BIOVAPOR MODEL FACT SHEET

Introduction

The BioVapor model is a one-dimensional steady-state compartmental model for vapor intrusion that incorporates oxygen-limited aerobic biodegradation. The BioVapor model is available, relatively straightforward to use, and through aerobic biodegradation allows users to simulate an important mechanism for attenuation of petroleum hydrocarbon (PHC) vapor flux into buildings. This fact sheet is intended to provide key information on model construction, site input parameters, and sensitivity.

The BioVapor model shares many characteristics and input parameters with the U.S. Environmental Protection Agency (USEPA) petroleum vapor intrusion screening model (the PVIScreen model). The focus on the BioVapor model in this fact sheet is not intended to exclude the application of the PVIScreen model. The users are encouraged to explore the use of PVIScreen, particularly when its unique characteristics are desirable, such as its features relating to parameter input distributions and probabilistic analysis.

Model Input Parameters

BioVapor is conceptually similar to the broadly applied Johnson and Ettinger model (J&E model) and share many similar (often identical) defined model parameters. Default values and applicable ranges for model input parameters, including the additional parameters specific to the BioVapor model, are discussed in the Chemical Concentrations section along with a qualitative description of the sensitivity of the BioVapor model to input parameters. Other guidance on the selection of J&E model input parameters is also available (Hers et al. 2003; USEPA 2004; Weaver and Tillman 2005; Johnson 2005).

Input parameters for the BioVapor model that affect biodegradation aspects of the model are listed below:

- Oxygen gas (O_2) supply beneath the building
- Chemical parameters and concentrations, including all PHC sources or degradation products with oxidative demand (such as methane)
- Chemical-specific first-order biodegradation rate constants
- Baseline rate for O_2 respiration in soils
- Minimum O_2 for aerobic respiration
- Distance from bottom of building foundation to contamination source
- Type of building foundation (this affects the O_2-supply boundary condition)

Information on key input parameters for biodegradation modeling is provided in the following sections.

O_2 Supply Below Building

BioVapor has three options for identifying the O_2 supply or flux below the building foundation:

- Constant airflow rate is typically used for solid foundations (basement or slab-on-grade), where air flow is induced by stack effect (or other mechanisms causing building depressurization) or by the effect of wind on buildings.

- Constant O_2 concentration at surface below the building applies to earthen-floor foundations or dirt-floor crawl spaces, or where sub-slab O_2 concentrations are measured.
- Fixed aerobic depth below grade applies when measurement data on this depth are available.

In the BioVapor model, two different airflow rates may be specified: airflow through the foundation (Q_s) and airflow under the foundation (Q_f). The Q_s parameter relates solely to soil vapor advection and is used to calculate the mass transfer of chemicals through the foundation as soil vapor is drawn into a depressurized building. The Q_f parameter describes the advective airflow rate to below the foundation (Figure 1) and is used solely for calculating the O_2 supply or flux into soil below the foundation that is available for aerobic biodegradation (based on airflow rate, assuming atmospheric O_2 concentration).

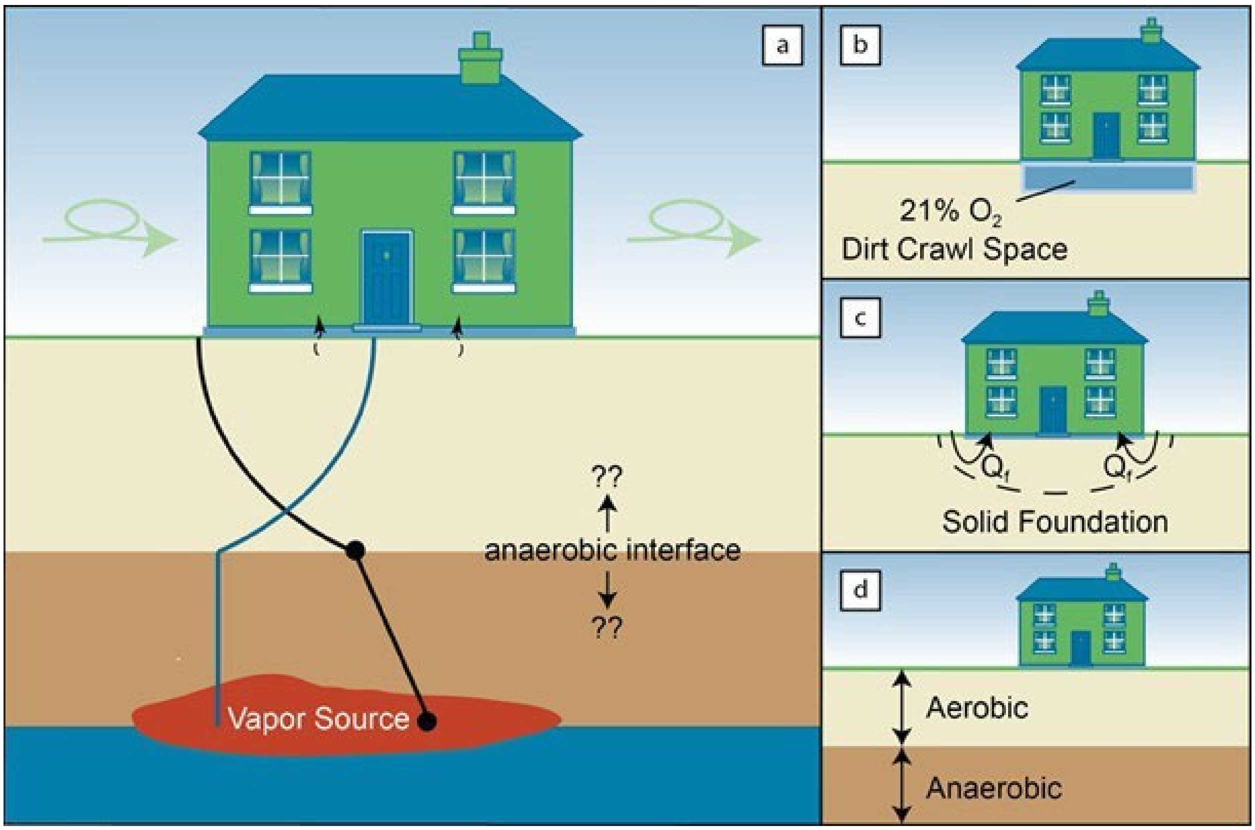

Figure 1. (a) BioVapor model biodegradation conceptualization; (b) O_2 boundary conditions consisting of constant O_2 concentration; (c) constant air flow; (d) fixed aerobic zone depth.

Source: Adapted from API (2010).

The BioVapor User's Guide (API 2012) recommends that Q_f be assumed greater or equal to Q_s because soil vapor advection below and into the building also supplies O_2. In addition, O_2 mass flux by diffusion, both through the building foundation and through lateral migration from the sides of the building, will also supply O_2 for biodegradation. Modeling by DeVaull (2012) showed that when the foundation permeability is low (and thus the soil vapor advection rate is low), the diffusive mass transport is proportionally high. In qualitative terms, this means that when Q_s is low, it generally is appropriate for Q_f to be higher than Q_s to account for O_2 diffusion.

Chemical Concentrations

The BioVapor model requires input of chemical concentrations for three groups of PHCs:

- Risk drivers (such as benzene, toluene, ethylbenzene, and xylenes [BTEX] or hexane)
- Other PHC compounds, which are not risk drivers but represent an oxygen demand
- Hydrocarbon surrogates, which include multiple chemicals (for example, hydrocarbon ranges) and which may also not be risk drivers, but represent an oxygen demand

It is important to include the risk drivers as well as the other PHC compounds and hydrocarbon surrogates as they all aerobically biodegrade and contribute to total oxygen demand in the subsurface.

Contaminant concentrations for soil vapor or groundwater sources may be entered, and new chemicals may be added to the database. Concentration data for groundwater may be used for a dissolved PHC source, but soil vapor data are recommended for a light nonaqueous-phase liquid (LNAPL) source.

The oxygen demand required by the total hydrocarbons in soil vapor should be accounted for by entering input data on PHC concentrations. The best practice for estimating source concentrations for BioVapor input uses PHC concentrations in soil vapor estimated by one of the following three methods:

1. Estimate concentrations of individual BTEX compounds and other risk drivers as warranted by an approved analytical method and use empirical relationships to estimate concentrations of other aliphatic and aromatic hydrocarbons. These estimates may be obtained from literature values that are based on representative total petroleum hydrocarbons (TPH) concentration for product type (API 2012) or measured TPH (such as USEPA Method TO-3). This method is acceptable when the type of product at the site is known.
2. Estimate concentrations of individual BTEX compounds and other risk drivers as warranted by an approved analytical method and measure aliphatic and aromatic hydrocarbon ranges (for example, Massachusetts air-phase petroleum hydrocarbon method for aliphatics and aromatics).
3. Use USEPA Method TO-15 analysis with an extended PHC chemical list, including tentatively identified compounds, modified to account for C5 and C6 aliphatics, to provide a reasonable accounting of total hydrocarbons present.

For all methods, methane and other fixed gas concentrations may be analyzed according to an accepted method.

Guidance on estimating petroleum vapor composition and vapor concentrations in LNAPL source zones is provided in **Table 1**. Estimated TPH concentrations in **Table 1** are directly above LNAPL zones. For dissolved-phase TPH plumes in groundwater, the concentrations of individual hydrocarbon components and TPH are generally at least 100 to 1,000 times lower (and often much greater than 1,000 times lower) than those within LNAPL source zones (USEPA 2013).

Table 1. Petroleum vapor composition.

Compound	Fresh Gasoline	Moderately Weathered Gasoline	Diesel
Benzene	0.25%–1%	1%–2%	<<1%
Toluene, ethylbenzene, xylene	1%–4%	5%–15%	<1%
Other aromatic hydrocarbons	<0.1%	<1%	<10%
Aliphatic hydrocarbons	95%–99%	83%–94%	>90%
Total hydrocarbons	≈200 mg/L	≈100 mg/L	≈1–5 mg/L

Note: mg/L = milligrams per liter.

Source: Adapted from API (2010).

First-Order Biodegradation Rate Constants

In the BioVapor model, degradation is defined in terms of a first-order water-phase aerobic degradation rate, k_w (hr^{-1}). Degradation is assumed to occur only in the water phase of the soil matrix (and only when O_2 is present) at a rate proportional to chemical concentrations in the water phase. A statistical compilation of first-order water-phase biodegradation rates from laboratory and field studies (DeVaull 2007; 2011) for air-connected vadose zone soils is shown in Table H-2 and Figure H-1 in **Appendix H**. The median or geometric mean rate constants in Figure H-1 or listed in Table H-2 are a reasonable starting point for modeling. As part of a sensitivity analysis, a range of rate constants should be simulated. The most likely rates in the distribution are the median (or geometric mean) values. The lowest rates in this empirical data set may have been derived, in some cases, for soils that were not actually uniformly aerobic soils.

Baseline Soil O_2 Respiration Rate

The baseline soil O_2 respiration accounts for the natural oxygen demand from the soil and may be specified directly or estimated from the soil organic carbon level (f_{oc}) based on an empirical relationship developed by DeVaull (2007), as follows:

$$\text{Baseline Soil } O_2 \text{ Respiration Rate} = 1.69\ (\text{mg } O_2/g_{oc} \text{ day}) \times f_{oc}$$

For the range $0.0004 < f_{oc} < 0.4$, errors in the O_2 respiration estimate are within a factor of approximately 10 of the correlation at a 95 percent confidence level (DeVaull 2007). This equation is the BioVapor default value and is recommended in the absence of site-specific data.

Minimum O_2 for Aerobic Respiration

The BioVapor model default of 1 percent is reasonable for modeling purposes. Evidence from field studies with detailed profiles indicates O_2 depletion to low concentrations (<<1 percent) and a corresponding reduction in petroleum vapor concentrations (Davis et al. 2009).

Model Sensitivity

The BioVapor model can show a large sensitivity to source zone concentration and vertical separation distance in cases where biodegradation is the primary attenuation mechanism (DeVaull 2007; Weaver 2012). For these conditions, parameters relating to subsurface O_2 availability (O_2 concentration, foundation airflow), the biodegradation rate and soil moisture can have a significant influence on model estimates (Weaver 2012). Table 2 provides a qualitative evaluation of model sensitivity and recommended data sources.

Table 2. BioVapor inputs parameters and sensitivity.

Parameter	Default Value	Normal Range	Parameter Sensitivity	Reference
Part A: Values for Building Parameters				
Indoor mixing height, L_{mix} (cm)	244 (residential, slab-on-grade) 366 (residential basement) 300 (commercial)	(-)	Medium	USEPA (2017)
Air exchange rate, ER (1/hour)	0.45 (residential) 1.5 (commercial)	(-)	Medium	USEPA (2017)
Foundation thickness, L_{crack} (cm)	10 (residential), 20 (commercial)	(-)	Low	USEPA (2017)
Foundation area, Ab (cm^2)	1.5E+6 (residential) 1.5E+7 (commercial)	(-)	Low to medium	USEPA (2017)
Foundation crack fraction, h (cm^2-cracks/cm^2-total)	0.001 (residential and commercial)	0–1	Low	USEPA (2017)
Total porosity (soil-filled cracks), q (cm^3-void/cm^3-soil) $T_{,crack}$	1.00	0–1	Low	USEPA (2004)*
Water-filled porosity (soil-filled cracks), q (cm^3-water/cm^3 soil) w_{crack}	0.00	0–1	Low	USEPA (2004) *
Airflow through foundation, Q_s (cm^3-air/second)	83 (residential)	Min: 0	Low (see discussion below)	Hers et al. (2003); USEPA (2004)*†

Note: cm = centimeters, min. = minimum.
* Not addressed in USEPA (2017) model user's guide.
† Q_{soil}/Q_{build} parameter is used.
Notes on the effect of building parameters on model results:

- Relatively insensitive, unless biodegradation is negligible.
- High sensitivity to airflow through foundation, Q_s, if O_2 in the subsurface (and therefore aerobic biodegradation) is limited. Q_s of 83 cm^3-air/sec is for a medium-sized single-family dwelling based on research in Hers et al. (2003). USEPA (2017) and DTSC (2024) specify input of Q_s/Q_b where Q_b = building ventilation rate. USEPA (2017) recommends a Q_s/Q_b value of 0.003. DTSC (2024) recommends a Q_s/Q_b value of 0.03. For nonresidential buildings, a site-specific Q_s/Q_b may be estimated (e.g., from empirical data), and Q_s obtained from estimates of Q_b.
- Residential: (single-family house, slab-on-grade, or basement); commercial: (small office or retail building, slab-on-grade).

Parameter	Default Value	Normal Range	Parameter Sensitivity	Reference
Part B: Values for Vadose Zone Parameters				
Soil porosity, q (cm^3-void/cm^3-soil) T	0.375 (sand)‡	0.1–0.5	High	USEPA (2017); Johnson (2005)
Soil water content, q (cm^3-water/cm^3-soil) w	0.054 (sand)	0–0.5	Very high	USEPA (2017); Johnson (2005)
Soil organic carbon fraction, f_{oc} (cm^3/cm^3-soil)	0.005	0.0001–0.1	Medium	See baseline O_2 respiration rate parameter
Soil density—bulk, r_s (g-soil/cm^3-soil)§	1.7	1.5–2	Low to medium	ASTM (2000)
Airflow through foundation, Q_s (cm^3-air/second)	83	(-)	High	Hers et al. (2003); USEPA (2004)

Parameter	Default Value	Normal Range	Parameter Sensitivity	Reference
Air flow underneath foundation, Q_f (cm^3-air/second)	(-)	≥ Q_s	Very high	No default, generally equal to or greater than Q_s
O_2 concentration below building, at soil surface (atmospheric, for dirt-floor, otherwise apply if measured below foundation)	Optional	0%–21%	High	
Aerobic depth, L_a (cm)	Optional	0–LT	High	
Minimum O_2 concentration for aerobic biodegradation, O_2-min	1%	0%–1%	Low	DeVault (2007)
Annual median soil temperature, T (°C)	10	3–25	Low to medium	USEPA (2017) for groundwater
Baseline soil O_2 respiration rate, L (mg-O /g-soil-sec); function base 2 of f_{oc}	1.956E-7	Min.: 0	Low to medium	DeVault (2007)
Depth to source (from bottom of foundation), LT (cm)	(-)	(-)	Low to medium for >200 cm, medium to high for <200 cm	None

Note: cm = centimeters, g = grams, mg = milligrams, min. = minimum.
‡ See USEPA (2017) for additional soil textures.
§ Used to calculate volumetric water content; hence it is a sensitive parameter.

Parameter	Default Value	Normal Range	Parameter Sensitivity	Reference
Part C: Values for Source Zone Parameters				
Chemical-specific source vapor concentration (mg/m^3)	Scenario-specific	0–100,000	Medium	
Total source vapor concentration (mg/m^3)	Scenario-specific	0–100,000	High	

Note: mg/m^3 = milligrams per cubic meter.
Notes on the effect of vadose zone parameters on model results:

- Generally, model results can be sensitive to soil vadose zone properties and air flow under the foundation (Q_f). When there are higher total source vapor concentrations, O_2 may be limited. Any source chemicals that may aerobically biodegrade contribute to total O_2 demand (including methane).
- The BioVapor model does not include input screens for physical-chemical parameters and first-order biodegradation rate, but these values can be adjusted in the BioVapor model database.

At sites where biodegradation is negligible, such as sites with high concentration sources and short vertical separation distances, the sensitivity of the BioVapor model is similar to that for the J&E model, which is applicable for nondegrading chemicals. For these conditions, parameters describing the building enclosure and foundation show a significant effect on model estimates (Weaver and Tillman 2005; Weaver 2012; Picone et al. 2012). These parameters include, most significantly, the building air exchange rate and the foundation air flow rate.

When using a petroleum vapor intrusion model such as BioVapor, conduct a sensitivity analysis by specifying known and nominally known parameters (such as source zone concentrations, vertical separation distance, and building dimensions) and varying these and other key input parameters to account for uncertainty and variability in nominal site conditions. The key parameters affecting subsurface fate and transport include the O_2 boundary conditions, the first-order decay rate, the PHC source vapor strength, and the soil moisture content. Appendix H includes a more detailed discussion of parameter estimates and input values.

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