Fact Sheet # 25

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 *Draft Guidance for Evaluating the Vapor Intrusion to Indoor Air Pathway from Groundwater and Soils* (EPA 2002) 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 2002).

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 W.S. 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.

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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.

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 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.state.wy.us/volremedi/index.asp

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 nonaqueous 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) located at http://www.epa.gov/superfund/health/conmedia/soil/pdfs/attachc.pdf. 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 available at
  http://www.epa.gov/superfund/resources/soil/introtbd.htm.

- EPA Superfund Chemical Data Matrix, Appendix A., available at
  http://www.epa.gov/superfund/sites/npl/hrsres/tools/scdm.htm

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. http://www.epa.gov/swerust1/rbdm/rbcafntm.pdf

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. http://www.epa.gov/superfund/sites/npl/hrsres/tools/scdm.htm

EPA, Soil Screening Guidance: Technical Background Document. 1996a. EPA/540/R95/128. May. http://www.epa.gov/superfund/resources/soil/introtbd.htm

EPA, Soil Screening Guidance: User's Guide. 2nd Edition, July 1996b, EPA/9355.4-23 http://www.epa.gov/superfund/resources/soil/ssg496.pdf Attachment C to this document at: http://www.epa.gov/superfund/health/conmedia/soil/pdfs/attachc.pdf

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. http://www.epa.gov/oswer/riskassessment/pdf/OSWERdirective9285.6-03.pdf

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

C. EVALUATING VAPOR INTRUSION USING THE JOHNSON AND ETTINGER MODEL

11. What is vapor intrusion?

Vapor intrusion is the migration of volatile chemical vapors from buried wastes, contaminated soil, contaminated groundwater, or free phase product, through the vadose zone and into overlying buildings. Vapors can migrate into buildings both with and without basements. The resulting indoor air concentrations may present a chronic health hazard due to long term exposure and, in some cases, (e.g., methane levels exceeding the LEL) could result in explosion hazards.

Vapor intrusion is generally only of concern when volatile chemicals (e.g., Henry's Law Constant > 10^{-5} atm m^3/mol) are present in the subsurface below or near occupied buildings (existing or future). Common volatile chemicals include volatile organic compounds (e.g., EPA Method 8260

or TO-15 compounds), naphthalene, and mercury. Vapor intrusion is unlikely to be of concern if existing or potential buildings are more than 100 feet from the edge of source (e.g., the edge of the dissolved plume in groundwater), and no unusual preferential pathways for vapor migration exist (EPA, 2002). For example, typical utility laterals and concrete and asphalt are not sufficient to create a preferential pathway.

The vapor intrusion pathway begins with partitioning of the volatile chemicals of concern from the source material (e.g., contaminated soil, dissolved plumes, and waste) to the vapor phase in the vadose zone. Vapors will then diffuse through the unsaturated soil in the direction of lower concentration (usually upwards) according to Fick's First Law of Diffusion. The rate of diffusion is controlled by the chemical gradient and the effective diffusivity of the soil which, in turn, is controlled by the air content of the soil. Higher levels of saturation (lower air content) will impede vapor diffusion, while lower levels of saturation (higher air content) will enhance vapor diffusion.

Once vapors come within a few feet of building foundations, they may be pulled into the building by the flow of air, or advection, whenever air pressures in the building are lower than ambient air pressures. Reduced building pressures can be caused by: (1) temperatures inside the building that are higher than outside temperatures, creating rising air currents or a "stack" effect; (2) strong winds blowing over the building; and (3) operation of heating and ventilation equipment, including oven hood and bathroom exhaust fans and clothes dryers. Vapors will migrate more freely into buildings with exposed earth floors, sumps or other large openings, and cracked or broken floor slabs and foundation walls (e.g., field stone walls).
Soil vapors that enter a building due to diffusion and/or advection will mix and become diluted by ambient air that flows through the building. The average air exchange rate in residential homes in the winter ranges from about one exchange every two hours in warm climates, to about one exchange every four hours in cold climates (EPA, 2004). Summer air exchange rates are generally higher.

The potential impact of vapor intrusion on human health depends on the toxicity of the chemical, the concentration in the air, the frequency and duration of exposure, and the receptor (e.g., adults versus children). See Fact Sheet #20 *Human Health Risk Assessment.*

12.   How should I evaluate the potential for vapor intrusion?

The first step in any vapor intrusion evaluation is determining whether an immediate safety hazard (e.g. explosion) or acute health risk exists. If these risks do not exist, the potential for long-term chronic health impacts should be evaluated. Although indoor air samples may be collected to directly evaluate the potential for vapor intrusion, DEQ recommends a step-wise screening process to avoid unnecessary testing and the complications that may arise when trying to interpret indoor air test results (due to the potential for background or indoor sources of many compounds).

EPA (2002) provides a general screening approach that is acceptable to DEQ if performed properly according to the most recent version of this guidance. The first step involves determining whether volatile chemicals are present in the vicinity of existing or future buildings; if the answer to both questions is no, vapor intrusion is not of concern. If vapor intrusion cannot be ruled out at step one, then concentrations of COCs in groundwater and/or soil vapor may be compared to generic or semi-site specific screening levels (based on depth and soil type). The screening levels in EPA (2002) should be modified, as necessary, to conform to toxicity criteria approved by DEQ. A one-in-one million risk level should be used for screening purposes; however, screening levels are not necessarily action or cleanup levels. Exceedance of a screening level only indicates the need for further evaluation.

Concentration data must be based on a sufficient number of representative samples collected according to DEQ approved procedures. For example, groundwater samples must be collected from wells screened across the water table with a screen length no deeper than 10 feet below the water table. Soil vapor samples should be collected from a depth of at least five feet below the ground surface and at or below the building foundation depth, following good sample collection practices (e.g., API 2005, NYSDOH, 2005).

If groundwater and/or soil vapor concentrations exceed EPA screening levels, more site-specific evaluation of the potential for vapor intrusion will be necessary. This may include:

- Collection of additional site specific data including groundwater concentrations, soil vapor concentrations, and/or sub-slab vapor concentrations; soil properties; and building and occupant information (existing or future);
- Use of the Johnson and Ettinger Model (EPA, 2004) incorporating site-specific data and information, as described below; and/or
- Indoor air testing (consult with DEQ regarding appropriate guidance and procedures).

The remainder of this fact sheet discusses DEQ's expectations when the Johnson and Ettinger Model is being used for vapor intrusion evaluations.

13.   What is the Johnson and Ettinger Model?

The Johnson and Ettinger Model (JE Model) is a one-dimensional screening-level model used to estimate the transport of contaminant vapors from a subsurface source to indoor air spaces, based on the work of Johnson and Ettinger (1991). The model considers diffusion and convection of vapors as well as building volume and air exchange rate to calculate indoor air concentrations, based on concentrations in soil vapor or groundwater and site-specific or default values for soil and building properties. A spreadsheet version of the JE model and guidance for its use are provided by EPA (2004).

Because of the simplicity of the model and the large number of soil and building parameters that can affect vapor intrusion, and the potential uncertainty associated with many of these parameters, the JE Model is generally considered to have a precision no greater than one order

of magnitude (EPA, 2004; Weaver and Tillman, 2005). Therefore, the model may over-predict or under-predict indoor air concentrations, by an order of magnitude, even if the model is applied correctly and representative media concentration values are input. Use of conservative input parameters will increase the odds that the model is over-predicting indoor air concentrations. Johnson (2002) recommends identifying the critical parameters associated with any modeled scenario and conducting sensitivity analyses for these parameters.

14. When should I use the JE Model?

The JE model can be used to identify sites or buildings which require a more detailed evaluation (e.g., indoor air testing) when the results of screening indicate further evaluation is warranted (see above). DEQ will also consider use of the JE Model in lieu of indoor air testing a) when site conditions do not preclude the model's use (see below), b) when the most up-to-date EPA version of the model has been applied correctly using representative or reasonable default values for all parameters, d) when sensitivity analyses have been conducted by varying the most critical parameters over reasonable ranges, e) when the results have been interpreted conservatively, and f) when indoor air testing would be difficult or potentially inconclusive. The JE Model will likely be necessary to evaluate the potential for vapor intrusion in future buildings, since indoor air tests cannot be conducted in buildings that do not exist (alternatively, appropriate institutional controls that require pre-emptive mitigation or testing of buildings when built can be considered).

15. Can the JE Model be used at my site?

Because the JE model was developed as a screening tool, it is based on a number of simplifying assumptions regarding contaminant distribution and occurrence, subsurface characteristics, transport mechanisms, and building construction. Therefore, use of the JE Model will not be allowed when site conditions are inconsistent with model assumptions. Specific conditions that will preclude the use of the JE Model (adapted from EPA 2004) include:

- The presence of residual or liquid free-product below or within 100 feet (horizontally) of the building.
- Contamination that is only present under a small portion of the building (more likely with large buildings).
- Geologic materials that do not behave like porous media (i.e., like soils), including fractured bedrock where the primary porosity occurs in the fractures, and karst formations. Finely fractured clays and weathered sedimentary bedrock may be modeled if fractures are so closely spaced, or the material so weathered, that it behaves more like a porous medium than a fractured rock.
- Sites where significant lateral flow of vapor occurs due to atypical preferential pathways or pressure-driven flow (e.g., landfill gas). Typical utilities, such as water and sanitary sewer

laterals running into a building are not considered to be preferential pathways precluding the use of the model.

- Very shallow groundwater where the basement is in contact with the groundwater or capillary zone.

In addition, temporal variability due to seasonal fluctuations or plume migration should be considered and long-term average or conservative conditions should be modeled (e.g., media concentrations, depth to groundwater, temperatures).

Although EPA (2002, 2004) does not recommend using the JE Model for buildings with crawl spaces, more recent evaluations have indicated that crawl spaces can be modeled by setting the floor thickness to 0 and the portion of the floor that is a "crack" to 1 (i.e., 100%). In many cases, diffusion of vapors through the underlying soil is the rate limiting factor and the presence or lack of a slab has little effect on predicted indoor air concentrations.

16.   Which version of the JE Model should I use?

DEQ accepts the use of the most current version of the JE Model on the EPA OSWER website (www.epa.gov/oswer/riskassessment/airmodel/johnson_ettinger.htm) at the time of the evaluation. Use of other versions or models must be approved in advance by DEQ.

17.   Who is qualified to run the JE Model?

Model users should have training and experience in the use of the JE Model and be familiar with current model guidance (e.g., EPA, 2004). Although the EPA spreadsheet version of the model is relatively easy to use, mistakes can be made and the significance of certain parameter selections and their interactions with other aspects of the model are not always obvious. Further, the modeling team should have sufficient skills in geology, hydrogeology, environmental chemistry, and risk assessment to select appropriate and representative values for all soil and concentration parameters and exposure assumptions.

18.   Does DEQ require sensitivity analyses when using the JE Model?

Yes. The following table from the draft EPA guidance describes the uncertainty involved in determining key model parameters and the sensitivity of the JE model to those parameters.

Table G-2. Uncertainty and Sensitivity of Key Parameters for the Johnson & Ettinger Model.

Input Parameter	Parameter Uncertainty or Variability Variability	Parameter Sensitivity			
		Shallower Contamination Building Underpressurized	Deeper Contamination Building Underpressurized	Shallower Contamination Building Not Underpressurized	Deeper Contamination Building Not Underpressurized
Total Porosity	Low	Low	Low	Low	Low
Unsaturated Zone Water-filled Porosity	Moderate to High	Low to Moderate	Moderate to High	Moderate to High	Moderate to High
Capillary Transition Zone Water-filled Porosity	Moderate to High	Moderate to High	Moderate to High	Moderate to High	Moderate to High
Capillary Transition Zone Height	Moderate to High	Moderate to High	Moderate to High	Moderate to High	Moderate to High
Soil Bulk Density	Low	Moderate to High	Low to Moderate	Low	N/A
Qsoil	High	Moderate to High	Low to Moderate	N/A	N/A
Soil air permeability	High	Moderate	Low to Moderate	N/A	N/A
Building Depressurization	Moderate	Low to Moderate	Low to Moderate	N/A	Low to Moderate
Henry's Law Constant (for single chemical)	Low to Moderate	Low	Low	Low to Moderate	Low
Free-Air Diffusion Coefficient (single chemical)	Low	Moderate	Moderate	Low	Moderate
Building Air Exchange Rate	Moderate	Moderate	Moderate	Moderate	Moderate
Building Mixing Height	Moderate	Low to Moderate	Low to Moderate	Moderate	Low to Moderate
Subsurface Foundation Area	Low to Moderate	Low	Low	Low to Moderate	Low
Depth to Base of Foundation	Low	Low	Low	Low	Low to Moderate
Building Crack Ratio	High	Low	Low	Moderate to High	Low
Crack Moisture Content	High			Moderate to High	
Building Foundation Slab Thickness	Low			Low	

For model parameters which have significant uncertainty (e.g., Qsoil, building air exchange rate, and moisture content) and to which the JE model exhibits a moderate, moderate to high, or high sensitivity it is recommended a sensitivity analysis be performed utilizing several values within the specified range of values to determine the magnitude of the effect on the model output.

19.   Does DEQ specify default values for input parameters?

Yes, DEQ recommends following the recommended reasonable conservative range of building-related and soil-dependent parameters as provided in the EPA draft *Guidance for Evaluating the Vapor Intrusion to Indoor Air Pathway from Groundwater and Soils*.

20.   Where can I find the JE Model?

JE Model spreadsheets can be downloaded from:
http://www.epa.gov/oswer/riskassessment/airmodel/johnson_ettinger.htm.

21.   Does the JE Model consider biodegradation?

No. However, DEQ is aware that aerobic biodegradation of petroleum hydrocarbons vapors in the vadose zone can be significant, often reducing the potential impacts on buildings. Sufficient oxygen must be available in the vadose zone, below the building of concern, for biodegradation to occur. In situations where high concentrations of petroleum (e.g., free phase product) are present below the building and the distance between the building and the groundwater table is relatively small compared to the size of the building, oxygen may be depleted, preventing further biodegradation. Biodegradation is more likely to occur when free phase product is not present, the distance to the water table is large compared to the building dimensions, and the soils are

permeable. To account for the effects of biodegradation, modeling should be conducted using soil vapor data that are representative of conditions below the building and at a depth where biodegradation has already taken place. Soil vapor samples could be collected under the building (e.g., sub-slab), or immediately adjacent to the building. In the latter case, samples should be collected from a depth below the lowest slab and oxygen levels should be measured. If the oxygen level is less than 10% by volume, sub-slab samples should be collected to ensure that oxygen has not been depleted below the building (rendering exterior soil vapor samples non-representative). For more information on the effects of aerobic biodegradation on vapor intrusion potential see Abreu and Johnson (2006).

Biodegradation of chlorinated organics is generally not significant in the vadose zone compared to petroleum compounds.

22. Does DEQ have any guidance on soil vapor sampling methods?

DEQ currently recommends following the guidance in API (2005). NYSDOH (2005) also provides useful guidance on soil vapor sampling methods, including the use of various tracer gases to ensure sample integrity.

23. Vapor Intrusion References

Abreu, Lillian D. V. and Paul C. Johnson, 2006. *Simulating the Effect of Aerobic Biodegradation on Soil Vapor Intrusion into Buildings: Influence of Degradation Rate, Source Concentration, and Depth*. Environ. Sci. Technol. 2006, 40, 2304-2315.

API, 2005. *Collecting and Interpreting Soil Gas Samples from the Vadose Zone: A Practical Strategy for Assessing the Subsurface Vapor-to-Indoor Air Migration Pathway at Petroleum Hydrocarbon Sites*. Regulatory Analysis and Scientific Affairs, API Publication Number 4741, November 2005.

EPA, 2002. *Draft Guidance for Evaluating the Vapor Intrusion to Indoor Air Pathway from Groundwater and Soils (Subsurface Vapor Intrusion Guidance)*. Office of Solid Waste and Emergency Response, U.S. Environmental Protection Agency. (Docket ID No. RCRA-2002-0033 November 2002). Available at http://www.epa.gov/correctiveaction/eis/vapor.htm

EPA, 2004. *User's Guide for Evaluating Subsurface Vapor Intrusion into Buildings*. Prepared by Environmental Quality Management, Inc. for USEPA, Office of Emergency and Remedial Response, Washington, D.C., Revised February 22, 2004. Available at http://www.epa.gov/oswer/riskassessment/airmodel/johnson_ettinger.htm

Johnson, Paul C. and Robert A. Ettinger, 1991. *Heuristic Model for Predicting the Intrusion Rate of Contaminant Vapors into Buildings*. Environ. Sci. Technol. 1991, 25, 1445-1452.

Johnson, Paul C., 2002. *Identification of Critical Parameters for the Johnson and Ettinger (1991) Vapor Intrusion Model.* API Bulletin No. 17, May 2002.

NYSDOH, 2005. *Guidance for Evaluating Soil Vapor Intrusion in the State of New York*, Public Comment Draft, New York State Department of Health, Center for Environmental Health, Bureau of Environmental Exposure Investigation, February 2005.

Weaver, James W. and Fred D. Tillman, 2005. *Uncertainty and the Johnson-Ettinger Model for Vapor Intrusion Calculations.* EPA Office of Research and Development, National Exposure Research Laboratory, EPA/600/R-05/110.

24.   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.state.wy.us/volremedi/index.asp.

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.

Soil Attenuation Model (**Equation 1**)
- 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.

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

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	EPA, 1991

Parameter/Definition (units)	Site-Specific	Default	Source for Default
		(except for mercury: use H x 41 where 41 is a conversion factor)	
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.

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

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}.

<u>**Definitions**</u>

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 5, 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 #5, Fact Sheet #25 for the definition.

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