Using Fate and Transport Models to Evaluate Cleanup Levels

In its 2000 session, the Wyoming Legislature created new opportunities, procedures, and standards for voluntary remediation of contaminated sites. These provisions, enacted as Articles 16, 17, and 18 of the Wyoming Environmental Quality Act and implemented by the Wyoming Department of Environmental Quality (DEQ), will govern future environmental cleanups in Wyoming.

This Fact Sheet provides guidelines for using fate and transport models to calculate site-specific soil cleanup levels protective of groundwater and to evaluate the potential for vapor intrusion impacts in buildings.

DEQ expects that for many smaller, simpler sites, the Volunteer will be able to utilize default values in Fact Sheet #12, (Soil Cleanup Levels) or Fact Sheet #14 (Ecological Risk Assessment) when establishing soil cleanup levels or may be able use a simple analytical model, considering sorption and biodegradation processes to calculate site specific cleanup levels protective of groundwater. For larger, complex sites where it is anticipated that a remedy agreement will be needed to address many contaminants in several different media with a range of remedial alternatives, DEQ expects that more complicated models may be used. These more complicated cleanups and the models needed to develop cleanup values or to ensure a remedy is performing will likely be memorialized in the remedy agreement and will provide the flexibility for these larger, complex sites.

A. INTRODUCTION

1. What are fate and transport models and how are they used?

A fate and transport model is an analytical, semi-analytical, or numerical method for predicting and quantifying constituent migration within the environment. For example, a fate and transport model may be used to predict contaminant leaching from soil into groundwater and vertical contaminant migration in the unsaturated zone to the groundwater table. Fate and transport models range from very simple equations requiring little data to very complex equations (or series of equations) requiring detailed site-specific information. One or more fate and transport processes affecting constituent migration, such as advection or biodegradation, may be incorporated into a fate and transport model.

In the VRP, fate and transport models approved by DEQ for that purpose may be used to calculate soil cleanup levels protective of the uppermost groundwater. Fate and transport models may be

appropriate in certain circumstances where the uppermost groundwater is present in fractured bedrock. However, these fate and transport models may only be used with prior DEQ approval. Fate and transport models approved by DEQ may also be used to estimate volatile chemical indoor air concentrations due to migration of vapors from contaminated soils and/or groundwater.

2. Do I have to use a fate and transport model to develop soil cleanup levels or evaluate vapor intrusion?

No. When evaluating the need for soil cleanup, a Volunteer may use the cleanup levels listed in Fact Sheet #12 (*Soil Cleanup Levels*), Table 1; may determine background concentration-based cleanup levels for metals at a specific site as described in Fact Sheet #24 (*Establishing Site Specific Background Metals Concentrations in Soil*); or may develop cleanup levels protective of groundwater for a specific site using a fate and transport model approved by DEQ for this purpose. If a fate and transport model is used to develop cleanup levels protective of groundwater, cleanup levels must be no greater than the cleanup levels protective of direct human contact (to a depth of twelve (12) feet) listed in Table 1, Fact Sheet #12. In addition, regardless of the method used for development, cleanup levels must be protective of ecological receptors as described in Fact Sheet #14 (*Ecological Risk Assessment*). Depth of cleanup for ecological receptors is dependent on identified environmental receptors. If a Volunteer is considering use of a fate and transport model to develop soil cleanup levels protective of groundwater, DEQ recommends the following approach be used. The Volunteer may use any one of the options or may use the options in a stepwise approach.

- ***Option 1 – Defaults:*** is use of the default cleanup levels protective for migration of contaminants to groundwater listed in Fact Sheet #12, Table 1. These cleanup levels are calculated using a simple soil/water partitioning model expected to provide conservative values protective at all VRP sites. If site concentrations do not exceed these values or if a Volunteer chooses to use these values, there is no reason to develop site-specific cleanup levels for protection of groundwater using a fate and transport model. In addition, cleanup levels protective of direct human contact (to a depth of twelve (12) feet) listed in Table 1, Fact Sheet #12 must be met and cleanup levels must be protective of ecological receptors, depth appropriate to receptor, as described in Fact Sheet #14. Meeting all of these cleanup levels would result in a final cleanup for which all cleanup requirements have been satisfied.

- ***Option 2 – Analytical Models:*** is determination of cleanup levels protective of groundwater using the Appendix A models described in question #7, below, with either the site-specific or default distance between the contaminated soil zone and groundwater and thickness of the contaminated soil zone. The DEQ encourages the use of site-specific data for other input parameters to calculate soil cleanup values using these equations, but has provided conservative default parameters for use when site-specific data are not available. In addition, cleanup levels protective of direct human contact (to a depth of twelve (12) feet) listed in Table 1, Fact Sheet #12 must be met, and cleanup levels must be protective of ecological receptors, depth appropriate to receptor, as described in Fact Sheet #14. Meeting all of these

requirements would result in a final cleanup for which all cleanup requirements have been satisfied, although DEQ may require groundwater monitoring to confirm that the cleanup levels determined using the model are protective of groundwater at the site.

- ***Option 3 – Semi-Analytical and Numerical Models***: allows the use of semi-analytical and numerical models to determine cleanup levels protective of groundwater with prior DEQ approval. A Volunteer may use some site-specific information, such as fraction organic carbon and depth to groundwater with default values for other parameters or may choose to determine site-specific values for all (or some) of the site-related input parameters. A remedy agreement and groundwater monitoring demonstrating that the model results are valid for the site and that groundwater is not impacted is required. Other models may be used with approval of DEQ.

When evaluating the potential for vapor intrusion impacts, a Volunteer may compare groundwater and/or soil vapor concentrations to the one in one-million (1×10^{-6}) screening levels in the EPA *Guidance for Evaluating the Vapor Intrusion to Indoor Air Pathway from Groundwater and Soils* (EPA 2015) or the most recent version. If concentrations in *representative* samples (both in time and space) are less than or equal to the EPA screening levels, no further evaluation of the vapor intrusion pathway should be necessary. However, when EPA screening levels are exceeded, Volunteers may elect to directly sample indoor air rather than attempt to predict indoor air concentrations based on soil and/or groundwater data and modeling. Indoor air samples should be collected and analyzed following DEQ approved protocols and methods, and any interpretations should consider the potential for seasonal variations and contributions of background sources (e.g., see EPA 2015).

B. DEVELOPING SOIL CLEANUP LEVELS USING FATE AND TRANSPORT MODELS

3. Can a fate and transport model be used to develop soil cleanup levels if the groundwater is already contaminated?

Volunteers should consult with DEQ if the groundwater at their site is already contaminated. In such cases, determination of soil cleanup levels protective of groundwater may be more complex than at sites where groundwater is not contaminated. Generally, contamination in the smear zone (from the top of the capillary fringe at the seasonal high water table level to the bottom of the capillary fringe at the seasonal low water table level) will be considered as part of groundwater contamination.

Under § 35-11-1605(e) compliance with soil cleanup levels must be monitored at locations determined by DEQ to ensure protection of human health and identified environmental receptors. Soil points of compliance must also ensure protection of surface water, groundwater, and air from

contamination resulting from any potential transfer of contaminants from soil to these other media. DEQ has limited flexibility when selecting remedies for soils that are acting as a source of contamination to groundwater. However, for contaminants that can be treated, such as hydrocarbons or other organic compounds, where it may be impractical to do physical removal because contamination is too wide-spread laterally and/or vertically, and where there are no unacceptable risks, longer term remedial measures (i.e., monitored natural attenuation) may be considered in the remedial strategy. For example, remedial measures may include active treatment or physical removal of highly contaminated soils in certain areas and use of other, less immediate remedial approaches for soils at other locations at the site. Points of compliance for soil may, in limited circumstances, reflect this flexibility. The rationale for points of compliance must be shown in the remedy agreement.

4. What processes may be considered in calculating site-specific cleanup levels?

Fate and transport processes that may be incorporated into models (without prior DEQ approval) to calculate cleanup levels protective of groundwater for VRP sites are sorption and biodegradation. Other fate and transport processes, such as volatilization and dilution of soil pore water as it enters an aquifer, may not be included in models used to develop cleanup levels for VRP sites without specific approval from DEQ. The Volunteer should consult with the DEQ about using models that incorporate fate and transport mechanisms not discussed in detail in this Fact Sheet. Some examples of fate and transport mechanisms not available with the models discussed in this Fact Sheet are advection, consecutive decay chains, and hydrodynamic dispersion. The DEQ recognizes that alternative models that include these mechanisms may be more appropriate for developing soil cleanup levels at certain VRP sites.

Sorption is the equilibrium partitioning of a constituent between the soil and water within the soil due to adsorption, absorption, solubility, and equilibrium chemical reactions. The importance of sorption in determining contaminant migration depends on many factors including the contaminants present, characteristics of the soil such as amount of organic material (fraction organic carbon) and bulk density, annual precipitation, and distance between the contaminants in soil and the groundwater. Sorption is likely to be an important process in determining migration of metals, especially at sites where the distance between the contaminants and groundwater is more than about ten feet. Sorption is also likely to be important for other contaminants that strongly partition to soil such as polycyclic aromatic hydrocarbons (PAHs) and polychlorinated biphenyls (PCBs). Sorption is typically not as important a process in determining the behavior of contaminants that are fairly soluble in water.

Biodegradation is the partial or complete decomposition of a constituent by indigenous microorganisms. Biodegradation may be important for organic or inorganic compounds. The importance of biodegradation during migration of a contaminant to groundwater depends on factors such as how easily a specific contaminant can be biologically degraded; whether a contaminant degrades aerobically or anaerobically, with aerobic degradation typically occurring more quickly than anaerobic degradation; the presence of electron receptors (oxygen for aerobic

degradation; nitrate, sulfate, ferric iron, and carbon dioxide for anaerobic degradation); and distance between the contaminants and groundwater (which affects the time available for biodegradation to occur). Biodegradation is likely to be an important process for contaminants that degrade aerobically relatively easily, such as benzene, especially if the distance to groundwater is large. Biodegradation is less likely to be a significant process at sites where the distance between the contaminants and groundwater is small or for compounds that degrade anaerobically, such as chlorinated solvents.

5. What considerations might be given when evaluating fate and transport modeling and site-specific data?

DEQ does have flexibility when reaching decisions about source zone[1] cleanup given the following considerations: a) DEQ can use a weight of evidence approach based on factors such as soil or waste contaminant concentrations, site-specific contaminant attenuation (fate and transport) modeling, and impacts noted in groundwater monitoring wells, located within or as close as reasonably possible to the source zone. For example, soil and/or waste contaminant concentrations and attenuation modeling may predict impacts to groundwater; however, groundwater sampling in the source zone may indicate that groundwater impacts don't exist. Using a weight of evidence approach for this example, DEQ can conclude that the soil and/or waste aren't contributing contaminants to groundwater. In other words, they are not 'sources'. In reaching this conclusion, factors such as the age, size and stability of impacted soils or waste in the vadose zone, and groundwater monitoring well location (monitoring within the source zone is preferred, but based on site circumstances may occur as close as reasonably possible to the source), construction, design and sampling protocol will need to be considered; b) in using a weight of evidence approach, it is not appropriate to conduct dilution calculations/modeling in the absence of groundwater data to determine whether a theoretical source zone well may be impacted by contaminant leachate from the source. However, it is appropriate to conduct dilution modeling to 'back-calculate' a source zone cleanup standard if a source zone well is impacted above groundwater cleanup standards. The back-calculation approach would need to consider the location (within or as close as reasonably possible to the source), construction, design, sampling protocol of and sampling results from monitoring wells; and c) in the context of groundwater cleanup, it should be noted that the point of compliance (POC) is an approach or tool used to determine the effectiveness of a groundwater cleanup remedy, and that ultimately applicable cleanup standards must be met throughout the groundwater plume.

6. What models may be used?

The DEQ has determined that the fate and transport models that may be used to develop soil cleanup levels protective of groundwater for VRP sites are the analytical models described in

1 Source zone is defined as contaminated vadose zone soil or waste that has the potential to migrate or release contaminants to another media in excess of acceptable cleanup levels. For the purpose of evaluating fate and transport mechanisms, this definition does not account for the presence of NAPL.

Appendix A (included as an appendix to this Fact Sheet). The analytical models are described below. Other analytical, semi-analytical or numerical models, which may be more appropriate for evaluating fate and transport of inorganic nutrients (e.g., a model that incorporates consecutive decay chains) or metals (e.g., a model that incorporates complexation), may be used with the approval of DEQ.

- **Appendix A analytical models.** The DEQ has selected the Soil Screening Level (SSL) models (with some modifications) developed by EPA (1996a and b) for evaluating fate and transport of organic and inorganic constituents through the migration to groundwater pathway. The models may be used with site-specific data or the conservative default values listed in Appendix A to determine cleanup levels protective of groundwater that, if met (along with cleanup levels protective of direct contact identified in Fact Sheet #12, Table 1 (to a depth of twelve (12) feet) and ecological receptors (depth appropriate to receptor) as described in Fact Sheet #14) would result in a final cleanup for which all cleanup requirements have been satisfied. The DEQ may require groundwater monitoring to confirm the model results. A modification to the SSL model includes the removal of the Dilution and Attenuation Factor (DAF) of 20 and its replacement with a soil attenuation factor to account for sorptive mass redistribution to underlying clean soil in the migration to groundwater pathway. An electronic spreadsheet for calculating cleanup levels using the Modified Organic SSL Model and the Modified Inorganic SSL Model is currently available at http://deq.wyoming.gov/shwd/voluntary-remediation-program/ .

A Volunteer may use other fate and transport models to develop soil cleanup levels with approval from DEQ. The models described in this fact sheet are not appropriate for modeling contaminant fate and transport for the migration to groundwater pathway when non-aqueous phase liquids (NAPL) are present. The Volunteer should consult with the DEQ about other approaches to developing cleanup levels including using more complex models appropriate for these scenarios. The only processes that may be incorporated into a fate and transport model without prior DEQ approval are sorption and biodegradation. The Appendix A Modified Inorganic and Organic SSL models incorporate sorption processes. Some examples of fate and transport mechanisms not available with the Appendix A analytical models are advection, consecutive decay chains, and hydrodynamic dispersion. The DEQ recognizes that alternative models that include these mechanisms may be more appropriate for developing soil cleanup levels at certain VRP sites. A summary and description of potentially applicable unsaturated zone fate and transport models is presented in EPA's soil screening guidance document (EPA 1996a).

7. How do I decide which model to use?

For most sites, it is advisable to use the options in a step-wise approach to using fate and transport models as described in question #2 above. If a Volunteer chooses to use a model to determine cleanup levels protective of groundwater, DEQ suggests starting by calculating cleanup levels using one of the Appendix A models described above with the site-specific or default values for input parameters. A Volunteer may also choose to allocate more resources to calculate cleanup levels that may be higher but still protective of groundwater, using a more complex model. The

selected modeling approach will likely be dependent on the concentration and extent of contamination at the site, the amount of site-specific information available, and the resources available to perform site-specific modeling. More complicated modeling approaches, require relatively detailed site information as modeling input. A well-documented site conceptual model is typically an appropriate first step prior to implementing a more complicated modeling approach.

If site-specific values rather than default parameters are used with the above models, groundwater monitoring will be required to confirm model results.

8. What are the chemical-specific model inputs that must be used?

All of the fate and transport models require input of parameters that are dependent on the contaminant and parameters that are dependent on site-specific conditions. There is limited flexibility in modifying chemical-specific parameters. Each contaminant has two chemical properties that are important for fate and transport modeling using this guidance. These properties are:

- The distribution coefficient (K_d) for metals or soil organic carbon-water distribution coefficient (K_{oc}) for organics
- Henry's law constant (atm-m^3/mol)

Default values of the distribution coefficients and Henry's law constant (atm-m^3/mol) for selected contaminants are presented in Attachment C (EPA, 1996b). The user must use these default values, if available, or get approval from DEQ to use alternate values.

Other chemical-specific model parameters that may be required as modeling input (depending on the model) are:

- Henry's law constant (dimensionless) (assumed to be zero for all metals except mercury)
- Solubility (mass/volume).

Values for contaminants or parameters not included in Appendix A should be obtained from the following references, listed in order of preference:

- EPA Soil Screening Guidance: Technical Background Document .

- EPA Superfund Chemical Data Matrix, Appendix A

9. What other model inputs are needed?

The Appendix A models also require input parameters that are dependent on site conditions. Please refer to Appendix A for the default values for selected parameters for the Appendix A models (Option 2 in question #2 above). The following are some additional, conservative default

values appropriate for many sites in Wyoming that Volunteers may elect to use in the absence of site-specific data:

- Default soil condition = sandy clay soil
- Volumetric soil moisture at field conditions = 0.321 mL/cm^3
- Precipitation infiltration = 0.5
- L_2 Distance from the top of contaminated soil zone to seasonal high groundwater = 6 ft (183 cm)
- L_1 Thickness of contaminated soil zone = 5 ft (152 cm)

To determine site-specific values of these parameters for use in the Appendix A models, use the thickest (i.e., greatest vertical extent) area of contamination (L_1) and the distance from the top of the contaminated soil zone to seasonal high groundwater (L_2). A site-specific distance from the top of the contaminated soil zone to seasonal high groundwater may generally be determined to be at least a minimum distance using site information from test pits or geoprobe investigations; however, the method for determining this distance should be discussed with DEQ.

If an alternative fate and transport model is selected to determine soil cleanup levels (e.g., a model is selected to determine fate and transport of inorganic nutrients), additional input parameters may be required to run the model. In such cases, DEQ approval will be required.

10. Soil Cleanup Modeling References

For additional information regarding fate and transport models for calculation of soil cleanup levels protective of groundwater, the Volunteer is referred to the following documents.

ATSM, RBCA Fate and Transport Models: Compendium and Selection Guidance, November 1998. Carsel, R.F., and R.S. Parrish. 1988. Developing joint probability distributions of soil water retention characteristics. Water Resources Research, 24(5):755-769.161

Connor, J.A., R.L. Bowers, S.M. Paquette, and C.J. Newell. 1997. Soil Attenuation Model for Derivation of Risk-Based Soil Remediation Standards, Groundwater Services, Inc., Houston, TX, sponsored by Partners in RBCA Implementation (PIRI).

Dragun, 1988; Lyman, et al., 1979; and Baes and Sharp, 1983

EPA Superfund Chemical Data Matrix, Appendix A - Chemical Data, Factor Values, and Benchmarks for Chemical Substances PDF. January 2004.

EPA, Soil Screening Guidance: Technical Background Document. 1996a. EPA/540/R95/128. May.

EPA, Soil Screening Guidance: User's Guide. 2nd Edition, July 1996b, EPA/9355.4-23 Attachment C to this document

EPA. 1991. Risk Assessment Guidance for Superfund, Volume I: Human Health Evaluation Manual (Part B, Development of Risk-Based Preliminary Remediation Goals). Interim. Publication 9285.7-01B. Office of Emergency and Remedial Response, Washington, DC. NTIS PB92-963333.

Howard, 1991. Handbook of Environmental Degradation Rates, CRC.

C. EVALUATING VAPOR INTRUSION

For additional information regarding assessing and mitigating the vapor intrusion pathway from subsurface vapor sources to indoor air, the Volunteer is referred to the following EPA guidance document.

EPA. 2015. Technical Guide for Assessing and Mitigating the Vapor Intrusion Pathway from Subsurface Vapor Sources to Indoor Air, U.S. Environmental Protection Agency, (OSWER Publication 9200.2-154) June 2015.

11. How can I get more information about the VRP?

For specific information to learn about VRP sites in your community, to obtain copies of other VRP Fact Sheets or other guidance documents, or to volunteer for the program, contact DEQ at (307) 777-7752 or through the VRP website at: http://deq.wyoming.gov/shwd/voluntary-remediation-program/

The VRP website includes all of the Fact Sheets and other guidance documents for the VRP. This website is updated frequently and includes the latest information about DEQ's progress in developing guidance, policy, and other supporting documents for the VRP.

Appendix A
Fate and Transport Models

The Soil Screening Guidance (U.S. Environmental Protection Agency (EPA), 1996a and b) addresses the migration to groundwater exposure pathways with simple equations that require a small number of easily obtained soil parameters, meteorologic conditions, and hydrogeologic parameters. These equations incorporate a number of conservative simplifying assumptions – an infinite source, no fractionation between pathways, and no biological or chemical degradation, conditions that can be addressed with more complicated models. The DEQ has selected the Inorganic and Organic Soil Screening Level (SSL) equations, with some modifications, as the Appendix A models for evaluating cleanup levels at Voluntary Remediation Program (VRP) sites. The DEQ recognizes that infinite source models can violate mass balance for certain contaminants (i.e., can release more contaminants than are present) and site conditions (e.g., small sources). Applying more complicated models can avoid these problems and more accurately define the risk of exposure via the migration to groundwater pathway, and, depending on site conditions, can lead to adjusted cleanup levels that are still protective. However, input data requirements and modeling costs make this option more expensive to implement than using the models in this Appendix.

The EPA developed the SSL equations, which combine exposure information assumptions with EPA toxicity data, for application at sites where future residential land use is anticipated (EPA, 1996a). The EPA Technical Background Document (EPA, 1996a) states that SSLs developed in accordance with this guidance can be used under State voluntary remediation programs (VRPs) to develop final cleanup levels based on the nine-criteria analysis described in the National Contingency Plan (Section 300.430 (e) (9) (iii)). The VRP has incorporated these criteria into the Remedy Selection Process (see VRP Fact Sheet #21).

The VRP has elected to use a Dilution and Attenuation Factor (DAF) of one (1) to develop its soil cleanup levels (see Fact Sheet #12). To remain consistent with this decision, the EPA SSL equations used in this Appendix were modified to remove the DAF of 20 (i.e., not allow modeling with a dilution factor) and instead, to incorporate a soil attenuation factor to account for sorptive mass redistribution to underlying clean soil in the migration to groundwater pathway.

1. Key Model Assumptions: The following model assumptions are inherent in the equations in this Appendix and should be reviewed for consistency with the conceptual site model to determine their applicability for the migration to groundwater pathway.

<u>Soil Attenuation Model (**Equation 1**)</u>

- Corresponds to movement of dissolved constituents through porous media
- No NAPLs present (if NAPLs are present, the Appendix A equations do not apply)
- The equation determines the maximum leachate concentration reaching the depth of groundwater, neglecting the effects of the diminishing source concentration over time as the leachate process continues

- Neglects the effects of competitive sorption of dissolved organic constituents

Modified Inorganic and Organic SSL Fate and Transport Models (**Equations 2 and 3**)

- Infinite source
- No contaminant attenuation by biodegradation or chemical degradation in the soil
- Instantaneous and linear equilibrium soil/water partitioning
- Unconfined, unconsolidated aquifer with homogeneous and isotropic hydrologic properties
- Receptor well at the downgradient edge of the source and screened within the plume
- No contaminant dilution or attenuation in the aquifer
- No NAPLs present (if NAPLs are present, the Appendix A equations do not apply)

2. Soil Attenuation Model Equations: The following equation, based on a model developed by Connor et al., 1997, corrects the equilibrium soil leachate concentration for the effect of sorptive mass loss as the leachate percolates downward toward the underlying water bearing unit. This adjustment can prove significant in deep groundwater systems, where a significant thickness of unaffected soils underlies the affected soil zone. Prior to reaching groundwater, percolating rainwater serves to redistribute this source mass among soil, air, and pore fluids throughout the full thickness of the surface soil column.

$$C_{w2}\ (\text{mg/L}) = C_{w1} \times \frac{L_2}{L_1} \qquad \textbf{(Eq 1)}$$

Soil Attenuation Model Input Parameters

Parameter/Definition (units)	Site-Specific	Default	Source
C_{w1} concentration of COC in soil leachate discharged to underlying water-bearing unit (mg/L)	-	Wyoming VRP Fact Sheet #13 groundwater cleanup values	EPA MCLs, WY DWELs
C_{w2} initial soil-water leachate concentration (mg/L) prior to adjustment for soil attenuation (the target soil-water leachate concentration)	-	-	Connor et. al., 1997
L_1 thickness of affected soil zone (cm)	allowed	152 cm	Connor et. al., 1997
L_2 distance from top of affected soil zone to top of water bearing unit (cm)	allowed	183 cm	Connor et. al., 1997

To determine site-specific values of these parameters for use in the Appendix A models, use the thickest (i.e., greatest vertical extent) area of contamination (L_1) coupled with the distance from the top of the contaminated soil zone to seasonal high groundwater (L_2). A site-specific distance from the top of the contaminated soil zone to seasonal high groundwater may generally be determined to be at least a minimum distance using site information from test pits or geoprobe investigations; however, the method for determining this distance should be discussed with DEQ.

3. Modified Inorganic SSL Fate and Transport Model: This model is based on the EPA SSL Soil-Water Partition Equation for Migration to Groundwater Pathway: Inorganic Contaminants (EPA, 1996). The Wyoming Department of Environmental Quality (DEQ) has eliminated the DAF of 20 that was used in the equation and has instead incorporated a simple soil attenuation factor equation based on a model by Connor et al., 1997 (in Eq 1). Although the DEQ encourages the use of site-specific data to calculate soil cleanup values using this equation (Eq 2), conservative default parameters are provided for use where site-specific data are not available.

$$C_t = C_{w2} \left\{ K_d + \frac{\theta_w + \theta_a H'}{\rho_b} \right\} \qquad \textbf{(Eq 2)}$$

Modified Inorganic SSL Fate and Transport Model Input Parameters

Parameter/Definition (units)	Site-Specific	Default	Source for Default
C_t cleanup level in soil (mg/kg)	-	-	-
C_{w2} target soil-water leachate concentration (mg/L)	allowed	Use value calculated from Eq 1	Connor et. al., 1997
K_d soil-water partition coefficient (L/kg)	-	chemical-specific	EPA, 1996b: Attachment C
θ_w water-filled soil porosity (L_{water}/L_{soil})	allowed	0.3 (30%)	U.S. EPA/ORD
θ_a air-filled soil porosity (L_{air}/L_{soil})	allowed	0.13	n - θ_w
n total soil porosity (L_{pore}/L_{soil})	allowed	0.43	$1 - \rho_b / \rho_s$
ρ_b dry soil bulk density (kg/L)	allowed	1.5	EPA, 1991
ρ_s soil particle density (kg/L)	allowed	2.65	EPA, 1991
H' dimensionless Henry's law constant	-	assume to be zero for inorganic contaminants (except for mercury: use H	EPA, 1991

		x 41 where 41 is a conversion factor)	
Parameter/Definition (units)	**Site-Specific**	**Default**	**Source for Default**
H Henry's law constant (atm-m^3/mol	-	chemical-specific (when calculating a value for mercury)	EPA, 1996b: Attachment C

4. Modified Organic SSL Fate and Transport Model: This model is based on the EPA SSL Soil-Water Partition Equation for Migration to Groundwater Pathway: Organic Contaminants (EPA, 1996). The Wyoming DEQ has eliminated the DAF of 20 that was used in the equation and has instead incorporated a simple soil attenuation factor equation based on a model by Connor et al., 1997 (in Eq 1). Although the DEQ encourages the use of site-specific data to calculate soil cleanup values using this equation (Eq 3), conservative default parameters are provided for use where site-specific data are not available.

$$C_t = C_{w2}\left\{\left(K_{oc}\ f_{oc}\right) + \frac{\theta_w + \theta_a\ H'}{\rho_b}\right\} \qquad \textbf{(Eq 3)}$$

Modified Organic SSL Fate and Transport Model Input Parameters

Parameter/Definition (units)	**Site-Specific**	**Default**	**Source**
C_t cleanup level in soil (mg/kg)	-	-	-
C_{w2} target soil-water leachate concentration (mg/L)	allowed	Use value calculated from Eq 1	Connor et. al., 1997
K_{oc} soil organic carbon-water partition coefficient (L/kg)	-	chemical-specific	EPA, 1996b: Attachment C
f_{oc} organic carbon content of the soil (kg/kg)	allowed	0.001 (0.1%)	Carel et al., 1988
θ_w water-filled soil porosity (L_{water}/L_{soil})	allowed	0.3 (30%)	U.S. EPA/ORD
θ_a air-filled soil porosity (L_{air}/L_{soil})	allowed	0.13	n - θ_w
n total soil porosity (L_{pore}/L_{soil})	allowed	0.43	$1 - \rho_b / \rho_s$
ρ_b dry soil bulk density (kg/L)	allowed	1.5	EPA, 1991
ρ_s soil particle density (kg/L)	allowed	2.65	EPA, 1991

H' dimensionless Henry's law constant	-	H x 41 where 41 is a conversion factor	EPA, 1991
H Henry's law constant (atm-m^3/mol	-	chemical-specific	EPA, 1996b: Attachment C

5. Sensitivity Analysis of Models: EPA conducted a sensitivity analysis to examine the effects of site-specific parameters on migration to groundwater SSLs (EPA, 1996a). The results indicated that for volatile chemicals, the model is somewhat sensitive to water content (e.g., up to 54% change in SSLs for chloroform), and less sensitive to bulk density (e.g., up to 18% change for chloroform). Organic carbon content has the greatest effect on SSLs for all chemicals except chloroform. As expected, the effect of f_{oc} increases with increasing K_{oc}.

Definitions

Advection: Advection involves the transfer of heat energy by means of horizontal mass motions through a medium. This is useful for dual-porosity systems allowing for preferential flow in fractures or macropores while storing water and dissolved chemicals in the matrix.

Biodegradation: Refer to Question 4, Fact Sheet #25 for the definition.

Cation Exchange: Chemical trading of cations between the soil minerals and organic matter with the soil solution and plant roots.

Complexation: Refers to molecules formed by the combination of ligands (usually organic ligands) and metal ions in soil solution. The properties of complexes depend on the metal, its oxidation number, and the number and type of the ligands.

Consecutive Decay Chains: The sequential application of decay equations repeated for organic or inorganic products of interest (e.g., Urea $\rightarrow NH_4^+ \rightarrow NO_3^- \rightarrow N_2$). Used for evaluating fate of nitrogen species, organic phosphates, pesticides, and radionuclides.

Convective transport: Convection involves the transfer of heat energy by means of vertical mass motions through a medium.

Diffusion: Molecular mixing of one substance into another substance.

Erosion: Transport of soil mineral particles and organic matter by wind, flowing water, or both.

Hydrodynamic Dispersion: Unsteady liquid flow and chemical reaction in soils and other porous materials resulting from pulse input. This causes extra spreading due to complicated flow paths around soil particles, differences in water velocity within single pores, and to differences in water velocity in adjacent pores.

Hydrolysis: Chemical weathering process that involves the reaction between mineral ions and the ions of water (OH- and H+), and results in the decomposition of the rock surface by forming new compounds, and by increasing the pH of the solution involved through the release of the hydroxide ions.

Oxidation: Loss of an electron during a chemical reaction from one atom to another.

Photolysis: Chemical decomposition (cleavage of one or more covalent bonds) of constituents in soils induced by light or other radiant energy.

Runoff: The topographic flow of water (generated by precipitation) from higher to lower elevations. It occurs when the infiltration capacity of an area's soil has been exceeded. It also refers to the water leaving an area of drainage. It is also called overland flow.

Sorption: Refer to Question #4, Fact Sheet #25 for the definition.

Volatilization: The process where a solid or liquid substance is converted into a gas.