--	--	--	--	--	--
Atomic Weight (g/mol)	65.4		65.4		--	--	--	--
Solubility Limit (gm/cc)	1.40E-03	EPA (2004), Page A-405.	1.00E+01	EPA (1996)	--	--	--	--
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	200 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	200 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	--	--
	2,400 (clay)		2,400 (clay)		--	--	--	--
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	--	--
Cs-137 - Atomic Weight 137 g/mol								
Half Life (years)	3.02E+01	Disposal Unit Source Term (DUST) default library	3.02E+01	--	--	--	None Specified	--
Atomic Weight (g/mol)	137		137		--	--	None Specified	
Solubility Limit (gm/cc)	3.40E-01	EPA (2004), Page A-71.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	280 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	280 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	280 (sand) 280 (waste) 1900 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	1,900 (clay)		1,900 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Tc-99 - Atomic Weight 99 g/mol								
Half Life (years)	2.13E+05	Disposal Unit Source Term (DUST) default library	2.13E+05	--	2.13E+05	Disposal Unit Source Term (DUST) default library	None Specified	--
Atomic Weight (g/mol)	99	--	99	--	99	EPA (1996)	None Specified	--
Solubility limit (gm/cc)	7.18E-03	Derived from geochemical database prepared by Lawrence Livermore National Laboratory and converted to PHREEQC format.	1.00E+01	EPA (1996) (Not Verified)	1.00E+01	EPA (1996) (Not Verified)	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	2.82E-01	DOE (2002a), Min: 5.27E-10 Max: 0.848 Mean: 0.282	0.2 (sand) 20 (clay)	Sheppard and Thibault (1990), not found table (sand - 0.1, clay - 1)	0.2 (sand) 1.0 (waste) 20 (clay)	Sheppard and Thibault (1990), not found table DOE 1997 and DOE (2002b)	0.2 (sand) 1.0 (waste) 20 (clay)	The distribution coefficients for Tc-99 are available in Table C.3.1. Chemical and physical properties of different classes of chemicals identified as COPCs for the C-746-U Landfill of DOE 2003b, page C3-301. Table 4.5 DUST model input parameters, page 4-12, has Kds for Tc-99. Table 4.5 references Sheppard and Thibault (1990).
Diffusion coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	None Specified	--
Ac-227 - Atomic Weight 227 g/mol								
Half Life (years)	22	ANL (2005)	21.8	--	--	--	None Specified	--
Atomic Weight (g/mol)	227		227		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E+01	No value found. Assume 10 gm/cc to prevent solubility from limiting migration.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	450 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	450 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	450 (sand) 450 (waste) 2400 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	2,400 (clay)		2,400 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Am-241 - Atomic Weight 241 g/mol								
Half Life (years)	4.32E+02	--	4.32E+02	--	--	--	None Specified	--
Atomic Weight (g/mol)	241		241		--	--	None Specified	
Solubility Limit (gm/cc)	8.00E-03	Derived from geochemical database prepared by Lawrence Livermore National Laboratory and converted to PHREEQC format.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	1900 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	1900 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	1900 (sand) 1900 (waste) 8400 (clay)	DOE 2003b, page C3-313 and Table Att. 1. Distribution coefficient of radionuclides and their daughter products in different zones, page C3-314.
	8400 (clay)		8400 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
Np-237 - Atomic Weight 237 g/mol								
Half Life (years)	2.14E+06	Disposal Unit Source Term (DUST) default library	2.14E+06	--	2.14E+06	Disposal Unit Source Term (DUST) default library	None Specified	--
Atomic Weight (g/mol)	237		237		237	EPA (1996)	None Specified	
Solubility Limit (gm/cc)	1.00E+01	No value found. Assume 10 gm/cc to prevent solubility from limiting migration.	1.00E+01	EPA (1996) (Not Verified)	1.00E+01	EPA (1996) (Not Verified)	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	5 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	5 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	70 (sand)	Sheppard and Thibault (1990), conflict with numbers in the table	70 (sand) 70 (waste) 144 (clay)	DOE 2003b, page C3-313 and Table Att. 1. Distribution coefficient of radionuclides and their daughter products in different zones, page C3-314. No Kd values for NP-237 reported in table.
	55 (clay)		55 (clay)		144 (clay)	DOE (1997) and DOE (2002b)		
Diffusion Coefficient (cm^2/sec)	1.00E-06	DOE (2003) (U-Landfill Report)	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Pa-231 - Atomic Weight 231 g/mol								
Half Life (years)	3.30E+04	ANL (2005)	3.28E+04	--	--	--	None Specified	--
Atomic Weight (g/mol)	231		231		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E+01	No value found. Assume 10 gm/cc to prevent solubility from limiting migration.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	550 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	550 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	550 (sand) 550 (waste) 2700 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	2,700 (clay)		2,700 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
Pb-210 - Atomic Weight 210 g/mol								
Half Life (years)	2.20E+01	ANL (2005)	2.20E+01	--	--	--	None Specified	--
Atomic Weight (g/mol)	210		210		--	--	None Specified	
Solubility Limit (gm/cc)	8.70E-04	EPA (2004), Page A-225	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	270 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	270 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	270 (sand) 270 (waste) 550 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	550 (clay)		550 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Pu-238 - Atomic Weight 238 g/mol								
Half Life (years)	8.78E+01	Disposal Unit Source Term (DUST) default library	8.78E+01	--	--	--	None Specified	--
Atomic Weight (g/mol)	238		238		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E+01	No value found. Assume 10 gm/cc to prevent solubility from limiting migration.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	550 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	550 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	550 (sand) 550 (waste) 5100 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	5100 (clay)		5100 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
Pu-239 - Atomic Weight 239 g/mol								
Half Life (years)	2.41E+04	Disposal Unit Source Term (DUST) default library	2.41E+04	--	--	--	None Specified	--
Atomic Weight (g/mol)	239		239		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E+01	No value found. Assume 10 gm/cc to prevent solubility from limiting migration.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	550 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	550 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	550 (sand) 550 (waste) 5100 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	5100 (clay)		5100 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Pu-240 - Atomic Weight 240 g/mol								
Half Life (years)	6.54E+03	Disposal Unit Source Term (DUST) default library	6.57E+03	--	--	--	None Specified	--
Atomic Weight (g/mol)	240		240		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E+01	No value found. Assume 10 gm/cc to prevent solubility from limiting migration.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	550 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	550 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	550 (sand) 550 (waste) 5100 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	5100 (clay)		5100 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
Ra-226 - Atomic Weight 226 g/mol								
Half Life (years)	1.60E+03	Disposal Unit Source Term (DUST) default library	1.60E+03	--	--	--	None Specified	--
Atomic Weight (g/mol)	226		226		--	--	None Specified	
Solubility Limit (gm/cc)	3.10E-01	EPA (2004), Page A-301	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	500 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	500 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	500 (sand) 500 (waste) 9100 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	9,100 (clay)		9,100 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Ra-228 - Atomic Weight 228 g/mol								
Half Life (years)	5.80E+00	Disposal Unit Source Term (DUST) default library	5.75E+00	--	--	--	None Specified	--
Atomic Weight (g/mol)	228		228		--	--	None Specified	
Solubility Limit (gm/cc)	3.10E-01	EPA (2004), Page A-303	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	500 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	500 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	500 (sand) 500 (waste) 9100 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	9,100 (clay)		9,100 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
Th-228 - Atomic Weight 228 g/mol								
Half Life (years)	1.90E+00	ANL (2005)	1.90E+00	--	--	--	None Specified	--
Atomic Weight (g/mol)	228		228		--	--	None Specified	
Solubility Limit (gm/cc)	2.80E-01	EPA (2004), Page A-343	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	3200 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	3200 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	3200 (sand) 3200 (waste) 5800 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	5800 (clay)		5800 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Th-229 - Atomic Weight 229 g/mol								
Half Life (years)	7.34E+03	Disposal Unit Source Term (DUST) default library	7.34E+03	--	--	--	None Specified	--
Atomic Weight (g/mol)	229		229		--	--	None Specified	
Solubility Limit (gm/cc)	2.80E-01	EPA (2004), Page A-345.	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	3200 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	3200 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	3200 (sand) 3200 (waste) 5800 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	5800 (clay)		5800 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
Th-230 - Atomic Weight 230 g/mol								
Half Life (years)	7.70E+04	ANL (2005)	7.70E+04	--	--	--	None Specified	--
Atomic Weight (g/mol)	230		230		--	--	None Specified	
Solubility Limit (gm/cc)	2.80E-01	EPA (2004), Page A-347	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	3200 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	3200 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	3200 (sand) 3200 (waste) 5800 (clay)	DOE 2003b, page C3-313 and Table Att. 1. Distribution coefficient of radionuclides and their daughter products in different zones, page C3-314.
	5800 (clay)		5800 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
Th-232 - Atomic Weight 232 g/mol								
Half Life (years)	1.40E+10	ANL (2005)	1.40E+10	--	--	--	None Specified	--
Atomic Weight (g/mol)	232		232		--	--	None Specified	
Solubility Limit (gm/cc)	2.80E-01	EPA (2004), Page A-351	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	3200 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	3200 (sand)	Sheppard and Thibault (1990), Table 1, Page 472	--	--	3200 (sand) 3200 (waste) 5800 (clay)	DOE 2003b, page C3-313 and Table Att. 1. Distribution coefficient of radionuclides and their daughter products in different zones, page C3-314.
	5800 (clay)		5800 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
U-233 - Atomic Weight 233 g/mol								
Half Life (years)	1.59E+05	Disposal Unit Source Term (DUST) default library	1.59E+05	--	--	--	None Specified	--
Atomic Weight (g/mol)	233		233		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E-04	EPA (2004), Page A-381	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	35 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	66.8 (sand)	Sheppard and Thibault (1990), does not match number in table	--	--	66.8 (sand) 410 (waste) 3640 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	1600 (clay)		3640 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
U-234 - Atomic Weight 234 g/mol								
Half Life (years)	2.40E+05	ANL (2005)	2.44E+05	--	--	--	None Specified	--
Atomic Weight (g/mol)	234		234		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E-04	EPA (2004), Page A-383	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	35 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	66.8 (sand)	Sheppard and Thibault (1990), does not match number in table	--	--	66.8 (sand) 410 (waste) 3640 (clay)	DOE 2003b, page C3-313 and Table Att. 1. Distribution coefficient of radionuclides and their daughter products in different zones, page C3-314.
	1600 (clay)		3640 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
U-235 - Atomic Weight 235 g/mol								
Half Life (years)	7.00E+08	ANL (2005)	7.04E+08	--	--	--	None Specified	--
Atomic Weight (g/mol)	235		235		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E-04	EPA (2004), Page A-385	1.00E+01	EPA (1996) (Not Verified)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	35 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	66.8 (sand)	Sheppard and Thibault (1990), does not match number in table	--	--	66.8 (sand) 410 (waste) 3640 (clay)	DOE 2003b, page C3-313 and Table Att. 1. Distribution coefficient of radionuclides and their daughter products in different zones, page C3-314.
	1600 (clay)		3640 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)
U-236 - Atomic Weight 236 g/mol								
Half Life (years)	2.34E+07	Disposal Unit Source Term (DUST) default library	2.34E+07	--	--	--	None Specified	--
Atomic Weight (g/mol)	236		236		--	--	None Specified	
Solubility Limit (gm/cc)	1.00E-04	EPA (2004), Page A-387	1.00E+01	EPA (1996)	--	--	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	35 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	66.8 (sand)	Sheppard and Thibault (1990), does not match number in table	--	--	66.8 (sand) 410 (waste) 3640 (clay)	"Project Communication" with the Waste Disposal Options Project Team from Paducah, KY.
	1600 (clay)		3640 (clay)		--	--		
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	--	--	None Specified	--
U-238 - Atomic Weight 238 g/mol								
Half Life (years)	4.50E+09	ANL (2005)	4.47E+09	--	4.47E+09	Disposal Unit Source Term (DUST) default library	None Specified	--
Atomic Weight (g/mol)	238		238		238	EPA (1996)	None Specified	
Solubility Limit (gm/cc)	1.00E-04	EPA (2004), Page A-389	1.00E+01	EPA (1996)	1.00E+01	EPA (1996)	Default	Yu et al, 2001.[3]
Unsaturated Soils, Waste, Saturated Materials (Vertical and Horizontal Flow) Kd (cc/gm)	35 (sand and all other materials)	Sheppard and Thibault (1990), Table 1, Page 472	66.8 (sand)	Sheppard and Thibault (1990), does not match number in table	66.8 (sand) 410 (organic) 3640 (clay)	Sheppard and Thibault (1990), does not match number in table DOE (1997) and DOE (2002b)	66.8 (sand) 410 (waste) 3640 (clay)	DOE 2003b, page C3-313 and Table Att. 1. Distribution coefficient of radionuclides and their daughter products in different zones, page C3-314. Table does not give references or justification for Kd values presented
	1600 (clay)		3640 (clay)					
Diffusion Coefficient (cm^2/sec)	1.00E-06	--	1.00E-06	No reference given. From DOE (2010), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	1.00E-06	No reference given. From DOE (2003), "Values obtained from DUSTMS model are insensitive to diffusion coefficient if the diffusional release fraction = 0."	None Specified	--

Table C1.3. Chemical Specific Parameters (Continued)

Parameters	PGDP Model Value	Reference(s)	Previous Draft Model Value (based on DOE 2010)	Reference(s)	U-Landfill (DOE 2003) Value	Reference(s)	ORISE RESRAD Model Value[2]	Reference(s)

Notes

1. -- Denotes information not available.
2. ORISE RESRAD Model Value information provided by personal communication (John Volpe email - 04/24/2011).
3. User's Manual for RESRAD Version 6. "The default value is assigned; however, it is not used by the code. This parameter is one of the options in RESRAD to derive distribution coefficients (Kds) when site-specific data is not available. In this case site-specific Kds are available and are used by the code; therefore, there was no need to use this option to derive them."
4. Kd - chemical specific distribution coefficient.
5. Koc - chemical specific octanol/water partition coefficient.
6. foc - fraction organic carbon.

References

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Table C1.4. HELP Model Input Parameters

Parameter	Units	Deterministic Value
Fraction of area allowing runoff	%	100% (18.94 acres)
Evaporative zone depth	inches	8 inches for Operational Period (low end of silts) 18 inches for Postclosure and Long-Term Modeling Periods (high end of silts)
Start of growing season	day	96th Julian Day
End of growing season	day	300th Julian Day
Average annual wind speed	mph	8.2
Average 1st quarter relative humidity	%	70
Average 2nd quarter relative humidity	%	67
Average 3rd quarter relative humidity	%	72
Average 4th quarter relative humidity	%	54
Normal mean monthly precipitation (Jan)	inches	3.27
Normal mean monthly precipitation (Feb)	inches	3.9
Normal mean monthly precipitation (Mar)	inches	4.92
Normal mean monthly precipitation (April)	inches	5.01
Normal mean monthly precipitation (May)	inches	4.94
Normal mean monthly precipitation (June)	inches	4.05
Normal mean monthly precipitation (July)	inches	4.19
Normal mean monthly precipitation (Aug)	inches	3.34
Normal mean monthly precipitation (Sept)	inches	3.69
Normal mean monthly precipitation (Oct)	inches	3
Normal mean monthly precipitation (Nov)	inches	4.32
Normal mean monthly precipitation (Dec)	inches	4.65
Normal mean monthly temperature (Jan)	^{o}F	32.6
Normal mean monthly temperature (Feb)	^{o}F	36.9
Normal mean monthly temperature (Mar)	^{o}F	47.5
Normal mean monthly temperature (April)	^{o}F	57.9
Normal mean monthly temperature (May)	^{o}F	66.7
Normal mean monthly temperature (June)	^{o}F	75.2
Normal mean monthly temperature (July)	^{o}F	78.8
Normal mean monthly temperature (Aug)	^{o}F	76.8
Normal mean monthly temperature (Sept)	^{o}F	70.2
Normal mean monthly temperature (Oct)	^{o}F	58.7
Normal mean monthly temperature (Nov)	^{o}F	47.9
Normal mean monthly temperature (Dec)	^{o}F	37.3
Solar Radiation Data Station Latitude	Decimal Degrees	37.1 N

Table C1.5. DUST-MS Model Input Parameters

Parameter	Units	Deterministic Value
Title and General Problem Definition		
Number of Nodes	n/a	298 (Site 11) 266 (Site 3A)
Number of Isotopes	n/a	Varies
Mass Units	grams	grams
Decay Chains	n/a	Varies
Time Parameters		
Number of Time Steps	n/a	10000
Initial Time Interval (yrs)	years	1.6 0.16 0.08
Fractional Change in Time Interval	n/a	0
Maximum Time Interval	years	1.6 0.16 0.08
Maximum Simulation Time	years	16000 1600 800
Number of Time Step Resets	n/a	0
Material Parameters		
Number of Materials	n/a	6 (Site 11) 5 (Site 3A)
Number of Material Changes	n/a	298 (Site 11) 266 (Site 3A)
K-d (Distribution Coefficient)	cc/gm	Chemical Specific
Density	gm/cc	Material - Density 1 - 1.34 2- 1.4 3 - 1.8 4 - 3.1 5 - 1.43 (Site 11) 5 - 1.41 (Site 3A) 6 - 1.43 (Site 11)
Dispersion Coefficient	cm	415 (Site 11) 366 (Site 3A)
Diffusion Coefficient	cm^2/s	Chemical Specific
Changes to Node Material Types	n/a	First Node to Last Node = Material 1 to 10 = 1 11 to 20 = 2 21 to 26 = 3 27 to 196 = 4 197 to 198 = 3 199 to 200 = 2 201 to 206 = 3 207 to 226 = 1 227 to 270 = 5 (Site 11) 227 to 266 = 5 (Site 3A) 271 to 298 = 6 (Site 11)
Change in Node Number	n/a	1

Table C1.5. DUST-MS Model Input Parameters (Continued)

Parameter	Units	Deterministic Value
Change in Material Type	n/a	0
Output Parameters		
Output for Time Steps	n/a	Print Concentrations at time step = 1 and every 999 time steps
Number of Concentration Traces	n/a	5 (Site 11) 4 (Site 3A)
Node Locations for Concentration Traces	n/a	1, 26, 206, 270, 298 (Site 11) 1, 26, 206, 266 (Site 3A)
Number of Flux Traces	n/a	5 (Site 11) 4 (Site 3A)
Node Locations for Flux Traces	n/a	1, 26, 206, 270, 298 (Site 11) 1, 26, 206, 266 (Site 3A)
Facility Dimensions		
Area of Facility	cm^2	7.67E+08
Node Coordinates		
First Node	n/a	1
Last Node	n/a	298 (Site 11) 266 (Site 3A)
Change in Node Number	n/a	1
Starting Location	cm	0
Change in Delta X	cm	15.24
Incremental Change in Delta X	n/a	0

Table C1.5. DUST-MS Model Input Parameters (Continued)

Parameter	Units	Deterministic Value
Initial Conditions		
First, Last Node, and Initial Concentration	g/cc	First Node to Last Node = Initial Concentration 1 to 26 = 0 27 to 196 = Chemical Specific 197 to 266 (Site 3A) or 298 (Site 11) = 0
Change in Node Number	n/a	1
Fractional Change in Concentration	n/a	0
Boundary Conditions		
Upper Boundary	$g/cm^2/s$	Total Flux = 0
Lower Boundary	g/cc	Concentration = 0
Number of Data Points	n/a	2
Use BC File	n/a	No - All
Water Velocity Parameters		
Number of Data Points	n/a	10 - Gradual Failure (BL) Scenario 4 - Instantaneous Failure (IF) Scenario 2 - No Failure (NF) Scenario
Time and Water Velocity Parameters	years and cm/s	Time - Water Velocity 0 - 2.458E-14 (BL, IF, NF) 170 - 2.458E-14 (BL, IF, NF) 195 - 1.217E-13 (BL) 220 - 6.030E-13 (BL) 320 - 3.626E-10 (BL) 395 - 3.962E-08 (BL) 470 - 3.636E-07 (BL) 520 - 3.889E-07 (BL) 570 - 3.901E-07 (BL, IF) 16000 - 3.907E-07 (BL, IF)

Table C1.5. DUST-MS Model Input Parameters (Continued)

Parameter	Units	Deterministic Value
Moisture Content		
First and Last Node - Initial Moisture Content	n/a	First Node to Last Node = Material 1 to 10 = 0.3098 11 to 20 = 0.0452 21 to 26 = 0.4251 27 to 196 = 0.3588 197 to 198 = 0.4112 199 to 200 = 0.1123 201 to 206 = 0.427 207 to 226 = 0.342 227 to 270 = 0.393 (Site 11) 227 to 266 = 0.3025 (Site 3A) 271 t0 298 = 0.445 (Site 11)
Change in Node Number	n/a	1
Incremental Change in Moisture Content	n/a	0
Container Failure Times		
Number of Containers	n/a	0
Number of Failure Types	n/a	none
Failure Times for Containers	n/a	none
Waste Forms		
Not used	n/a	Not used
Sources		
Number of Source/Sink Nodes	n/a	0

Table C1.6. AT123D Model Input Parameters

Parameter	Units	Deterministic Value
Aquifer Tab		
Hydraulic Conductivity	m/hr	35.6 (Site 11) 1.18 (Site 3A)
Hydraulic Gradient	m/m	0.00066 (Site 11) 0.0032 (Site 3A)
Effective Porosity	n/a	0.3
Soil Bulk Density	kg/m^3	1670 (Site 11) 1560 (Site 3A)
Longitudinal Dispersivity	m	15
Transverse Dispersivity	m	1.5
Vertical Dispersivity	m	0.15
Aquifer Width	m	Infinite
Aquifer Depth	m	10.8 (Site 11) 4.572 (Site 3A)
Number of Eigenvalues	n/a	500
Steady-State Error Tolerance	n/a	0.01
Input Tab		
Release Coordinates	m	Site 11 X - Start = -113.1, End = 113.1 Y - Start = -169.6, End = 169.6 Z - Start = 0, End = 0 Site 3A X - Start = -124.8, End = 124.8 Y - Start = -153.6, End = 153.6 Z - Start = 0, End = 0
Soil organic carbon content	%	0
Koc - Organic carbon adsorption coefficient	(ug/g)/ (ug/ml)	0
Kd - Distribution Coefficient	m^3/kg	Chemical Specific
Water Diffusion Coefficient	m^2/hr	Chemical Specific
First-Order Decay Coefficient	1/hr	Chemical Specific

Table C1.6. AT123D Model Input Parameters (Continued)

Parameter	Units	Deterministic Value
Output Tab		
Starting Time Step		1
Ending Time Step		10001
Time Step		1
X-Axis Coordinates	m	Site 11 - 113.1, 213.1, 225.9, 1356.3, 3907.6 Site 3A - 124.8, 224.8, 242.6, 625.7, 1000
Y-Axis Coordinates	m	0
Z-Axis Coordinates	m	0
Load Tab		
Initial Concentration	mg/L	0
Single Mass Load	kg	not used
Model Time Step	hrs	14025.6 1402.56 701.28
Continuous = 0, >1 Varying	n/a	10000
Water Density	kg/m^3	1000
Release Type	n/a	Continuous Release
Load Release Rate	kg/hr	Varies by Chemical

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Comment Response Summary

Comments on Appendix C to the Work Plan for CERCLA Waste Disposal Alternative Evaluation Remedial Investigation/Feasibility Study (DOE/LX/07-0099&D2/R1) Paducah Gaseous Diffusion Plant

Comment 1: Attachment C1 to this Appendix contains HELP modeling input parameters but fails to include any of the inputs to DUSTMS. Please add a listing of the input parameters used in the DUSTMS program and include a figure or table that illustrates how the twenty HELP layers and ten DUSTMS material layers interrelate.

Response 1: Input parameter values for use in DUSTMS are included in Attachment C1. Tables C1.4, C1.5, and C1.6 have been added to Attachment C1.

The following sentence has been added to Section C.3.2.1 to refer to new figures C.2 and C.3:

"Figures C.2 and C.3 provide an illustration of how the HELP layers and DUSTMS material layers interrelate for Sites 11 and 3A, respectively."

The remaining figures in the text have been updated as appropriate to account for the insertion of these figures.

Comment 2: Section C.3.2, Page C-7, Point No. (2), Lines 3-6: The text implies that fate and transport modeling to be conducted in support of PWAC development will rely upon "predicted contaminant mass from the analytical waste profile" and that this mass will be assumed to be uniformly distributed in the soil. In fact, a unit concentration (corresponding to a certain mass) for each contaminant is being used as initial input to the DUSTMS code to predict contaminate concentrations at downgradient exposure points. These concentrations are then used in conjunction with MCLs or risk/hazard-based values to back-calculate the PWAC for each contaminant of concern. The PWAC will then be compared (in the FS Report) against predicted inventories of any given contaminant of concern derived from the analytical waste profile for the site in order to assess the feasibility of constructing an onsite waste repository at Paducah. Please modify the text such that it more accurately reflects how the modeling is being conducted. Also, the text should make clear that the material assumed to contain homogeneously distributed contamination is not soil, but is an artificial construct having a bulk density of 3.1 g/cc.

Response 2: The referenced text has been modified as follows to include a description of the modeling process:

"Disposal Unit Source Term-Multiple Species (DUSTMS) modeling will be performed for each metal, radionuclide, and indicator chemical under the gradual failure scenario to predict the contaminant flux entering the aquifer over time. A unit concentration for each contaminant will be used as an initial input to DUSTMS. This unit concentration is converted to an initial contaminant mass within the landfill. The contaminant mass will be assumed to be contained in a homogenized soil. The entire landfill volume will be assumed to be filled with a single contaminant embedded in the soil waste. DUSTMS is used to calculate initial groundwater concentrations based on this initial mass/concentration. Once downgradient groundwater concentrations are obtained from the Analytical Transient 1-, 2-, 3-Dimensional (AT123D) model and initial PWAC concentrations are calculated, DUSTMS is rerun using the initial PWAC concentrations to obtain new initial groundwater concentrations. (DUSTMS modeling also will be performed for selected contaminants as part of an uncertainty analysis under the immediate and no failure scenarios.)"

As was discussed and agreed-upon in the April 13, 2011, modeling subgroup conference call, the bulk density of 3.1 g/cm^3 was selected to be representative of a soil/debris mixture.

Comment 3: Section C.3.2.1.1, Page C-9, 1st Paragraph, Lines 4-5: It is stated that contaminants present in leachate generated during the landfill's operational period are assumed to be removed from the landfill. This is in fact what will occur. However, it was agreed during the June 13-14, 2011 modeling subgroup meeting held in Nashville, Tennessee that mass removed would no longer be added to the initially calculated PWAC. In other words, the final PWAC will not be increased to reflect the mass removed. Please remove this sentence or make it clear in the text, as agreed, that credit for mass removal will not be taken.

Response 3: As noted by the reviewer, it was agreed in the June 13–14, 2011, modeling subgroup meeting that chemical mass removed via the leachate collection system during the operational period will not be added back into the system. This decision was made after submittal of the Work Plan Appendix C on June 3, 2011. The referenced lines have been modified as follows:

"During this period, contaminant mass removed via the leachate collection system is assumed to be collected and removed from the landfill; however, the mass removed by the leachate collection system will not be taken into account during calculation of the PWAC."

Comment 4: Section C.3.2.1.1, Page C-10, 4th Paragraph, Line 1: The prior two paragraphs refer to the "no failure" and "instantaneous failure" scenarios, respectively. This paragraph clearly refers to the "gradual failure" scenario. However, the first sentence does not make this clear. In the interest of clarity, consider modifying the first sentence such that it explicitly states that this paragraph refers to the gradual failure scenario.

Response 4: The text has been clarified per the reviewer comment as follows:

"For the gradual failure scenario, at 200 years the HDPE geomembrane components of the cap and liner system would commence to degrade (i.e., all antioxidants are depleted and the induction time for the start of degradation is completed)."

Comment 5: Section C.3.2.1.1, Page C-10, 6th Paragraph, Line 1: This sentence pertains to the Lee equation that was used to model the effects of engineered barrier degradation upon percolation rates through the landfill during the 200 to 600 year post-closure period. The decay constant α used in the Lee equation is listed as 0.059 year-1. The modeling subgroup has agreed upon a value of α of 0.064 year-1. Please correct the text accordingly.

Response 5: A value of α of 0.064 yr^{-1} will be used for the modeling per the modeling subgroup agreement. The value has been updated as appropriate:

" α = decay constant (0.064 year^{-1})

The decay constant, α, was set at 0.064 year^{-1}, which results in failure of the engineered barrier system at 600 years postclosure."

Comment 6: Section C.3.2.1.2, Page C-11: This section in part provides a description of the DUSTMS code. It is suggested that the text be modified slightly to indicate that this modeling effort is being performed assuming that no containers exist.

Response 6: Discussion and agreement on not using waste containers in the DUSTMS modeling occurred after submittal of the Work Plan Appendix C on June 3, 2011. The following discussion has been added to the referenced section:

"As the waste is not expected to be containerized during waste placement, and because it is assumed for the purposes of modeling that the contaminants are readily available for transport and not packaged or treated to decrease leachability, containers will not be simulated."

Comment 7: Section C.3.3, Page C-17, 3rd Paragraph: It is somewhat unclear what is being stated. What is meant by "the greater of cumulative ELCR and/or HI targets?" The word "targets" appears to refer to the 1E-05 ELCR risk based target and the HI=3 hazard-based target. Since it is cumulative risk or hazard that are being addressed here, an exceedence of one or the other of the "targets" as predicted by the models would require that the major risk or hazard driver be identified and that it's PWAC be adjusted downward in order to lower the cumulative risk or hazard curve below the appropriate target. Please elaborate in the text what is meant by "the greater of the cumulative ELCR and/or HI targets" or simply reword the sentence.

Response 7: For clarity, the sentence has been modified as follows:

"The increased cumulative ELCR and/or HI targets of 1E-05 and 3, respectively, are used beyond 1,600 years at the boundary of the WDF and DOE property line to address the uncertainties in exposure (e.g., receptor location relative to ground water flow) and constituent release and migration."

Comment 8: Section C.3.4, Page C-18, 1st Paragraph, Line 4: The PWAC is described here as a maximum number of curies that could be placed in the landfill "or the single contaminant limit per COPC." Use of the word "limit" is nonspecific. Please reword this portion of the sentence to read as follows: "or the single contaminant mass limit (in grams or Kg) per COPC."

Response 8: The text has been modified as requested:

"Additionally, the PWAC is the total contaminant amount, such as maximum curies permitted in the cell or the single contaminant mass limit (in grams or kilograms) per COPC."

Comment 9: Section C.3.4, Page C-19, Line 5: The bulk density listed here for the purpose of calculating total mass or curies permitted in the cell is 1.5 g/cm3. This bulk density is typical of soil. However, the modeling subgroup has agreed to use a homogeneous wasteform bulk density of 3.1 g/cm3. This is a volume-weighted number that takes into consideration the presence of wasteforms in the cell that are denser that soil. The bulk density used in this equation should be consistent with that used to derive the modeled PWAC. If 1.5 g/cm3 will be used in this equation then it should also be used as the waste bulk density input to DUSTMS. Please modify the text as necessary.

While this comment is made for the sake of consistency, the appropriate value to use for bulk density is in question. The 3.1 g/cm3 was derived assuming that a certain amount of waste would be steel. The presence of steel, having a higher bulk density than soil, raises the average bulk density. The difficulty arises in that the steel is not uniformly distributed throughout the waste but is expected to be placed into the facility whole. Soil having a high bulk density is not the same as soil having an average bulk density and a hunk of metal in it. Therefore, the bulk density of the transport media within the unit is artificially increased raising the PWAC.

Response 9: As was discussed and agreed-upon in the April 13, 2011, modeling subgroup conference call, the bulk density of 3.1 g/cm^3 was selected to be representative of a soil/debris mixture.

The text has been modified as follows:

"ρ_b = bulk density (3.1 g/cm^3)"

Comment 10: Section C.3.5, Page C-19, 4th Paragraph: The paragraph suggests that pore water concentrations computed using DUSTMS will require further scrutiny following completion of the modeling to insure that the concentrations do not exceed assumed solubility limits for particular contaminants. This additional scrutiny should not be required. DUSTMS accounts for the solubility limits of individual contaminants. Therefore, pore water concentration in waste should never exceed the solubility limits for any particular contaminant. Please remove this paragraph from the document.

Response 10: DUSTMS does account for the solubility limits of individual contaminants. Also, pore water concentration in waste should not exceed the solubility limits for any particular contaminant. However, because of the back calculation of the chemical-specific PWAC from the predicted groundwater concentrations, it is possible to calculate a PWAC that would exceed solubility limits. Therefore, the solubility check to ensure free liquid is not simulated as being emplaced in the facility is valid.

No change has been made to the text.

Comment 11: Section C.3.5, Page C-19, 6th Paragraph, 3rd Sentence: While it is acceptable to base the calculated PWAC on a modeling period limited to 10,000 years, a subsequent forward run should be performed such that all radionuclide peaks are captured, as agreed to during Paducah WDO Modeling Sub-Group discussions. It is recognized that a modeling period of this length would have too much associated uncertainty to be used directly in the PWAC calculation, but it is essential to capture the theoretical maximum impact of wastes that greatly increase in radioactivity over hundreds of thousands of years (especially considering the "permanent" nature of the disposal method). Please make appropriate changes to the text.

Response 11: The sentence in the text Section C.3.5:

"Also, it is acknowledged that some radionuclide contaminants (and possibly their daughter products) will not reach their peak concentrations at the point of compliance during the 10,000-year period of interest; however, simulations will be performed only for a maximum 10,000 years in accordance with the performance evaluation period."

has been replaced with the following:

"Also, because some radionuclide contaminants (and decay products from ingrowth) will not reach their peak concentration prior to 10,000 years, an uncertainty analysis examining ingrowth and risk beyond 10,000 years will be completed for uranium-238 (U-238) (parent compound) and thorium-230 (Th-230) (progeny). This analysis will use a forward run of the transport model for the gradual failure scenario to the peak concentrations for U-238 and Th-230 and the selected initial PWAC for U-238 and Th-230 as the source term concentration. Due to modeling software constraints, the time step used in this analysis will be larger than that used for development of the PWAC."

Comment 12: Attachment C.1, Proposed Modeling Parameters, Tables C1.1 and C1.2: These two tables' list HELP model inputs for the 30 to 200 year post-closure period and the 600 + year long-term monitoring period, respectively. Both tables contain variations (some larger than others) in initial moisture content and Site 3A loess and native clay thicknesses relative to the final parameter list submitted in a Geosyntec memo dated May 6, 2011. Kentucky does not necessarily take issue with the

parameter changes. However, these deviations from the originally proposed values should be explained. In particular, Kentucky is interested in learning how or why the initial moisture contents for layers 10 through 14 as listed in Table C1.1 were increased and why the initial moisture contents for the top three layers in Table C1.2 were decreased. Were these values generated by the HELP model or were they specified by the modeler? What was the basis for the changes? Please respond to these questions in the Comment Response Summary.

Response 12: Site 3A Layer 19 and 20 thicknesses were updated after submittal of the May 6, 2011, memo to better match the thicknesses for the PGDP Waste Disposal Options Conceptual Landfill Design (Paducah Fact Sheet dated June 2010). This update was reflected in the Layer 19 and 20 thicknesses presented in Table C1.1. The combined thickness of Layers 19 and 20 were not modified from their original value of 360 inches.

Initial moisture content values listed in Tables C1.1 and C1.2 were assigned as follows: when available, final calculated moisture content values from the previous time period are carried over and used as initial moisture content values for the subsequent time period; if previous time periods are not available, the initial moisture contents are estimated directly by HELP.

For example, the initial moisture contents for Layers 10–20 during the Post-closure Period (Table C1.1) are those calculated by HELP at the end of the Operational Period. Layers 1–9, which do not exist during the Operational Period, have initial moisture contents that are explicitly estimated by HELP.

The Long-term Monitoring Period initial moisture content values (Table C1.2) are specified as being equal to the Post-closure Period's final moisture content values.