

**Appendix C**  
**Technical Background Document**  
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This appendix is intended to provide supporting documentation for the OIS Tier 1 and Tier 2 process. The first section, 1.0, presents the equations used and assumptions made in Tier 1 and Tier 1A. Section 2.0 presents a summary of the models allowed in Tier 2.

## **1.0 Tier 1**

The following sub-sections 1.1 through 1.5 describe the Colorado RBCA Tier 1 exposure pathways, input parameters, equations used, and input variables that can be changed in the Tier 1A process.

### **1.1 Tier 1 Exposure Pathways**

In this section each of the exposure pathways/RBSLs will be discussed. The assumptions made for each exposure pathway are listed, as well as the input variables that are unique to the pathway.

#### **1.1.1 Surficial Soil: Ingestion/Dermal Contact/Inhalation**

Surficial soil is defined as the top 1 meter of soil. The RBSLs for surficial soil assume that all four of the following potential exposure scenarios occur simultaneously:

- ingestion of soil;
- dermal contact with soil;
- inhalation of vapors in outdoor air; and
- inhalation of particulates in outdoor air.

The four doses from these exposure scenarios are added together to obtain an overall dose from surficial soil, from which the RBSL is then calculated. This is the only RBSL that accounts for multiple exposure pathways with a single RBSL. The RBSL equations for carcinogens and for non-carcinogens, residential and commercial scenarios are presented in Section 1.3.

Ingestion and dermal contact with soil are direct pathways: the receptor is assumed to come in contact with the chemical of concern in the source medium (i.e., surficial soil).

Inhalation of vapors and inhalation of particulates are indirect pathways: the receptor is assumed to come in contact with the chemical of concern outside of the source medium (i.e., not in the surficial soil). For the inhalation scenarios, a concentration in soil is calculated below which air quality in the breathing zone is not jeopardized. Two volatilization factors are employed to account for the chemical moving from soil to outdoor air: in one case as a vapor; in the other as a particulate. The equations for these two volatilization factors are presented in Section 1.3.

The assumptions made in the calculation of this RBSL are:

- The risk is additive from four pathways: ingestion of soil, dermal contact with soil, inhalation of vapors and inhalation of particulates.
- The concentration in surficial soil is assumed to be uniformly distributed (constant) with depth.
- The concentration does not change over the exposure duration.

- Dermal absorption rates remain constant over the exposure duration.
- The distribution of chemical in the various phases (sorbed, dissolved and vapor) in the soil is assumed to follow linear, equilibrium partitioning.
- There is no biodegradation in any of the chemical phases in the soil.
- The outdoor air is assumed to be well mixed in the breathing zone “box”.
- If the volatilization factor calculated exceeds the total amount of chemical estimated to be in the soil, the volatilization factor is determined using a mass balance approach where it is assumed that all of the mass volatilizes from the surficial soil during the exposure duration.

The input parameters that are (somewhat) unique to this pathway are listed below:

<i>Soil ingestion rate</i>	<i>Depth of surficial soil</i>	<i>Particulate emission rate</i>
<i>Skin surface area exposed</i>	<i>Air diffusion coefficient</i>	<i>Average wind speed</i>
<i>Outdoor inhalation rate</i>	<i>Moisture content</i>	<i>Width of source</i>
<i>Time spent outdoors</i>	<i>Air content</i>	<i>Height of breathing zone</i>
<i>Dermal absorption</i>	<i>Porosity</i>	<i>Fraction organic carbon</i>
<i>Soil adherence to skin</i>	<i>Henry’s law coefficient</i>	<i>Soil bulk density</i>

This list does not include those input parameters that are common to every pathway (e.g. toxicity values, exposure duration, body weight, etc.).

### 1.1.2 Subsurface Soil: Ingestion Of Groundwater Impacted By Leachate

Subsurface soil is defined as the unsaturated soil that is deeper than 1 meter below ground surface and extends to the water table. In this pathway, the RBSL in soil is calculated so that concentrations in groundwater 10 meters downgradient from the source will not exceed MCLs. The distance of 10 meters away from the source area was chosen to account for some of the dilution processes that would occur in a pumping well. The ASTM approach assumes that the groundwater in the upper 2 meters of the aquifer directly underneath the source is the groundwater that the receptors would come in contact with. The concentration actually measured in a well would be much lower than the actual concentration in the aquifer for several reasons: (1) water wells used to supply water for domestic or other purposes usually have screen lengths much greater than 2 meters and (2) a pumping well pulls water in radially (from upgradient, downgradient and below the well screen). In Tier 1, putting the well 10 meters downgradient of the source had very little impact on the RBSLs in soil because the attenuation factor calculated between the source and 10 meters downgradient was close to 1 for all chemicals of concern. This approach was chosen so that in Tier 1A, site-specific parameters could be accounted for easily and a more realistic attenuation factor calculated.

Ingestion of groundwater impacted by leachate from subsurface soil is an indirect pathway meaning that a transfer from one media to another occurs. A leaching factor is calculated to account for partitioning in the unsaturated zone and to get the source concentration in groundwater. The Domenico groundwater model is then used to estimate groundwater concentrations in the aquifer 10 meters downgradient from the source. This pathway uses the same leaching factor as presented by the ASTM. The approach differs from the ASTM in two ways: the point of exposure in groundwater is assumed to occur 10 meters downgradient of the source (at the water table) and the concentration in

groundwater at the point of exposure is assumed to be the MCL for the chemical of concern, not a calculated RBSL in groundwater as is the case in the ASTM approach.

The Domenico model is a simple groundwater dispersion model that can account for three-dimensional dispersion and first-order degradation.

The assumptions made in the calculation of this RBSL are:

- The concentration in the subsurface soil is assumed to be uniformly distributed (constant) from 1 meter below ground surface to the water table.
- The concentration in soil does not change over the exposure duration, it does not deplete.
- No losses due to degradation or volatilization occur in the unsaturated zone.
- The distribution of chemical in the various phases (sorbed, dissolved and vapor) in the unsaturated and saturated zones is assumed to follow linear, equilibrium partitioning.
- The flow in the aquifer is uniform and constant.
- The aquifer and unsaturated zone properties are homogeneous.
- A minimum first-order degradation rate is assumed in the aquifer for each chemical. Section 1.3 presents the values used and the rationale for choosing them.
- If the RBSL calculated exceeds the value for which the equilibrated vapor and dissolved pore-water phases become saturated (residual level), a “RES” is entered as the RBSL indicating that the MCL cannot be reached or exceeded for that compound given the specified exposure scenario.

The input parameters that are unique to this exposure pathway are:

<i>Fraction organic carbon</i>	<i>Soil bulk density</i>
<i>Width of source</i>	<i>Dispersivity in the aquifer</i>
<i>Moisture content</i>	<i>Degradation rate</i>
<i>Air content</i>	<i>Thickness of mixing zone (in the aquifer)</i>
<i>Porosity</i>	<i>Hydraulic conductivity and gradient (Darcy velocity)</i>
<i>Henry's law coefficient</i>	<i>Distance downgradient</i>
<i>Infiltration rate</i>	

### 1.1.3 Soil Vapor: Inhalation of Indoor Air Vapors

In this exposure pathway, RBSLs are calculated in soil vapor that are protective of inhalation of indoor air. Soil vapor measurements, taken very near the soil source, are then compared to the soil vapor RBSLs calculated for Tier 1.

The RBSL in soil vapor is calculated by estimating an attenuation factor that accounts for diffusion in the unsaturated zone and building foundation and dilution and mixing with the air in the building. In order to calculate the RBSL in soil vapor, an acceptable risk-based indoor air concentration is calculated first. Then the attenuation factor is applied to calculate the soil vapor concentration. The equations used to estimate the risk-based concentration in air are presented in Section 1.4. The Johnson & Ettinger (1991) model was used to calculate the attenuation factor. This model considers advection (pressure-driven vapor flow) as well as diffusion processes. Pressure-driven vapor flow arises when the basement of the building is under-pressurized relative to the surrounding soil vapor. This condition causes the soil vapor surrounding the building to be drawn into the basement by advection (with flow of air). Under-pressurization can occur when running a heater in the building.

The ASTM equations for calculating RBSLs in soil, protective of indoor air, consider diffusion only. The Johnson and Ettinger model could be considered more conservative than the diffusive only model used by ASTM. The attenuation equation (considering both advection and diffusion) are presented in section 1.4.

The assumptions made in the calculation of this RBSL are:

- The soil vapor concentration in the subsurface soil near the source is assumed to be constant and does not deplete with time (infinite source).
- No mass is lost due to degradation or leaching.
- The soil vapor migrates into the building due to pressure-driven flow and diffusive transport.
- The distribution of chemical in the various phases (sorbed, dissolved and vapor) in the unsaturated and saturated zones is assumed to follow linear, equilibrium partitioning.
- The air in the building is well mixed and can be estimated by assuming a fresh air exchange rate.
- The unsaturated zone properties are homogeneous.
- The diffusion through the building foundation is assumed to occur in soil-filled cracks in the foundation.

The input parameters that are unique to this exposure pathway are:

<i>Fraction organic carbon</i>	<i>Henry's law coefficient</i>	<i>Diffusion coefficient in air</i>
<i>Soil bulk density</i>	<i>Thickness of the foundation</i>	<i>Diffusion coefficient in water</i>
<i>Moisture content</i>	<i>Fraction of cracks</i>	<i>Ceiling height in building</i>
<i>Air content</i>	<i>Air content in cracks</i>	<i>Air exchange rate in building</i>
<i>Distance to the building</i>	<i>Water content in cracks</i>	<i>Pressure difference</i>
<i>Intrinsic permeability of soil</i>	<i>Distance from basement to soil vapor source</i>	

### 1.1.4 Groundwater: Inhalation of Indoor Air Vapors

Inhalation of indoor air vapors volatilizing from groundwater is an indirect pathway. This RBSL is used for the case where groundwater may be contaminated but the soil is not contaminated. Otherwise it is expected that volatilization from soil will drive the selection of a RBSL. This RBSL would only be used for non-potable aquifers since the MCL is expected to be lower than the RBSL calculated here.

The RBSL is calculated using an attenuation factor that considers diffusion through a capillary fringe, the unsaturated zone, and the building foundation. In this scenario, the contaminant source is the dissolved concentrations in groundwater and so advection of soil vapor is not considered to increase the release of the contaminants—only diffusion processes are considered in the equations.

The assumptions made in the calculation of this RBSL are:

- A depth-weighted effective diffusion coefficient is calculated considering diffusion in the capillary fringe, the unsaturated zone, and the building foundation.
- The contaminant moves up through the unsaturated zone by diffusion only (no advective flow).
- The concentration in groundwater remains constant (and dissolved) throughout the exposure duration.
- No mass is lost from the aquifer due to degradation, dispersion or advection (plume moving away).
- No mass is lost while the chemical is diffusing upwards to the building.
- The distribution of chemical in the various phases (sorbed, vapor and dissolved) at the water table-unsaturated zone interface is assumed to follow linear, equilibrium partitioning.
- The air in the building is well mixed and can be estimated by assuming a fresh air exchange rate.
- The unsaturated zone properties are homogeneous.
- The diffusion through the building foundation is assumed to occur in soil-filled cracks in the foundation.
- If the calculated RBSL exceeds the pure component solubility for any individual component, “>SOL” is entered in the RBSL table to indicate that the selected risk level or hazard quotient cannot be reached or exceeded for that compound and the specified exposure scenario.

The input parameters that are unique to this exposure pathway are:

<i>Moisture content (capillary)</i>	<i>Henry’s law coefficient</i>	<i>Diffusion coefficient in air</i>
<i>Air content (capillary)</i>	<i>Thickness of the foundation</i>	<i>Diffusion coefficient in water</i>
<i>Moisture content (unsat. zone)</i>	<i>Fraction of cracks</i>	<i>Ceiling height in building</i>
<i>Air content (unsaturated zone)</i>	<i>Air content in cracks</i>	<i>Air exchange rate in building</i>
<i>Depth to groundwater</i>	<i>Water content in cracks</i>	<i>Thickness of capillary fringe</i>
<i>Thickness of unsaturated zone</i>		

### 1.1.5 Groundwater Ingestion

Ingestion of groundwater is a direct pathway. The Colorado Tier 1 RBSLs for the “groundwater: ingestion” exposure pathway are not calculated using a risk-based model; rather, they are based on MCLs recommended by EPA (ASTM 1995). The concentrations in groundwater 10 meters downgradient of the source will be compared to the groundwater RBSLs (MCLs).

## 1.2 Tier 1 Equations

The Colorado Tier 1 approach calculates RBSLs by manipulating the human health risk assessment equations to solve for the RBSL concentration. Instead of calculating the risk (either individual excess lifetime cancer risk or hazard quotient), a target risk level is plugged into the equations along with the other input parameters. This method of calculating RBSLs is sometimes called the “back-calculation”.

Table C-1 (at the end of Section 1.0) presents the equations used to calculate the Colorado RBSLs.

## 1.3 Tier 1 Input Parameters

Table C-2 (at the end of Section 1.0) presents the parameter definitions and parameter values employed in the Colorado Tier 1 RBSL calculations. Note, a residential exposure is assumed for properties that are zoned commercial because commercial property in Colorado may be used for residences as well.

The Colorado RBCA diverges from the ASTM (1995) protocol by accounting for child exposure to chemicals of concern in a residential scenario. The Colorado Tier 1 child exposure parameter values are based on EPA Region 9 defaults (1996). The Colorado Tier 1 adult exposure values differ from the ASTM (1995) default values for two parameters only: exposure time for outdoor air and target risk. The ASTM assumes the exposure time for outdoor air is 24 hours/day.

The basis for choosing the default values for the Colorado-specific input parameters are discussed below.

### 1.3.1 Depth to Groundwater, Thickness of Unsaturated Zone

Depth to groundwater measurements were collected from 76 sites around the state of Colorado. From these measurements an average depth to groundwater of 15.8 feet was calculated with a standard deviation of 12.7. However, the majority of the sites surveyed have depths to groundwater between 2 and 25 feet. Therefore, a more appropriate average depth was calculated using only the sites that fall within the standard deviation. The average from these sites was 12.5 ft (380 cm).

Since site-specific measurements of capillary fringe thickness are not generally practical to obtain, the ASTM default of 5 cm was adopted. Using this value, and the average depth to groundwater, the resulting thickness of the unsaturated zone is 375 cm.

### 1.3.2 Groundwater Darcy Velocity

The default value of 1800 cm/yr for Darcy Velocity is based on site-specific measurements of saturated hydraulic conductivity and groundwater gradient. Measurements of these parameters were collected from a total of 12 sites, however only 7 of the sites had hydraulic conductivities within a range that is reasonable for a sandy clay loam. These conductivities ranged between  $7.2 \times 10^{-4}$  and  $2.2 \times 10^{-2}$  cm/sec, with an average value of  $4.7 \times 10^{-3}$  cm/sec. The Darcy velocity was calculated for each of these sites and was found to range from 132 to 5396 cm/yr. The mean value was 1800 cm/yr.

### 1.3.3 Average Wind Speed

Based on NOAA data, an average annual wind speed of 3.7 m/s (370 cm/s) was chosen for the Tier 1 default value. This value represents the mean value from 5 weather stations evaluated in Colorado (Denver, Colorado Springs, Pueblo, Alamosa, and Grand Junction).

### 1.3.4 Fraction Organic Carbon

The equations used to calculate RBSLs use fraction organic carbon (Foc) to predict the amount of sorption occurring in the soil. The equations assume that the product of Foc and Koc equals the distribution coefficient. In reality, there are other processes occurring in soil that cause organic chemicals to sorb to soil (e.g. presence of silts and fine-grained materials, and electro-magnetic molecular forces also cause chemicals to sorb even if no organic carbon is present). While the Foc is one of the most important components it is only a partial predictor of the total amount of the amount of sorption occurring. It is however, the only process considered in the equilibrium partitioning equation used to calculate the RBSLs. For that reason, it is important to not underestimate Foc, or use an adjusted Foc to account for all of the partitioning processes.

Fraction organic carbon (Foc) was measured in soils collected from 5 sites using the Walkley-Black Test Method. The average of the Foc values from these sites was 0.009 g oc/g soil. This value is very close to the ASTM default value of 0.01 g oc/g soil. The default value was chosen to be 0.009 g oc/g soil for the Tier 1 tables. This value could be considered conservative for most soils.

### 1.3.5 Infiltration Rate

The infiltration rate is defined here as the total amount of water that infiltrates through the unsaturated zone and recharges groundwater. It is also called the groundwater recharge rate.

A common rule-of-thumb used in groundwater modeling is to assume that infiltration can be estimated to be equal to 10% of the average annual precipitation. Walton (1988) presents groundwater recharge data from different researchers for many sites in Illinois, Wisconsin, Alberta, Wyoming, Nebraska, and Ohio. The recharge rate estimated for these sites ranged from 18% of precipitation (for a sandy soil) to 2% of precipitation. All of the sites but one had values that were less than 10% of the total precipitation.

Precipitation records were evaluated for 48 weather stations throughout Colorado. At least one 30-year average precipitation record was available in each of the regions. The 30-year averages from the different regions of Colorado ranged between 23 cm/yr and 50 cm/yr (9 to 20 inches/yr). Ten percent of the maximum average precipitation of 50 cm/yr yields an infiltration rate of 5 cm/yr.



## 1.4 Chemical Parameters

Colorado Tier 1 RBSLs are calculated for the following chemicals of concern: benzene, ethylbenzene, toluene and xylenes. Table C-3 presents the chemical parameter values employed in the Colorado Tier 1 RBSL calculations.

**Table C-3. State of Colorado Tier 1 Chemical Parameter Values**

Input Parameter	Benzene	Ethyl- benzene	Toluene	Xylenes
Oral RfD (mg/kg-day)	1.7E-3	0.10	0.20	2.0
Inhalation RfD (mg/m <sup>3</sup> )	1.7E-3	0.29	0.114	0.2
Oral Slope Factor (mg/kg-day) <sup>-1</sup>	2.9E-2	ND	ND	ND
Inhalation Slope Factor (mg/kg-day) <sup>-1</sup>	2.9E-2	ND	ND	ND
Solubility (mg/L)	1750	169	526	198
Carbon-water Sorption Coefficient (log K <sub>oc</sub> )	58.9	363	182	240
Henry's Law Constant ([cm <sup>3</sup> H <sub>2</sub> O]/[cm <sup>3</sup> air])	0.228	0.323	0.272	0.290
Diffusion coefficient in air (cm <sup>2</sup> /s)	8.8E-02	7.5E-02	8.7E-02	7.2E-02
Diffusion coefficient in water (cm <sup>2</sup> /s)	9.8E-06	7.8E-06	8.6E-06	8.5E-06
MCL (mg/l)	5.0E-3	0.7	1	10
Degradation rate in groundwater (1/day)	0.00096	0.003	0.025	0.0019

The default values for the chemical input parameters were obtained from EPA's Soil Screening Guidance (1994). The degradation rates were chosen by selecting the minimum values presented for each chemical in Howard (1991) for dissolved phase degradation rates.

## **1.5 Input Variables That Can Be Modified In Tier 1A**

In Tier 1A, Site-Specific Target Levels (SSTLs) may be calculated using the exact same equations as were used in Tier 1 but with site-specific values substituted for the Tier 1 default values. This section discusses each of these site-specific parameters and how the data may be obtained.

Table C-4 presents the site-specific input parameters that may be modified in Tier 1A based on site-specific data.

Two additional parameters may be modified upon prior approval by the OIS: degradation rates in the saturated zone, and the areal fraction of cracks in the building foundation.

### **1.5.1 Degradation Rates in the Saturated Zone (1/day)**

In the Tier 1 tables, the chemical specific degradation rates are assumed to be zero. In performing a Tier 1A, the OIS may allow minimal degradation rates to be used in determining site-specific RBSLs. These minimal degradation rates are currently being studied and may be included in the next version of this document.

### **1.5.2 Areal Fraction of Cracks in Building Foundations (cm<sup>3</sup>/cm<sup>3</sup>)**

The OIS may consider allowing the areal fraction of cracks to be changed from the default value of 0.01 under two types of scenarios. First, if a site is being redeveloped and a future building is planned, the OIS may allow a value of 0.001 to reflect the fact that a new structure would be expected to have much less cracking than an older structure. Second, for existing structures, if the foundation can be inspected and the degree of cracking determined, the actual fraction may be used.

**Table C-4. Site-Specific Input Parameters that Can Be Modified in Tier 1A.**

Variable	Input Parameter Description(s)	Conditions Under Which It Should Be Modified
$L_s$	Depth to subsurface soil source zone (cm)	The measured depth from the ground surface to the subsurface soil source exceeds one meter. This parameter should only be used for the RBSL in soil to protect outdoor air.
$L_{gw}$	Depth to groundwater (cm)	The measured depth to groundwater should be substituted if it is not equal to the Tier 1 default.
$h_{cap}$ $h_v$	Thickness of the capillary fringe (cm) Thickness of the unsaturated zone (cm)	These two parameters added together must equal the depth to groundwater. The thickness of the capillary fringe should be changed if the soil is not a sandy soil. 5 cm (the Tier 1 default) should be considered a minimum value.
$W$	Width of source area parallel to wind or groundwater flow direction (cm)	The width of the source should be modified to reflect the measured width of contaminated soil.
$\theta_T$ $\theta_{ws}$ $\theta_{as}$	Total soil porosity ( $cm^3/cm^3$ ) Unsaturated zone water content ( $cm^3/cm^3$ ) Unsaturated zone air content ( $cm^3/cm^3$ )	The total porosity should be measured. The water and air contents added together must equal the total porosity. Water content may be measured or estimated using a van Genuchten type equation (see Tier 2 appendix).
$F_{oc}$	Fraction organic carbon ( $F_{oc}$ ) in soil (g/g)	Fraction organic carbon may be measured using the Walkley-Black method.
$U_{gw}$	Groundwater Darcy velocity (cm/yr)	This is the product of the hydraulic conductivity and gradient in the groundwater aquifer. The hydraulic conductivity may be estimated based on literature values for various soil types, or it may be measured in the field using an aquifer test. The gradient must be estimated from site data.
$\rho_s$	Soil bulk density ( $g/cm^3$ )	This parameter should be estimated in the lab.
$X$	Distance to point of exposure in groundwater (cm)	This parameter may be modified to equal the distance from the source to the property boundary in the direction of groundwater flow.
$\eta$	Areal fraction of cracks in building foundation ( $cm^3/cm^3$ )	If the building is non-existent today (it is a future construction) this value may be set to 0.001.

Table C-1. Equations Used to Calculate Colorado RBSLs. (1 of 6)

<p>Equations for Surficial Soil RBSL</p>	<p>RBSLs for carcinogenic contaminants (residential/commercial) [mg/kg]</p>	$RBSL_{surfsoil} = \frac{TR}{\left[ \frac{EF_c \times ED_c}{BW_c \times AT_{carc} \times 365 \frac{d}{yr}} \left[ \left( SF_o \times 10^{-6} \frac{kg}{mg} \times (ING(soil)_c \times RAF_o + SSA(soil)_c \times M \times RAF_d) \right) + \left( SF_{inh} \times INH(outair)_c \times \left( \frac{ET(out)_c}{24(hr/d)} \right) \times (VF_{ss} + VF_p) \right) \right] \right] + \left[ \frac{EF_a \times ED_a}{BW_a \times AT_{carc} \times 365 \frac{d}{yr}} \left[ \left( SF_o \times 10^{-6} \frac{kg}{mg} \times (ING(soil)_a \times RAF_o + SSA(soil)_a \times M \times RAF_d) \right) + \left( SF_{inh} \times INH(outair)_a \times \left( \frac{ET(out)_a}{24(hr/d)} \right) \times (VF_{ss} + VF_p) \right) \right] \right]}$	<p>C1</p>
	<p>RBSLs for carcinogenic contaminants (industrial) [mg/kg]</p>	$RBSL_{surfsoil} = \frac{TR \times BW_i \times AT_{carc} \times 365 \frac{d}{yr}}{EF_i \times ED_i \left[ \left( SF_o \times 10^{-6} \frac{kg}{mg} \times (ING(soil)_i \times RAF_o + SSA(soil)_i \times M \times RAF_d) \right) + \left( SF_{inh} \times INH(outair)_i \times \left( \frac{ET(out)_i}{24(hr/d)} \right) \times (VF_{ss} + VF_p) \right) \right]}$	<p>C2</p>
	<p>RBSLs for non-carcinogenic contaminants (residential/commercial) [mg/kg]</p>	$RBSL_{surfsoil} = \frac{THQ \times BW_c \times AT_{haz} \times 365 \frac{d}{yr}}{EF_c \times ED_c \left[ \frac{\left( 10^{-6} \frac{kg}{mg} \times (ING(soil)_c \times RAF_o + SSA(soil)_c \times M \times RAF_d) \right)}{RfD_o} + \frac{\left( INH(outair)_c \times \left( \frac{ET(out)_c}{24(hr/d)} \right) \times (VF_{ss} + VF_p) \right)}{RfD_{inh}} \right]}$	<p>C3</p>
<p><i>continued</i></p>	<p>RBSLs for non-carcinogenic contaminants (industrial) [mg/kg]</p>	$RBSL_{surfsoil} = \frac{THQ \times BW_i \times AT_{haz} \times 365 \frac{d}{yr}}{EF_i \times ED_i \left[ \frac{\left( 10^{-6} \frac{kg}{mg} \times (ING(soil)_i \times RAF_o + SSA(soil)_i \times M \times RAF_d) \right)}{RfD_o} + \frac{\left( INH(outair)_i \times \left( \frac{ET(out)_i}{24(hr/d)} \right) \times (VF_{ss} + VF_p) \right)}{RfD_{inh}} \right]}$	<p>C4</p>

Table C-1. Equations Used to Calculate Colorado RBSLs. (2 of 6)

<p>Equations for Surficial Soil RBSL</p>	<p>Volatilization factor from surficial soils to outdoor air (vapors) [(mg/m<sup>3</sup>air)/(mg/kg soil)]</p>	$VF_{ss} = \frac{2Wr_s}{U_{air}d_{air}} \sqrt{\frac{D_s^{eff}H}{p(q_{ws} + k_s r_s + Hq_{as})t}} \times 10^3 \frac{cm^3kg}{m^3g}$ <p>or :</p> $VF_{ss} = \frac{Wr_s d}{U_{air}d_{air}t} \times 10^3 \frac{cm^3kg}{m^3g}; \quad \text{whichever is less}$	<p>C5</p>
<p><i>concluded</i></p>	<p>Volatilization factor from surficial soils to outdoor air (particulates) [(mg/m<sup>3</sup>air)/(mg/kg soil)]</p>	$VF_p = \frac{P_e W}{U_{air}d_{air}} \times 10^3 \frac{cm^3kg}{m^3g}$	<p>C6</p>
<p>Equations for Soil Leaching to Ground-water RBSL</p>	<p>RBSLs for carcinogenic and non-carcinogenic contaminants (residential/commercial and industrial) [mg/kg]</p>	$RBSL_{sub\ soil} = \frac{RBSL_{gw}}{LF_{sw}}$	<p>C7</p>
<p><i>continued</i></p>	<p>Leaching factor from subsurface soil to groundwater [(mg/l H<sub>2</sub>O)/(mg/kg soil)]</p>	$LF_{sw} = \frac{DAF \cdot r_s}{[q_{ws} + k_s r_s + Hq_{as}] \left(1 + \frac{U_{gw}d_{gw}}{IW}\right)} \times \frac{cm^3kg}{lg}$	<p>C8</p>

Table C-1. Equations Used to Calculate Colorado RBSLs. (3 of 6)

<p>Equations for Soil Leaching to Ground-water RBSL <i>concluded</i></p>	<p>Dilution Attenuation Factor along the centerline of a dissolved plume [(mg/l)/(mg/l)]</p>	$DAF = \frac{C_{(x)}}{C_{source}} = \exp\left[\left(\frac{X}{2a_x}\right) \cdot \left(1 - \sqrt{1 + \frac{4IRq_{eff} a_x}{U_{gw}}}\right)\right] \cdot \operatorname{erf}\left[\frac{W}{4 \cdot \sqrt{a_y X}}\right] \cdot \operatorname{erf}\left[\frac{d_{gw}}{4 \cdot \sqrt{a_z X}}\right]$	<p>C9</p>
<p>Equations for Soil Vapor RBSL (Soil Vapor to Indoor Air)</p>	<p>RBSLs for carcinogenic and non-carcinogenic contaminants (residential/commercial and industrial) [mg/m<sup>3</sup>]</p>	$RBSL_{soil\ gas} = \frac{RBSL_{ind\ air}}{AF_{seps}} \times 10^{-3} \frac{mg}{mg}$	<p>C10</p>
<p><i>continued</i></p>	<p>RBSLs in indoor air for carcinogenic contaminants (residential/commercial) [mg/m<sup>3</sup>]</p>	$RBSL_{ind\ air} = \frac{TR}{\left[ \frac{ED_c \times EF_c \times INH(ind\ air)_c \times \left(\frac{ET(ind)_c}{24}\right) \times SF_{inh}}{BW_c \times AT_{carc}} + \frac{ED_a \times EF_a \times INH(ind\ air)_a \times \left(\frac{ET(ind)_a}{24\ (hr/d)}\right) \times SF_{inh}}{BW_a \times AT_{carc}} \right]} \times 365 \frac{d}{yr} \times 10^3 \frac{mg}{mg}$	<p>C11</p>
<p><i>continued</i></p>	<p>RBSLs in indoor air for carcinogenic contaminants (industrial) [mg/m<sup>3</sup>]</p>	$RBSL_{ind\ air} = \frac{TR \times AT_{carc} \times BW_i}{SF_i \times EF_i \times ED_i \times INH(ind\ air)_i \times \left(\frac{ET(ind)_i}{24\ (hr/d)}\right)} \times 365 \frac{d}{yr} \times 10^3 \frac{mg}{mg}$	<p>C12</p>

Table C-1. Equations Used to Calculate Colorado RBSLs. (4 of 6)

Equations for Soil Vapor RBSL (Soil Vapor to Indoor Air)	RBSLs in indoor air for carcinogenic contaminants (residential/commercial) [mg/m <sup>3</sup> ]	$RBSL_{ind\ air} = \frac{THQ \times AT_{haz} \times BW_c \times RfD_{inh}}{EF_c \times ED_c \times INH(ind\ air)_c \times \left( \frac{ET(ind)_c}{24(hr/d)} \right)} \times 365 \frac{d}{yr} \times 10^3 \frac{mg}{mg}$	C13
	RBSLs in indoor air for non-carcinogenic contaminants (industrial) [mg/m <sup>3</sup> ]	$RBSL_{ind\ air} = \frac{THQ \times AT_{haz} \times BW_i \times RfD_{inh}}{EF_i \times ED_i \times INH(ind\ air)_i \times \left( \frac{ET(ind)_i}{24(hr/d)} \right)} \times 365 \frac{d}{yr} \times 10^3 \frac{mg}{mg}$	C14
	Attenuation factor from soil vapor to indoor (enclosed-space) air [(mg/m <sup>3</sup> air)/(mg/m <sup>3</sup> soil vapor)]	$AF_{seep} = \frac{\left[ \frac{D_s^{eff} A_B}{Q_{B-LT}} \right] \exp\left( \frac{Q_{soil} L_{crack}}{D_{crack}^{eff} h A_B} \right)}{\exp\left( \frac{Q_{soil} L_{crack}}{D_{crack}^{eff} h A_B} \right) + \left[ \frac{D_s^{eff} A_B}{Q_{B-LT}} \right] + \left[ \frac{D_s^{eff} A_B}{Q_{soil L_T}} \right] \left( \exp\left( \frac{Q_{soil} L_{crack}}{D_{crack}^{eff} h A_B} \right) - 1 \right)}$ from Johnson and Ettinger (1991)	C15
	Advective flow rate from soil into the building, [cm <sup>3</sup> /s]	$Q_{soil} = \frac{2p \cdot DP \cdot k_v \cdot X_{crack}}{m \cdot \ln\left[ 2 \cdot Z_{crack} / (h \cdot A_B / X_{crack}) \right]}$	C16
	Effective diffusion coefficient in soil based on vapor-phase concentration [cm <sup>2</sup> /s]	$D_s^{eff} = D^{air} \frac{q_{as}^{3.33}}{q_T^2} + D^{water} \left( \frac{1}{H} \right) \frac{q_{ws}^{3.33}}{q_T^2}$	C17
	Effective diffusion coefficient through foundation cracks [cm <sup>2</sup> /s]	$D_{crack}^{eff} = D^{air} \frac{q_{acrack}^{3.33}}{q_T^2} + D^{water} \left( \frac{1}{H} \right) \frac{q_{wcrack}^{3.33}}{q_T^2}$	C18

concluded

Table C-1. Equations Used to Calculate Colorado RBSLs. (5 of 6)

<p>Equations for Ground-water RBSL (Ground-water to Indoor Air)</p>	<p>RBSLs for carcinogenic and non-carcinogenic contaminants (residential/commercial and industrial) [mg/l]</p>	$RBSL_{gw} = \frac{RBSL_{ind\ air}}{VF_{wesp}} \times 10^{-3} \frac{mg}{mg}$ <p>RBSLind air are defined in equations A11 through A14</p>	<p>C19</p>
	<p>Volatilization factor from groundwater to indoor (enclosed space) air [(mg/m<sup>3</sup> air)/(mg/l H<sub>2</sub>O)]</p>	$VF_{wesp} = \frac{H \left[ \frac{D_{ws}^{eff}/L_{gw}}{ER L_B} \right]}{1 + \left[ \frac{D_{ws}^{eff}/L_{gw}}{ER L_B} \right] + \left[ \frac{D_{ws}^{eff}/L_{gw}}{(D_{crack}^{eff}/L_{crack}) h} \right]} \times 10^3 \frac{l}{m^3}$ <p>Deffcrack is defined by equation A18</p>	<p>C20</p>
	<p>Effective diffusion coefficient through capillary fringe [cm<sup>2</sup>/s]</p>	$D_{cap}^{eff} = D^{air} \frac{q_{acap}^{3.33}}{q_T^2} + D^{water} \left( \frac{1}{H} \right) \frac{q_{wcap}^{3.33}}{q_T^2}$	<p>C21</p>
<p><i>concluded</i></p>	<p>Effective diffusion coefficient between groundwater and soil surface [cm<sup>2</sup>/s]</p>	$D_{ws}^{eff} = \frac{(h_{cap} + h_v)}{\left[ \frac{h_{cap}}{D_{cap}^{eff}} + \frac{h_v}{D_s^{eff}} \right]}$	<p>C22</p>



Table C-1. Equations Used to Calculate Colorado RBSLs. (6 of 6)

Equations for Ground-water RBSLs Ingestion	RBSLs for carcinogenic and non-carcinogenic contaminants (residential/commercial and industrial) [mg/l]	$RBSL_{gw} = MCL$	C23
Equation for Soil Saturation Concentration	Soil concentration at which dissolved pore-water and vapor phases become saturated [mg/kg]	$C_{sat} = \frac{S}{r_s} [q_{ws} + k_s r_s + Hq_{as}] \times \frac{1g}{cm^3kg}$	C24
Equation for Sorption	Chemical-specific sorption to soil	$k_s = F_{oc} K_{oc}$	C25
Retardation Factor	Chemical-specific retardation coefficient in the saturated zone.	$R = 1 + \frac{k_s r_s}{q_{eff}}$	C26

Table C-2. Parameters Used in the RBSL Equations (1 of 5)

<i>Variable</i>	Parameter	Units	Parameter Value(s)
$A_B$	Surface area for enclosed space	$\text{cm}^2$	Residential: 7.40E+05 Industrial: 1.16E+06
$AF_{\text{seesp}}$	attenuation factor- subsurface soils to indoor air	$(\text{mg}/\text{m}^3)/(\text{mg}/\text{m}^3)$	Calculated value (Eqn. C15)
$AT_{\text{carc}}$	averaging time for carcinogens	yr	Residential adult = 70 Residential child = 70 Industrial = 70
$AT_{\text{haz}}$	averaging time for non-carcinogens	yr	Residential adult = 24 Residential child = 6 Industrial = 30
$B_{\text{vol}}$	building (enclosed space) air volume	$\text{cm}^3$	Residential = 3.60E+08 Industrial = 5.60E+08
$BW_{\text{c,a,i}}$	body weight <small>child, adult, worker</small>	kg	Residential adult = 70 Residential child = 15 Industrial = 70
$C_{\text{sat}}$	saturated soil concentration	yr	Calculated value (Eqn. C24)
$d$	lower depth of surficial soil zone	cm	100
DAF	dilution attenuation factor	$\text{g}/\text{cm}^3 - \text{H}_2\text{O}/$ $\text{g}/\text{cm}^3 - \text{H}_2\text{O}$	Calculated value (Eqn. C27)
$D^{\text{air}}$	diffusion coefficient in air	$\text{cm}^2/\text{s}$	Chemical-specific
$D_{\text{crack}}^{\text{eff}}$	effective diffusion coefficient in foundation cracks	$\text{cm}^2/\text{s}$	Calculated value (Eqn. C18)
$D_{\text{s}}^{\text{eff}}$	effective diffusion coefficient in unsaturated zone soils	$\text{cm}^2/\text{s}$	Calculated value (Eqn. C17)
$D^{\text{water}}$	diffusion coefficient in water	$\text{cm}^2/\text{s}$	Chemical-specific
$ED_{\text{c,a,i}}$	exposure duration <small>child, adult, worker</small>	yr	Residential adult = 24 Residential child = 6 Industrial = 25
$EF_{\text{c,a,i}}$	exposure frequency <small>child, adult, worker</small>	d/yr	Residential adult = 350 Residential child = 350 Industrial = 250

Table C-2. Parameters Used in the RBSL Equations (2 of 5)

<i>Variable</i>	Parameter	Units	Parameter Value(s)
ER	indoor air exchange rate with outside air	s <sup>-1</sup>	Residential = 1.4E-04 Industrial = 2.3E-03
ET(ind) <sub>c,a,i</sub>	exposure time to indoor air <small>child, adult, worker</small>	hr/d	Residential adult = 24 Residential child = 24 Industrial = 8
ET(out) <sub>c,a,i</sub>	exposure time to outdoor air <small>child, adult, worker</small>	hr/d	Residential adult = 8 Residential child = 8 Industrial = 8
F <sub>oc</sub>	fraction organic carbon in soil	g OC/g soil	0.009
H	Henry's law coefficient	cm <sup>3</sup> H <sub>2</sub> O/cm <sup>3</sup> air	Chemical-specific
h <sub>cap</sub>	capillary fringe thickness	cm	5
h <sub>v</sub>	unsaturated zone thickness	cm	375
I	infiltration rate through the unsaturated zone	cm/yr	5
ING(gw) <sub>c,a,i</sub>	groundwater ingestion rate <small>child, adult, worker</small>	l/d	Residential adult = 2 Residential child = 2 Industrial = 1
ING(soil) <sub>c,a,i</sub>	soil ingestion rate <small>child, adult, worker</small>	mg/d	Residential adult = 100 Residential child = 200 Industrial = 50
INH(ind air) <sub>c,a,i</sub>	indoor inhalation rate <small>child, adult, worker</small>	m <sup>3</sup> /d	Residential adult = 15 Residential child = 15 Industrial = 20
INH(out air) <sub>c,a,i</sub>	outdoor inhalation rate <small>child, adult, worker</small>	m <sup>3</sup> /d	Residential adult = 20 Residential child = 15 Industrial = 20
k <sub>oc</sub>	carbon-water sorption coefficient	cm <sup>3</sup> H <sub>2</sub> O/g OC	Chemical-specific
k <sub>s</sub>	soil-water sorption coefficient	cm <sup>3</sup> H <sub>2</sub> O/g soil	Calculated value (Eqn. C25)
k <sub>v</sub>	Soil air permeability	cm <sup>2</sup>	1.00E-8
L <sub>B</sub>	indoor air volume/floor area (infiltration area) ratio	cm	Residential = 486 Industrial = 4,828

Table C-2. Parameters Used in the RBSL Equations (3 of 5)

<i>Variable</i>	Parameter	Units	Parameter Value(s)
$L_{\text{crack}}$	foundation thickness	cm	15
LF	leaching factor	(mg/l)/(mg/kg)	Calculated value (Eqn. C8)
$L_{\text{gw}}$	depth to groundwater ( $h_{\text{cap}}+h_{\text{v}}$ )	cm	380
$L_{\text{s}}$	depth to subsurface soil sources	cm	100
$L_{\text{T}}$	depth from building foundation to soil vapor source	cm	100
M	soil to skin adherence factor	mg/cm <sup>2</sup>	0.5
$P_{\text{e}}$	particulate emission rate	g/cm <sup>2</sup> /s	6.9E-14
$Q_{\text{B}}$	enclosed space air exchange rate calculated from: $Q_{\text{B}}=ER*B_{\text{vol}}$	cm <sup>3</sup> /s	Calculated value
$Q_{\text{soil}}$	soil vapor flow rate into enclosed space due to under-pressurization	cm <sup>3</sup> /s	Calculated value (Eqn. C16)
$RAF_{\text{d}}$	dermal relative absorption factor	mg/mg	0.5
$RAF_{\text{o}}$	oral relative absorption factor	mg/mg	1.0
$RfD_{\text{inh}}$	inhalation chronic reference dose	mg/kg/d	Chemical-specific
$RfD_{\text{o}}$	oral chronic reference dose	mg/kg/d	Chemical-specific
S	pure chemical solubility in water	mg/l	Chemical-specific
$SF_{\text{inh}}$	inhalation slope factor	1/(mg/kg/d)	Chemical-specific
$SF_{\text{o}}$	oral slope factor	1/(mg/kg/d)	Chemical-specific
$SSA(\text{soil})_{\text{c,a,i}}$	skin surface area exposed to soil <small>child, adult, worker</small>	cm <sup>2</sup>	Residential adult = 3160 Residential child = 2190 Industrial = 3160
THQ	target hazard quotient	unitless	1.0
TR	target individual excess lifetime cancer risk	unitless	1.0E-06
$U_{\text{air}}$	wind speed above ground surface in outdoor air mixing zone	cm/s	370

Table C-2. Parameters Used in the RBSL Equations (4 of 5)

<i>Variable</i>	Parameter	Units	Parameter Value(s)
$U_{gw}$	groundwater Darcy velocity	cm/yr	1800
$VF_p$	volatilization factor from surficial soils to outdoor air-particulates	$(\text{mg}/\text{m}^3)/(\text{mg}/\text{kg})$	Calculated value (Eqn. C6)
$VF_{ss}$	volatilization factor from surf. soils to outdoor air-vapors	$(\text{mg}/\text{m}^3)/(\text{mg}/\text{kg})$	Calculated value (Eqn. C5)
$VF_{wesp}$	volatilization factor from groundwater to indoor air	$(\text{mg}/\text{m}^3)/(\text{mg}/\text{l})$	Calculated value (Eqn. C20)
$W$	width of source area parallel to wind or groundwater flow direction	cm	1340 (44 feet)
$X$	distance from soil column to downgradient point of exposure in groundwater	cm	1,000
$X_{crack}$	Total floor-wall seam perimeter distance	cm	Residential: 3.70E+03 Industrial: 4.60E+03
$Z_{crack}$	Distance below ground surface of the basement cracks	cm	244
$\alpha_x, \alpha_y, \alpha_z$	longitudinal, transverse and vertical dispersivity	fraction of distance downgradient	0.1, 0.0333, 0.0005
$\delta_{air}$	outdoor air mixing zone height	cm	200
$\delta_{gw}$	groundwater mixing zone thickness	cm	200
$\Delta P$	Pressure difference between soil and building	$\text{g}/\text{cm}\cdot\text{s}^2$	10
$\eta$	areal fraction of cracks in building foundation/walls	$\text{cm}^2\text{cracks}/\text{cm}^2\text{ area}$	0.01
$\lambda$	chemical-specific degradation rate	1/d	Chemical-specific
$\mu$	Air viscosity	$\text{g}/\text{cm}\cdot\text{s}$	1.80E-04
$\pi$	pi		3.1416

Table C-2. Parameters Used in the RBSL Equations (5 of 5)

<i>Variable</i>	Parameter	Units	Parameter Value(s)
$\theta_{\text{acrack}}$	volumetric air content in foundation/wall cracks	cm <sup>3</sup> air/cm <sup>3</sup> soil	0.26
$\theta_{\text{as}}$	volumetric air content in unsaturated zone soils	cm <sup>3</sup> air/cm <sup>3</sup> soil	0.26
$\theta_{\text{T}}$	total soil porosity	cm <sup>3</sup> voids/cm <sup>3</sup> soil	0.38
$\theta_{\text{wcap}}$	volumetric water content in capillary fringe soils	cm <sup>3</sup> H <sub>2</sub> O/cm <sup>3</sup> soil	0.342
$\theta_{\text{wcrack}}$	volumetric water content in foundation/wall cracks	cm <sup>3</sup> H <sub>2</sub> O/cm <sup>3</sup> soil	0.12
$\theta_{\text{acap}}$	volumetric air content in capillary fringe soils	cm <sup>3</sup> air/cm <sup>3</sup> soil	0.038
$\theta_{\text{ws}}$	volumetric water content in unsaturated zone soils	cm <sup>3</sup> H <sub>2</sub> O/cm <sup>3</sup> soil	0.12
$\rho_{\text{s}}$	soil bulk density	g/cm <sup>3</sup>	1.64
$\tau$	averaging time for vapor flux	s	9.46E+08

## 2.0 Tier 2

Tier 2 allows Site Specific Target Levels (SSTLs) to be calculated when Tier 1 or 1A RBSLs are exceeded and remediation to Tier 1 or 1A levels is expensive and/or engineered or institutional controls are not reasonable. In Tier 2, site-specific data is used in more sophisticated models to estimate the exposure concentrations (and hence the risk levels). The Tier 2 models can handle a wider variety of spatial conditions and also consider source depletion.

The following table presents the SSTL media (the media in which clean-up levels are being calculated), the exposure pathways considered and type of fate and transport model needed.

Table C-5. Exposure Pathways Associated with Each SSTL Media and Type of Fate and Transport Model Needed.

<b>SSTL Media</b>	<b>Exposure Pathways</b>	<b>Type of Fate and Transport Model Needed</b>
Soil (surficial or subsurface) and	Inhalation of indoor air (soil vapor intrusion)	Soil to indoor air model
	Inhalation of soil emissions (outdoors)	Unsaturated zone model, or Volatilization model
Soil Vapor	Ingestion of groundwater (leaching to groundwater and groundwater transport)	Unsaturated zone model coupled with a saturated zone model
	Inhalation of particulate emissions (outdoors)	Particulate emission model
	Inhalation of indoor air (leaching to groundwater, groundwater transport and volatilization from groundwater to indoor air)	Unsaturated zone model linked with a saturated zone model linked with a groundwater to indoor air model
Groundwater	Ingestion of groundwater (downgradient from the source)	Saturated zone model
	Inhalation of indoor air (vapors emanating from groundwater)	Groundwater to indoor air model, or Saturated zone model linked with groundwater to indoor air model

In selecting appropriate models for Colorado's Tier 2, three of the most common risk assessment software packages were evaluated. Table C-6 lists the models contained in these three packages for each of the pathways listed above.

**Table C-6. Fate and Transport Models Contained in Three Commercial Risk Assessment Software Packages**

Pathway	Commercial Software Package			Comments
	BP RISC	API DSS	GSI Tier 2 Toolkit	
Soil to Indoor Air	Johnson-Ettinger, or Depleting Source Model	None	Diffusion only model (Johnson-Ettinger minus advection)	The diffusion only model is the same as Johnson-Ettinger when run without advection (pressure difference)
Soil to Groundwater and Groundwater Transport (ingestion, dermal contact, shower)	VADSAT-like unsaturated zone model, or Saturated Soil Model	VADSAT, or Jury linked with AT123D, or SESOIL linked with AT123D	LEACH (Tier 1 Leaching Factor-LF), linked with Domenico (no unsaturated zone model)	LEACH is the Leaching Factor specified in the ASTM Tier 1 equations. GSI offers a new software that contains a unsaturated zone model called SAM. SAM is similar to LEACH, however it can consider degradation.
Soil to Outdoor Air	VADSAT-like unsaturated zone model linked with Box	VADSAT linked with Box Jury linked with Box SESOIL linked with Box Farmers linked with Box Thibodeaux-Hwang linked with Box Or, any of the above linked with a Gaussian model	Farmers (Tier 1 Volatilization Factor-VF) linked with Box Farmers linked with Gaussian	The Farmers algorithm is the same as the volatilization factor (VF) algorithm used in the ASTM Tier 1 equations. The box model is for onsite exposures and the Gaussian model is for offsite exposures.
Soil Particulate Emissions	None	Cowherd model linked with Box or Gaussian model	User-specified emission rate considered as part of the surficial soil RBSL.	
Soil to Groundwater and Groundwater Transport and Emissions from Groundwater to Indoor Air	VADSAT-like unsaturated zone model linked with Farmers	None	None	
Groundwater Transport (For ingestion, dermal contact, shower)	AT123D	AT123D	Domenico	
Groundwater Transport and Emissions from Groundwater to Indoor Air	AT123D linked with Farmers	None	None	



The unsaturated zone model in BP RISC is based on the paper by Ünlü et al. (1992) which is the same paper that presents the equations used by VADSAT.

It should be noted that the groundwater to indoor air pathway is almost always modeled using the Farmer algorithm. That means that the volatilization rate is calculated from the concentration gradient between the groundwater and building and the effective diffusion coefficient for the chemical being modeled. The effective diffusion coefficient is estimated for each different “soil horizon” found between the groundwater and the building: capillary fringe, the native unsaturated zone, a lens (for BP RISC only), and the building foundation. While the equations used by both the GSI Tier 2 Tool Kit and BP RISC are the same, BP RISC gives you the option of using the groundwater concentration calculated by a fate and transport model as the source term. This is very important because it allows you to evaluate exposure to a receptor located downgradient from the source.

Table C-7 highlights the processes simulated by the unsaturated zone (leaching) and groundwater models. VF and LF designate “Volatilization Factor” and “Leaching Factor” respectively.

**Table C-7. Processes Simulated by Each Fate and Transport Model.**

<b>Process Description</b>	<b>VADSAT</b>	<b>SESOIL</b>	<b>Jury</b>	<b>LEACH, Tier 1 LF</b>	<b>Thibodeaux- Hwang</b>	<b>Farmer, Tier 1 VF</b>	<b>AT123D</b>	<b>Domenico</b>
<b>Soil to Outdoor Air</b>								
Finite source (conserves mass?)	Y	Y	Y	Y	Y	N		
Homogeneous/isotropic soil	N <sup>1</sup>	N	Y	Y	Y	Y		
Constant depth to source	Y	N	N	N	N	Y		
<b>Soil Leaching to Groundwater</b>								
Finite source (conserves mass?)	Y	Y	Y	N				
Homogeneous/isotropic soil	Y	N	Y	Y				
Considers biodegradation	Y	Y	Y	N				
Uniform chemical distribution for source	Y	N	Y	Y				
Considers presence of NAPL	Y	Y <sup>2</sup>	N	N				
Considers dispersion	Y	N	Y	N				
User specifies moisture content	N	N	Y	Y				
<b>Groundwater Transport</b>								
Steady-state flow field	Y						Y	Y
Can handle variable leaching rate?	Y						Y	N
Transient concentrations	Y						Y	N
Constant source only	N						N	Y
Considers degradation	Y						Y	Y
Considers dispersion	Y						Y	Y

<sup>1</sup>The VADSAT model in RISC can consider heterogeneities in the soil column for purposes of calculating an effective diffusion coefficient for volatilization processes.

<sup>2</sup>The SESOIL model does limit the chemical to the effective solubility, however, the user must calculate the effective solubility and enter it as an input value.

Each of the models and algorithms listed in Table C-7 were evaluated for performance and sensitivity. The criteria evaluated were:

- Ease of use.
- The potential to generate unrealistic scenarios (for example unrealistic moisture contents and infiltration rates in SESOIL).
- The data requirements and ease of obtaining the data required.
- The ability to handle residual levels of contamination (especially important for petroleum hydrocarbons).

- Ease of understanding the model and model output.

Based on the review, the OIS has chosen the VADSAT model (as part of BP RISC or part of API DSS) to be the only unsaturated zone and groundwater models allowed for Tier 2 analyses. Indoor air risk may be evaluated under Tier 2 using the indoor air model in BP RISC. These models are easy to use, have a minimum amount of data requirements, and can handle residual levels of contamination automatically.

Detailed summaries, that list data requirements and features of the VADSAT models are provided in the following sections. Detailed summaries of the other models reviewed, are available for review by request of the OIS.

## **2.1 VADSAT Model Description (Unsaturated Zone)**

### **2.1.1 Overview**

The VADSAT model can be used to estimate volatile emissions to outdoor air, leaching to groundwater, and groundwater transport. VADSAT is available as part of BP RISC and API DSS, or as a standalone model from the American Petroleum Institute. The standalone version has a Windows interface and it fairly easy to use. The standalone version allows the use of Monte Carlo simulations. Neither BP RISC or the API DSS allows the VADSAT model to be run in a Monte Carlo mode. The VADSAT model consists of a unsaturated zone model and a groundwater model linked together. The groundwater portion of the model is identical to running AT123D. This section (2.1) will only cover the unsaturated zone portion of the VADSAT model. The saturated zone portion of the model will be described under the AT123D model description (section 2.1).

VADSAT was developed specifically to handle petroleum hydrocarbons that are part of mixtures (such as production wastes, gasoline, diesel, etc.). It does this by calculating the mole fraction of each individual constituent being modeled and then calculating the individual chemical's effective solubility.

### **2.1.2 Features of the VADSAT (Unsaturated Zone) Model**

- Homogeneous unsaturated zone properties.
- Uniform moisture content.
- Steady state, uniform infiltration rate (percolation rate).
- Calculates moisture content from residual water content, hydraulic conductivity and van Genuchten's  $n$  parameter.
- Can handle residual levels (NAPL) of contamination.
- Calculates effective solubility internally.
- Considers degradation in the dissolved phase.
- Conserves mass (finite source).
- Volatile emissions are calculated using a Farmers-type algorithm at each time step.
- Considers dispersion in the direction of percolation (internally calculated).

### 2.1.3 Discussion of Model

#### 2.1.3.1 Lens in BP RISC

The unsaturated zone model in BP RISC is based on the equations used in the VADSAT model with one change. BP RISC allows the user to specify a “lens” or soil unit between the source and the surface that can have a different moisture content than the native unsaturated zone. This feature is useful to “slow down” the emission rate. Most unsaturated zone models overestimate the volatile emission rate because they assume that the moisture content is constant at the long term average. In reality, any wetting front or lower permeability lens will have a higher than average moisture content and will seriously impede the amount of volatilization occurring. Some unsaturated zone models (SESOIL and the standalone VADSAT) give you the option to “turn down” the emissions by specifying an arbitrary fraction of emissions allowed, in BP RISC a lens is used. When a unsaturated zone model overestimates emissions, it will underestimate the amount of contaminant reaching groundwater and therefore may underestimate concentrations in a down-gradient well. The volatilization mechanism is a very important part of the model even if the purpose of the modeling effort is to estimate leaching to groundwater.

#### 2.1.3.2 Estimating Moisture Content

Moisture content is an easy parameter to measure in the field, however, the value obtained may not be very reasonable when used as the input for a model based on long-term average conditions (such as the models used for risk assessment). On the other hand, *residual* moisture content is an easy parameter to measure for soils and is not subject to fluctuations from season to season or length of time since a rain event. For those reasons, VADSAT estimates moisture content from the residual moisture content and other user-supplied inputs.

The moisture content in the unsaturated zone is a very important parameter for two reasons. Most important, it is used to calculate the effective diffusion coefficient for volatilization. Less important, the actual pore water velocity depends on the moisture content as it is calculated by dividing the infiltration rate by the moisture content.

The relative permeability of unsaturated zone soil varies with the moisture content. Unsaturated soil is less permeable than saturated soil of the same type. As a soil becomes more and more saturated its permeability approaches that of the saturated soil. This relationship, however, is not usually linear, i.e. a soil at 20% saturation does not have twice the permeability of the same soil at 10% saturation. In fact, this relationship is different for different soil types. One way of relating the permeability to the moisture content for various soils is to use a “fitting algorithm” where one of the fitting parameters can be measured for different soil types. The VADSAT model uses the Brooks and Correy (1964) model relating moisture content, infiltration rate, and hydraulic conductivity. This model is probably the most widely used model relating soil moisture and permeability in analytical unsaturated zone models. One of the inputs required for the Brooks and Correy model is van Genuchten’s  $n$  parameter which has been measured by Carsel and Parrish for a number of different soil types. VADSAT estimates moisture content by first solving the Brooks and Correy algorithm for relative permeability from the specified

infiltration rate and hydraulic conductivity. Then the moisture content is estimated using the van Genuchten algorithm for relative permeability and moisture content.

The reader is referred to Appendix A of the BP RISC User's Manual or Unlu et al. (1992) for the details and equations used in this calculation.

#### 2.1.4 Data Requirements

Obtaining the data required for VADSAT is fairly simple since some of the input parameters can be looked up in databases (van Genuchten's  $n$ , residual moisture content, hydraulic conductivity). BP RISC has databases built into the software interface providing soil parameter values. Table C-8 lists the data requirements for the unsaturated portion of the VADSAT model.

Table C-8. Data Requirements for VADSAT.

<b>MEDIA-SPECIFIC PARAMETERS</b>	<b>UNITS</b>	<b>SOURCE OF DATA</b>
Porosity	cm <sup>3</sup> pores/cm <sup>3</sup> soil	measured or use default
Residual (or Irreducible) Water Content	cm <sup>3</sup> water/cm <sup>3</sup> soil	measured or use default
Fraction Organic Carbon	g /g soil	measured or use default
Hydraulic Conductivity	m/day	measured or use default
Soil Bulk Density	g/cm <sup>3</sup>	measured
van Genuchten Parameter	dimensionless	use default
Unsaturated Zone Thickness	m	measured
<b>SOURCE PARAMETERS</b>		
Length of Contaminated Zone	m	estimated
Width of Contaminated Zone	m	estimated
Thickness of Contaminated Zone	m	estimated
<b>TPH DATA</b>		
Molecular Weight of TPH	g/mol	use default
Concentration of TPH	mg/kg	measured
<b>CHEMICAL SPECIFIC DATA (individual chemical component)</b>		
Molecular Weight	g/mol	use default
Concentration	mg/kg	measured
Solubility	mg/l	use default
Diffusion Coefficient in Air	cm <sup>2</sup> /s	use default
Diffusion Coefficient in Water	cm <sup>2</sup> /s	use default
Koc	ml/g	use default
Degradation Rate	1/d	measured, use default
Henry's Law Constant	(mg/l)/(mg/l)	use default

### 2.1.5 Sensitivity Discussion

For BTEX type contaminants, the unsaturated zone model is probably most sensitive to the ***degradation rate*** if there is a significant amount of travel time between the source and water table. For this input parameter, in the absence of site data, it is recommended to use a value on the lower end of the published range of degradation rates.

Other input parameters that can create fairly large variations in leaching rates to groundwater or volatilization rates to outdoor air are the ***input parameters that govern the estimation of moisture content***. Most of the parameters that affect this are easily measured or can be obtained from the literature (hydraulic conductivity, porosity, and residual moisture content) and the input values for the rest (van Genuchten's n) are chosen based on characterization of soil type and published values. It is important to perform a sensitivity study on any Tier 2 analysis by

changing the input values for these parameters over the range that is reasonable for the soil types found at the site.

The results of the model are also sensitive to the *concentration of TPH* for the chemicals of concern at UST sites (BTEX and other petroleum hydrocarbons). The reason for this is that BTEX constituents typically only comprise up to 14% of the total mass of organic chemicals found at the site. Benzene, for example, is usually found at levels ranging from zero to 3% of the TPH. The difference between benzene at 1% vs. 2% of the TPH is a difference between an effective solubility of 17.5 mg/l vs. 35 mg/l. This effective solubility will be the leachate concentration leaving the source area if the concentrations are high enough to be solubility limited (residual levels).

***Infiltration rate*** is another input parameter that is very difficult to measure or obtain site-specific data and can affect model results. Generally, the effects of changes in the infiltration rate are linear, that is, if the infiltration rate is doubled, twice as much water (and therefore dissolved contaminant eventually) reaches the water table. When degradation is being considered, the results are not necessarily linear. For example, if the infiltration rate is reduced, the travel time through the unsaturated zone is slower and degradation has a longer time to work. Since degradation losses are not linear with time, the resulting leaching rate is not affected linearly.

All models are sensitive to the ***source concentration*** in certain ranges. If the travel time is fairly large from the source to the water table and degradation is being considered, there might be a large range of source concentrations that still do not generate any breakthrough to the water table. On the other hand, if degradation is not being considered, or the distance to the water table is small, the model results will be much more sensitive to the source concentrations.

Depending on the Koc value of the chemical being simulated, the model results will be sensitive to ***fraction organic carbon***. The higher the Koc, the more sensitive the results up to a point, then at high Koc values no transport occurs at all.

#### 2.1.6 Comparison of VADSAT And The Tier 1 Leaching Factor (LEACH) and Volatilization Factor (Farmers)

Using the VADSAT unsaturated zone model yields very different results than the leaching and volatilization factors used in the ASTM Tier 1 algorithms (and the GSI Tier 2 Tool Kit). The main reasons that the resulting leachate and volatilization calculated by VADSAT will be different are:

- The VADSAT model has a finite source. That is, it allows leaching and volatilization to continue as long as there is still mass left in the source, after the source is gone, leaching from the source stops. This can have a large effect on the time averaged groundwater concentrations in a downgradient well used in the risk assessment.
- There may be a separation of the source and the water table. The Tier 1 leaching algorithm assumes the source reaches to the water table.
- The VADSAT model is transient. If there is a separation from the source to the water table (of clean unsaturated zone) then there will be a time-delay between the time when the model

starts and the leachate containing the modeled constituent reaches the water table. It is important to run the model long enough to reach steady-state, or until the peak concentrations have passed the well.

- The VADSAT model accounts for losses due to degradation in the liquid phase.

If the VADSAT model is set up with a source that reaches the water table, a large initial concentration, no degradation, and input parameters such that the moisture content matches that used in the Tier 1 Leaching Algorithm, then the resultant leachate concentrations from the two algorithms should be equal.

## **2.2 AT123D Model Description**

### 2.2.1 Overview

The AT123D model is a saturated zone model for predicting concentrations in groundwater at a location down-gradient from a source. AT123D can be used on its own by specifying a source in groundwater, or it can be linked with a unsaturated zone model such as VADSAT, SESOIL, LEACH, or Jury. The groundwater model included in the VADSAT model and BP RISC is identical to AT123D and so this appendix also applies to those other models as well.

AT123D stands for “Analytical, Transient, 1-, 2-, and 3-Dimensional” model. It simulates the dispersion of a contaminant in uniform flow field. The source can be a point, line or rectangle in shape. When AT123D is run using a constant source in the vertical plane, the steady state solution should equal that calculated with the Domenico model.

The standalone AT123D code is available as a compiled FORTRAN code (without a user interface) from the International Groundwater Modeling Center for about \$50. AT123D is included in BP RISC, API DSS, and RiskPro.

### 2.2.2 Features

- Transient model.
- Three-dimensional dispersion (longitudinal, lateral, and vertical). Dispersion values are a user input.
- One dimensional uniform flow field.
- Considers linear, reversible equilibrium adsorption (retardation).
- Considers degradation.
- Source may be instantaneous, constant release, or variable release (when linked with a unsaturated zone model).

### 2.2.3 Discussion

AT123D is a fairly simple groundwater model in that it considers a steady-state, uniform flow field. The transport of the contaminant is non-uniform and transient. It cannot consider water

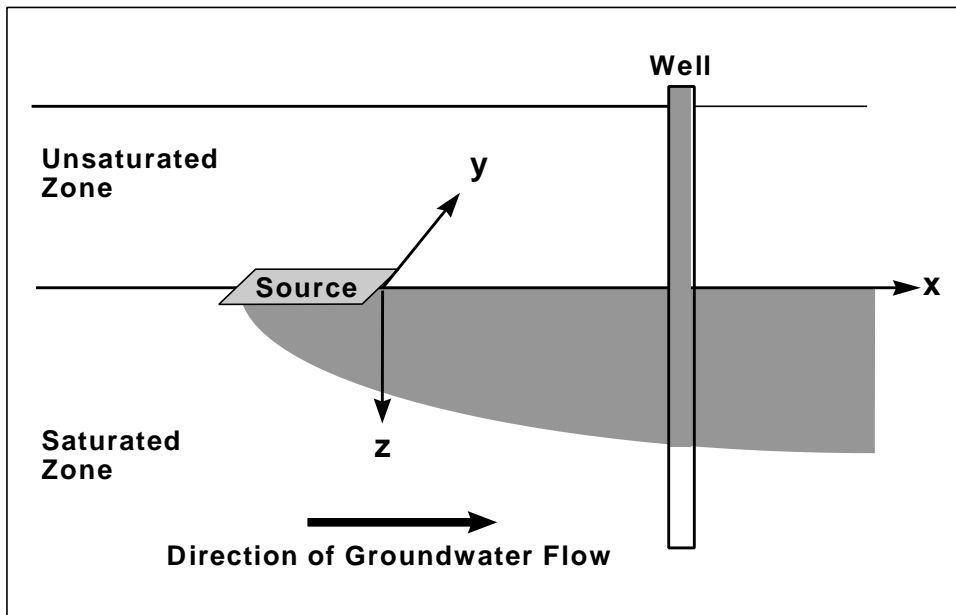


tables that are fluctuating and does not account for dilution from infiltration (down-gradient of the source region).

### 2.2.3.1 Source Geometry when Linked With a Unsaturated Zone Model

A horizontal planar source is most often used when AT123D is linked with a unsaturated zone model (VADSAT, and all of the unsaturated zone models in API DSS). This “works” mathematically in that mass is conserved, however it has little physical reality because in the real situation infiltration from the unsaturated zone would also carry water (or a volume) with it when it enters the water table. When AT123D is used with a planar source, the concentrations predicted in the groundwater may actually exceed the leachate concentrations very close to the source and at the very top of the aquifer (at the water table). To avoid this problem, a volume source is used in BP RISC. The size of the source is calculated to correspond with the infiltration volume so that if a well is placed adjacent to the source at the top of the aquifer, the concentration estimated at this location will equal the leachate concentration predicted by the unsaturated zone model.

The following figure shows AT123D model geometry and a horizontal, planar source at the water table.



**AT123D Model Geometry**

## 2.2.4 Data Requirements

The data requirements for AT123D are fairly straightforward with the exception of dispersion coefficients. These are usually estimated to be some fraction of the distance from the source to the “point of interest” (the down-gradient well). In the standalone AT123D and in RISKPRO softwares the dispersion coefficients are entered as a distance (not as a fraction) so it is important to scale these values appropriately. The rule-of-thumb commonly used is to assume longitudinal dispersivity is  $1/10^{\text{th}}$  the distance from the source to the well, transverse dispersivity to be  $1/3^{\text{rd}}$  of the longitudinal and vertical dispersivity to be  $1/10^{\text{th}}$  of the longitudinal.

**Data Requirements for AT123D**

<b>PARAMETER DEFINITION</b>	<b>UNITS/OPTIONS</b>
Time step	(yr)
<b>Source Parameters</b>	
Length in the x-direction (direction of groundwater flow)	(m)
Length in the y-direction	(m)
Thickness in the z-direction	(m)
Duration of the pulse (only for pulse source)	(yr)
Chemical release rate or concentration	(kg/yr) or (mg/L)
<b>Media Parameters</b>	
Effective porosity	( $\text{cm}^3/\text{cm}^3$ )
Hydraulic conductivity	(m/yr)
Hydraulic gradient	(m/m)
Longitudinal dispersivity	(m)
Transverse dispersivity	(m)
Vertical dispersivity	(m)
Bulk density of soil	( $\text{g}/\text{cm}^3$ )
Fractional organic carbon content	(g/g)
Thickness of aquifer	(m)
Width of aquifer	(m)
<b>Chemical Parameters</b>	
Organic carbon partition coefficient	( $\text{mg}/\text{g}$ )/( $\text{mg}/\text{cm}^3$ )
Overall decay rate	(1/day)
Diffusion coefficient in water	( $\text{cm}^2/\text{s}$ )
<b>Receptor Well Data</b>	
x-coordinate of well (in direction of groundwater flow)	(m)
y-coordinate of well	(m)
z-coordinate of well	(m)

Note, not all of these inputs are available in all software. For example, in VADSAT and BP RISC, the time step is fixed and the aquifer is assumed to be infinitely wide and deep.

### 2.2.5 Sensitivity Discussion

When simulating the transport of BTEX chemicals, results predicted by AT123D will be most sensitive to changes in **degradation rate**. This is because the BTEX compounds have fairly high degradation rates on average.

**Fraction organic carbon** ( $F_{oc}$ ) is also a sensitive input parameter as it affects travel time of the chemical.  $F_{oc}$  is very sensitive if it is changed while also considering degradation. The same applies to input parameters affecting groundwater flow velocity: **hydraulic conductivity, gradient, and effective porosity**.

The effect of changing **source concentration** on calculated down-gradient concentrations will most likely be linear. **Hydraulic conductivity, gradient, and effective porosity** will also affect the solution linearly in the absence of degradation.

The model is not very sensitive to dispersion coefficients when they are varied over a realistic range (scaled to the problem simulated).

### 2.2.6 Comparison of AT123D with Tier 1 Algorithms

There is no groundwater model specified in the ASTM Tier 1 equations for estimating concentrations away from the source. The ASTM Tier 1 RBSL for soil leaching to groundwater uses a simple mixing algorithm (sometimes called the Summers model) to estimate concentrations in the very top of the aquifer directly underneath the unsaturated zone source. This mixing model accounts for dilution only. AT123D can account for dispersion, degradation, retardation, and mass balance. The Colorado OIS approach for calculating Tier 1 RBSLs does combine the Domenico model with the steady-state leaching factor calculated for the unsaturated zone. The only difference between AT123D and Domenico models is that AT123D can handle a variable (transient) source term.

If AT123D were set up with using all of the same input parameters, the results will be identical to those calculated in the Colorado Tier 1 algorithm. It is important to note, however, that AT123D may produce unstable results for a well located that close to the source. This instability is due to the fact that AT123D is actually a finite difference model in the time dimension and so the results can be unstable when the time step is too large considering the distance to the well and the velocity of groundwater flow.