Batch Test Leaching Model Equations

The equations discussed below are incorporated into the Excel-based Batch Test Leaching Model that accompanies this technical memorandum. Figure 5 in the main text depicts the first page of the model (April 2007 version). The model will be updated as needed in the future.

Step 1. Calculate a partition coefficient for each chemical of potential concern.

The results of the SPLP test can be used to develop a sample-specific partition coefficient (Kd) for each chemical of potential of concern. The partition coefficient is calculated as follows (after Roy et. al, 1992; see also McClean and Bledsoe, 1992, and USEPA 1999):

$$Kd\ (L/kg) = \frac{Concentration_{sorbed}\,(\mu g/Kg)}{Concentration_{solution}\,(\mu g/L)} \tag{1}$$

where Concentration$_{sorbed}$ is the concentration of the contaminant that remained sorbed to the soil following the batch test and Concentration$_{solution}$ is the resulting concentration of the contaminant in the batch test solution. The term Kd is commonly reported in equivalent units of (ug/g)/(ug/cm^3) or cm^3/g, based on an assumed batch test solution density of 1.0 g/cm^3.

The sorbed concentration of the contaminant is calculated as follows:

$$Concentration_{sorbed}(ug/kg) = \frac{Mass_{sorbed}\,(\mu g)}{Sample\ Mass\,(kg)}. \tag{2}$$

where Mass$_{sorbed}$ is the mass of the contaminant still sorbed to the soil following the batch test. The mass of the sample called for in the SPLP batch test is 100 grams or 0.1 Kg (USEPA 1994).

The mass of the contaminant sorbed to the soil is calculated by subtracting the mass of the contaminant that went into the batch test solution from the initial, total mass of the contaminant in the soil sample:

$$Mass_{sorbed}\,(\mu g) = Mass_{total}\,(\mu g) - Mass_{solution}\,(\mu g) \tag{3}$$

where Mass$_{total}$ is original, total mass of the contaminant in the soil sample and Mass$_{solution}$ is the mass of the contaminant in the batch test solution. The total mass of the contaminant in the soil sample is calculated as:

$$Mass_{total}(\mu g) = Concentration_{total}\ (mg/kg) \times \left(\frac{1{,}000\,\mu g}{1mg}\right) \times Sample\ Mass(kg) \tag{4}$$

where Concentration$_{total}$ is the reported total concentration of the contaminant in the soil sample that used in the batch test (tested on a split sample). The mass of the contaminant in the batch test solution is calculated as:

$$Mass_{solution}(\mu g) = Concentration_{solution}(\mu g/L) \times Solution\,Volume(L)\,. \tag{5}$$

The default volume of solution used in SPLP batch tests is two liters (USEPA 1994).

Note that use of the batch test method to estimate Kd values is not longer valid if the solubility limit of the contaminant is exceeded in the batch test solution (refer to section on Leaching of Heavily Contaminated Soils in the main text). Exceeding the contaminants solubility suggests that free product is present in the soil (either liquid or dry). As a precautionary measure, a cutoff of 75% the assumed contaminant solubility is used in the Batch Test Leaching Model spreadsheet to identify if free product may be present in the batch test solution. The free product acts as a second reservoir of contaminant mass that will bias the true equilibrium concentration of the contaminant in the dissolved and sorbed phases. To accurately calculate desorption coefficients, batch test analyses must be run samples with lower concentrations of the contaminant in soil.

Step 2. Estimate the concentration of the contaminant in source-area leachate.
Once the soil-specific Kd value for a target contaminant has been determined, it is relatively simple to estimate the concentration of the contaminant in the soil moisture or "leachate" within the main body of contaminated soil or the leachate "source area"). This is done by incorporating the calculated Kd into a simple equilibrium partitioning equation and assuming default (or site-specific) soil properties (after USEPA 2001):

$$C_{total} = C_{leachate} \times \left(Kd + \left(\frac{\theta_w + (\theta_a \times H')}{\rho b} \right) \right) \times \left(\frac{1mg}{1000\mu g} \right) \qquad (6)$$

where: C_{total} = Total concentration of chemical in sample (mg/kg);

$C_{leachate}$ = Dissolved-phase concentration of chemical (µg/L);

Kd = Estimated or measured partition coefficient L/kg;

$Theta_w$ = water-filled porosity (L_{water}/L_{soil});

$Theta_a$ = air-filled porosity (L_{air}/L_{soil});

H' = Henry's Law Constant at 25°C ((µg/L-vapor)/(µg/L-water)); and

p_b = Soil bulk density (Kg/L).

Table H in Appendix 1 of the HDOH EAL document provides a summary of "dimensionless" Henry's Law Constants (H') for common volatile contaminants (HDOH 2005). For the purpose of calculating Tier 1 action levels, Kd is calculated as the chemical's published organic carbon partition coefficient (koc) times the fraction organic carbon in the soil (foc). This is discussed in Appendix 1 of the HDOH Environmental Action Levels document (HDOH 2005). Note that in this equation Kd and p_b are expressed in units of L/Kg and Kg/L, respectively, rather than in equivalent units of cm^3/g and g/cm^3. A default soil density of 1.5 Kg/L and soil porosity of 43% (0.43) are typically used in Tier 1 risk assessment models (e.g., USEPA 2001, 2004).

Equation 6 can be rearranged to solve for $C_{leachate}$ as follows:

$$C_{leachate} = C_{total} \div \left(\left(Kd + \left(\frac{\theta_w + (\theta_a \times H')}{\rho b} \right) \right) \times \left(\frac{1mg}{1000\mu g} \right) \right). \qquad (7)$$

This equation is incorporated into the "Batch Test Leaching Model" worksheet of the Excel file that accompanies this technical memo. The sorption coefficient should be used to estimate the dissolved-phase concentration of the contaminant in a hypothetical, saturated sample of soil at equilibrium and at the same contaminant concentration as the SPLP test. Since the soil is assumed to be fully saturated with water, the vapor-phase term of the equation "θ_a x H'" goes to zero.

Step 3. Tier 3 calculation of ultimate contaminant concentration in groundwater.

A conservative estimate of the contaminant concentration in groundwater that cuold be impacted by the leachate is made by dividing the calculated concentration of the contaminant in leachate by an assumed groundwater:leachate dilution factor (DF):

$$C_{groundwaater} = \frac{C_{leachate}}{DF} \qquad (8)$$

$$DF = \frac{\text{Volume Impacted Groundwater}}{\text{Volume Leachate}}. \qquad (9)$$

where: $C_{groundwater}$ = Concentration of chemical in groundwater (µg/L);
$C_{leachate}$ = Concentration of chemical in leachate (µg/L); and
DF = Groundwater/Leachate dilution factor (m^3/m^3).

This equation is incorporated into the Batch Test Leaching Model spreadsheet that accompanies this technical memo. A default DF of 20 is considered appropriate for sites less than or equal to 0.5 acres in size (USEPA 2001). A more site-specific DF factor can be calculated if needed, based on the following equation (USEPA 2001):

$$\text{Dilution Factor} = 1 + \left(\frac{K \times i \times d}{I \times L} \right) \qquad (10)$$

where "K" is the aquifer hydraulic conductivity (m/year), "i" is the regional hydraulic gradient, "d" is the assuming mixing zone depth (default is two meters), "I" is the surface water infiltration rate (m/year" and "L" is the length of the contamianted soil area that is parallel to groundwater flow (m).

Note that this equation does not consider an expected reduction in contaminant concentrations as the leachat migrates downward. This component of the evalaution can be included in more site-specific evaluations as needed.

Soil Gas Leaching Model

For volatile contaminants, soil gas data offer an alternative approach for estimation of contaminant concentrations in leachate as well as a method to evaluate the threat posed to groundwater by downward migrating vapor plumes. The relationship between vapor-phase and dissolved-phase volatile chemicals under equilibrium conditions is relatively straightforward:

$$H' = \frac{Cvapor\ (ug/L)}{Cleachate\ (ug/L)}. \qquad (11)$$

where: H'=Henry's Law Constant at 25°C;

C_{vapor}= Vapor-phase concentration in soil gas;

$C_{leachate}$= Dissolved-phase concentration in soil pore waters.

Table H in Appendix 1 of the HDOH EAL document provides a summary of "dimensionless" Henry's Law Constants (H') for common volatile contaminants (HDOH 2005). To calculate the concentration of the contaminant in the soil moisture the equation is rearranged to solve for "$C_{leachate}$." The C_{vapor} term is also adjusted to units of ug/m3 to correspond with the units typically reported in site data:

$$Cleachate\ (ug/L) = \frac{Cvapor\ (ug/m3) \times \frac{1\,m3}{1{,}000\,L}}{H'}. \qquad (12)$$

Equation 8 above can be used to estimate potential impacts to groundwater with respect to soil gas-based estimates of contaminant concentrations of the in leachate.

Soil gas "action levels" for protection of groundwater can be developed by rearranging the equation to solve for C_{vapor} and setting $C_{leachate}$ equal to a target leachate goal (e.g., groundwater action level times appropriate groundwater:leachate dilution factor):

$$\text{Cvapor (ug/m3)} = \text{Cleachate (ug/L)} \times \text{H}' \times \frac{1{,}000\ \text{L}}{1\ \text{m3}} \times \text{AF} \qquad (13)$$

The term "AF" is an attenuation factor that describes the anticipated decrease in contaminant concentrations over time as the vapor migrates to and eventually impacts groundwater (e.g., via natural degradation, resorption to soil particles or migration into soil moisture). Approaches for calculation of site-specific, vapor attenuation factors are not well established and beyond the scope of this technical memorandum.