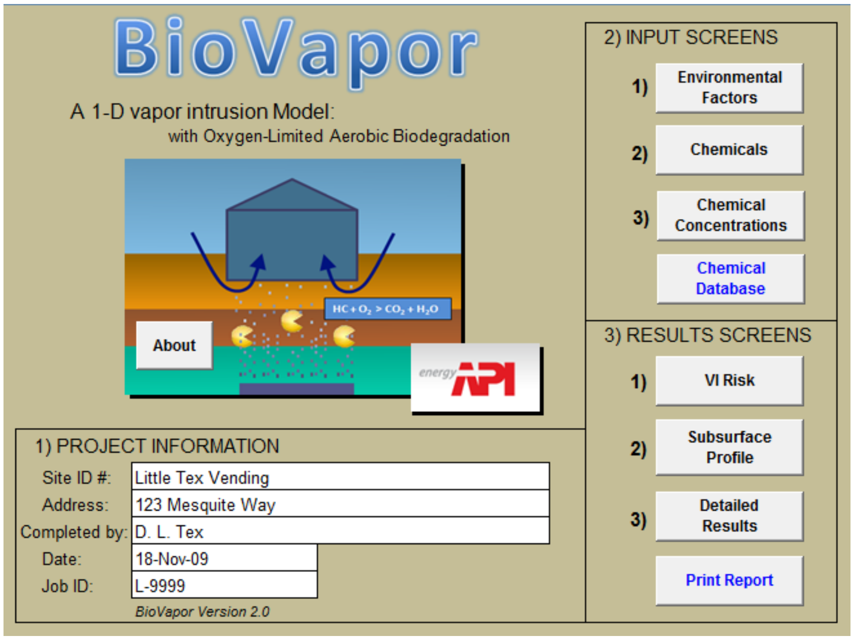
USERS MANUAL

BioVapor

A 1-D Vapor Intrusion Model with Oxygen-Limited Aerobic Biodegradation



BioVapor

A 1-D vapor intrusion Model:
with Oxygen-Limited Aerobic Biodegradation

1) PROJECT INFORMATION
Site ID #: Little Tex Vending
Address: 123 Mesquite Way
Completed by: D. L. Tex
Date: 18-Nov-09
Job ID: L-9999

BioVapor Version 2.0

Version 2.1

Prepared by GSI Environmental Inc. **November 2012**
2211 Norfolk, Suite 1000, Houston, Texas 77098-4054

VERSION 2.1 RELEASE NOTE

BioVapor 2.1 is a minor update of BioVapor 2.0. The changes made are detailed on Page 25 of this manual.

SPECIAL NOTES

Users of the model shall have a license to use the model only for the intended use as described in page one of the User's Manual. Resale or commercial use the model is strictly forbidden.

Neither API nor any of API's employees, subcontractors, consultants, or other assigns make any warranty or representation, either express or implied, with respect to the accuracy, completeness, or utility of the information contained herein, or assume any liability or responsibility for any use, or the results of such use, of any information or process disclosed in this publication, or represent that its use would not infringe upon privately owned rights.

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Where applicable, authorities having jurisdiction should be consulted.

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ACKNOWLEDGEMENTS

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API STAFF CONTACT

Roger Claff, Regulatory Analysis and Scientific Affairs Department (RASA)

MODEL AUTHOR

George DeVaull, Shell Global Solutions

SOFTWARE DEVELOPMENT

Thomas McHugh, GSI Environmental
Paul Newberry, GSI Environmental

REVIEWERS AND TESTERS

Harley Hopkins, ExxonMobil Corporation
Matt Lahvis, Shell Global Solutions (U.S.), Inc.
Todd Ririe, Chevron Corporation
Lynn Spence, Spence Environmental Engineering

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LIST OF ACRONYMS

Acronym	**Definition**
ASHRAE	American Society of Heating, Refrigerating and Air-Conditioning Engineers
ASTM	American Society for Testing and Materials
BTEX	Benzene, Toluene, Ethyl Benzene, Xylene
COCs	Constituents of Concern
NAPL	Non-Aqueous Phase Liquid
RBSL	Risk Based Screening Level
TPH	Total Petroleum Hydrocarbons
USEPA	U.S. Environmental Protection Agency
VI	Vapor Intrusion
VOC	Volatile Organic Compound

INTRODUCTION

BioVapor is a user-friendly spreadsheet implementation of the *Indoor Vapor Intrusion with Oxygen-Limited Biodegradation* model presented in DeVaull, 2007. This algebraic model incorporates a steady-state vapor source, diffusion-dominated soil vapor transport in a homogeneous subsurface soil layer, and mixing within a building enclosure. The soil is divided into a shallow aerobic layer including first-order biodegradation and a deeper anaerobic layer in which biodegradation is neglected. Model equations are provided in Appendix B of this guide. The user has three options for specifying the oxygen supply below the building foundation: 1) direct entry of the depth of the aerobic zone below the building foundation, 2) constant oxygen concentration below the building foundation, or 3) constant flow of atmospheric air below the building foundation. For Options 2 or 3, the model is solved by iteratively varying the aerobic depth to match oxygen demand (due to baseline soil respiration and biodegradation of chemicals) to oxygen supply. In the absence of aerobic biodegradation, the model is essentially equivalent to the Johnson and Ettinger (1991) vapor intrusion model. Although other analytical models have accounted for biodegradation with 1st-order decay, ***BioVapor*** improves on this method by accounting for limited oxygen availability.

This manual provides the computer system requirements for operation of ***BioVapor***, step-by-step user instructions, and information on scientific considerations required to identify appropriate input values and obtain valid model results. For additional details on development of the algebraic model, see DeVaull, 2007.

LIMITATIONS AND INTENDED USE OF BIOVAPOR

The ***BioVapo***r model is a steady-state 1-D analytical model intended to provide the user with an improved understanding of the potential affect of aerobic biodegradation in the vadose zone on the vapor intrusion pathway. The model does not directly account for spatial or temporal variations in parameter values. As a result, the model is not expected to provide highly accurate predictions when a single set of input parameter values is used to represent a single site. Rather, the model is expected to help the user identify a reasonable range of potential outcomes that result from varying key input parameter values to account for the uncertainty and variability associated with site conditions.

Some required or optional model input parameters such as oxygen concentration below the building foundation and baseline soil oxygen respiration rate are not commonly measured during the site investigation. When practical, this manual provides guidance concerning available methods to estimate reasonable values for these parameters. However, the user should conduct a sensitivity analysis in order to evaluate the effect of input parameter value uncertainty on the model results.

For some scenarios, the ***BioVapor*** model can predict acceptable petroleum hydrocarbon concentrations in indoor air when high concentrations of petroleum hydrocarbons are present in the subsurface. When interpreting these results, the user should consider the uncertainty associated with the model inputs, along with the potential effects of spatial and temporal variability. When free-phase hydrocarbons are present in the subsurface in close proximity to the target building, the user is cautioned against relying on ***BioVapor*** model results as the primary line of evidence that vapor intrusion is not a concern. In this case, BioVapor model results are more appropriately considered as a secondary or supporting line of evidence when other investigation results also indicate no vapor intrusion concern. In addition, the user is reminded that ***BioVapor*** does not evaluate other potential exposure routes (besides vapor intrusion) migration pathways, or potential risks (such as fire and explosion) other than health toxicity. The user is responsible for evaluation of these other considerations.

BIOVAPOR QUICK START

MINIMUM SYSTEM REQUIREMENTS

BioVapor requires a computer running Microsoft® Windows 2000, Windows XP or Vista. Additionally, the software requires Microsoft® Excel v2002 (XP), Microsoft® Office Excel 2003 or Microsoft® Office Excel 2007. To ensure proper operation, the user should install all software updates for Office Excel released by Microsoft®. The ***BioVapo***r model should run well on any personal computer (PC) computer capable of running Microsoft® Excel for Windows; however, ***BioVapor*** will not run properly using Excel for Mac.

INSTALLATION

BioVapor consists of an enhanced Microsoft® Excel workbook (Biovapor.xls) and help file (BioVapor_Help.chm). These two files may be delivered via electronic media such as e-mail, internet download, etc. The two files may be placed in a convenient location on your computer, but care should be taken to ensure that the two files are kept together in the same folder.

PROGRAM START-UP

- *Open* `“BioVapor.xls”`

To start ***BioVapor***, double-click on the file *BioVapor.xls.*

TROUBLESHOOTING

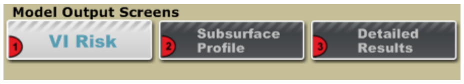
Although **BioVapor** is fully compatible with Microsoft Excel 2007, there are some security configurations that may cause it to malfunction. If problems are encountered in normal operation, it is suggested to save the BioVapor.xls file as a macro-enabled workbook (.xlsm).

DATA INPUT AND OUTPUT

The user interface of ***BioVapor*** is spreadsheet-based. Input values are entered into spreadsheet cells and navigation among the cells on each individual input screen can be performed using the arrow keys or the mouse, just as with any spreadsheet. The individual screens of the ***BioVapor*** tool may be printed using the buttons provided or using the “Print” (Ctrl+P) command in Microsoft® Excel.

On each input screen, white cells indicate primary input values, while black cells indicate calculated results. On the input screens, values can only be entered into white cells (all other cells are locked). When entered numbers are displayed in a red font color, the value entered is outside of normally accepted bounds (see Tables 1-5).

Where necessary, the general order of tasks to be completed is indicated by the numbers identifying each section of input data. Navigation to another screen is performed by clicking the appropriate labeled button (e.g., “Home”, “Next”, etc.) in the “Commands and Options” section.



Additionally, each screen has a navigation graphic at the top to indicate steps in the process. There are separate graphics for both the Input and Output section of the tool.

ON-LINE HELP

- *Click on the "?" buttons located throughout the software.*

Each input and output screen is described in further detail in this manual and in the on-line Help text. To access on-line help for a particular input section, click on the small question mark buttons located throughout the software or the "Help" button located on each input screen.

BIOVAPOR STEP-BY-STEP

How Do I Use *BioVapor*?

1) ***Home Screen:*** Enter project information. This screen serves as a point from which to access any and all other screens in the tool. Initially, it is necessary to begin with the Environmental Factors screen and proceed step-wise through the software. Once the process is complete, this screen serves as navigation point from which to review input and output data, as well as print a report.

2) ***Environmental Factors:*** Choose an Oxygen Boundary Condition. Provide input values for all parameters with white data input cells. Choose Default Values if desired. Select Next to specify chemicals.

3) ***Chemical Selection:*** Choose which chemicals ***BioVapo***r will analyze. Chemicals are divided into Potential Risk Drivers, Other Hydrocarbons, and Hydrocarbon Surrogates. In order to ensure a proper oxygen mass balance, all hydrocarbons in the source must be represented as risk drivers, other hydrocarbons, or hydrocarbon surrogates. To review or edit chemical properties (including 1st-order biodegradation rates), access the chemical database by choosing "Edit Chemicals." Select Next to specify chemical concentrations.

4) ***Chemical Concentrations:*** Input the concentration of the chemical(s) chosen. In order to ensure a proper oxygen mass balance, the Total Entered Hydrocarbon Concentration must equal the total hydrocarbon concentration in the source. Select Next to view the Vapor Intrusion (VI) Risk screen.

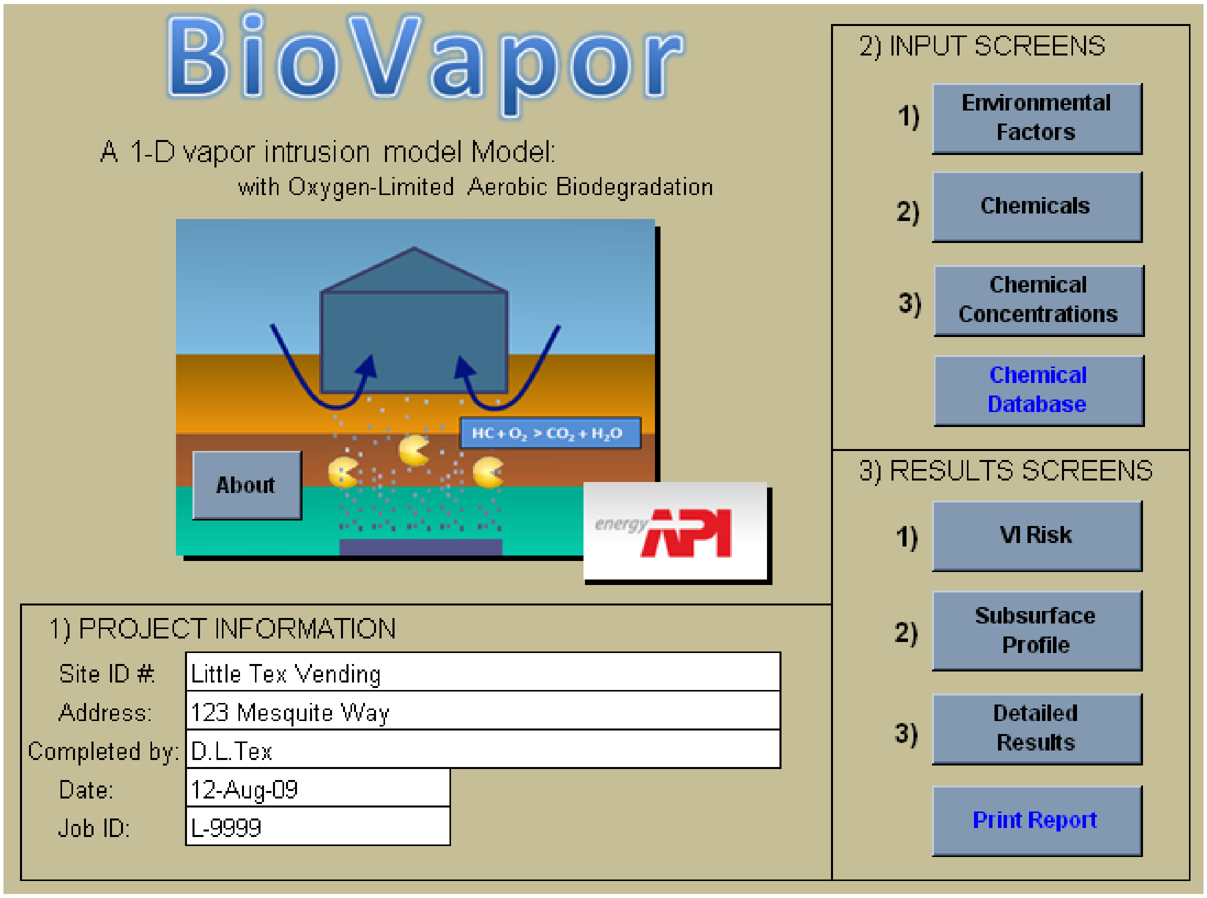
5) ***Vapor Intrusion Risk Results:*** This screen only displays results for chemicals in the Potential Risk Drivers database.

6) ***Subsurface Profile:*** Select a chemical from the dropdown menu and select "Update Charts" to see that chemical displayed on both the Concentration vs. Depth and Flux vs. Depth charts.

7) ***Detailed Results:*** This screen is divided into two sections: i) the upper General Results section displays data that is not related to individual chemicals, and ii) the lower Chemical Specific Results section displays both parameters that are chemical-specific and total values for all chemicals.

HOME SCREEN

The Home screen is the hub of the user interface, and is automatically opened at startup (see Figure 1). Most of the input and output screens are accessed from and return to this screen. On this screen, the user enters project information and is able to begin the ***BioVapor*** process by navigating to the appropriate input and output screens. Initially, it is necessary to proceed through the process in a step-wise fashion, but later, results can be accessed directly from this screen. Detailed reports can also be printed from this screen.



Site ID #: Little Tex Vending
Address: 123 Mesquite Way
Completed by: D.L.Tex
Date: 12-Aug-09
Job ID: L-9999

Figure 1: Home Screen

A) Project Information

Basic site and project information entered here will be displayed on all print-outs for easy identification and record-keeping.

B) Input Screens

These navigation buttons allow the user to access the screens used for entry of the required inputs: environmental factors, chemicals, and chemical concentrations.

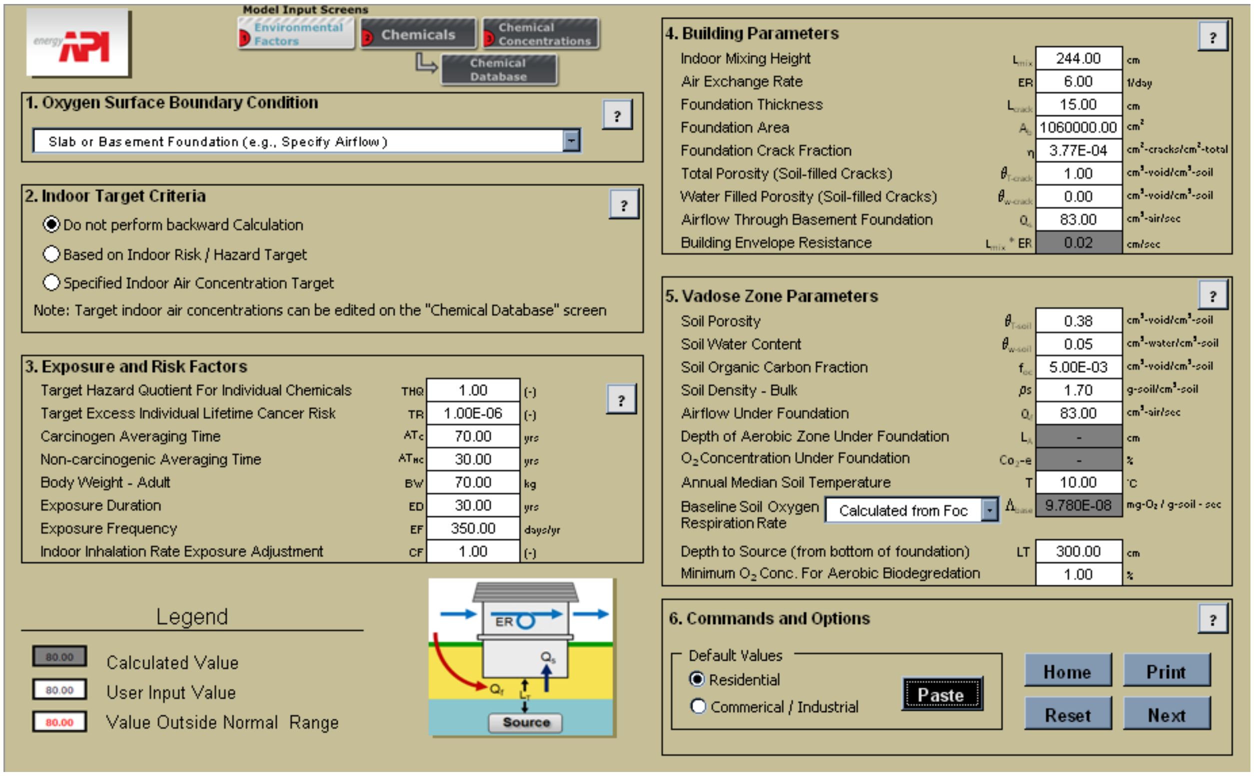
C) Results Screens

The navigation buttons allow the user to access the model results: vapor intrusion risk, subsurface profile, and detailed results.

INPUT SCREENS

ENVIRONMENTAL FACTORS

This screen is accessed by clicking “Environmental Factors” on the Home screen. On this screen, the user specifies: i) oxygen boundary condition; ii) backward calculation; iii) exposure and risk factors for each complete pathway; iv) building parameters and v) vadose zone parameters.



1. Oxygen Surface Boundary Condition

Slab or Basement Foundation (e.g., Specify Airflow)

2. Indoor Target Criteria

● Do not perform backward Calculation
○ Based on Indoor Risk / Hazard Target
○ Specified Indoor Air Concentration Target

Note: Target indoor air concentrations can be edited on the "Chemical Database" screen

3. Exposure and Risk Factors

Target Hazard Quotient For Individual Chemicals	THQ	1.00	(-)
Target Excess Individual Lifetime Cancer Risk	TR	1.00E-06	(-)
Carcinogen Averaging Time	AT_C	70.00	yrs
Non-carcinogenic Averaging Time	AT_{NC}	30.00	yrs
Body Weight - Adult	BW	70.00	kg
Exposure Duration	ED	30.00	yrs
Exposure Frequency	EF	350.00	days/yr
Indoor Inhalation Rate Exposure Adjustment	CF	1.00	(-)

Legend

80.00	Calculated Value
80.00	User Input Value
80.00	Value Outside Normal Range

4. Building Parameters

Indoor Mixing Height	L_{mix}	244.00	cm
Air Exchange Rate	ER	6.00	1/day
Foundation Thickness	L_{crack}	15.00	cm
Foundation Area	A_b	1060000.00	cm^2
Foundation Crack Fraction	η	3.77E-04	cm^2-cracks/cm^2-total
Total Porosity (Soil-filled Cracks)	$\theta_{T\text{-}crack}$	1.00	cm^3-void/cm^3-soil
Water Filled Porosity (Soil-filled Cracks)	$\theta_{w\text{-}crack}$	0.00	cm^3-void/cm^3-soil
Airflow Through Basement Foundation	Q_s	83.00	cm^3-air/sec
Building Envelope Resistance	L_{mix} * ER	0.02	cm/sec

5. Vadose Zone Parameters

Soil Porosity	$\theta_{T\text{-}soil}$	0.38	cm^3-void/cm^3-soil
Soil Water Content	$\theta_{w\text{-}soil}$	0.05	cm^3-water/cm^3-soil
Soil Organic Carbon Fraction	f_{oc}	5.00E-03	cm^3-void/cm^3-soil
Soil Density - Bulk	ρs	1.70	g-soil/cm^3-soil
Airflow Under Foundation	Q_f	83.00	cm^3-air/sec
Depth of Aerobic Zone Under Foundation	L_A	-	cm
O_2 Concentration Under Foundation	Co_2-e	-	%
Annual Median Soil Temperature	T	10.00	°C
Baseline Soil Oxygen Respiration Rate: Calculated from Foc	Λ_{base}	9.780E-08	mg-O_2 / g-soil - sec
Depth to Source (from bottom of foundation)	LT	300.00	cm
Minimum O_2 Conc. For Aerobic Biodegredation		1.00	%

6. Commands and Options

Default Values
● Residential
○ Commerical / Industrial

Figure 2: Environmental Factors Screen

1) Oxygen Boundary Condition

The user must choose one of three options: a) constant concentration, b) constant air flow, or c) directly specify depth of aerobic zone. Options (a) and (b) specify a maximum downward oxygen flow into the soils below a building foundation. The constant concentration option is most appropriate for open soils (e.g., dirt floor crawl space). The constant airflow option is most appropriate for solid foundations (e.g., concrete slab). Depth of aerobic zone (c) is most appropriate when vertical profile measurements have been used to directly estimate the depth of the aerobic zone.

a) Earthen Floor Foundation (e.g., specify oxygen surface concentration)

When this option is selected, maximum oxygen availability is limited by the user specified oxygen concentration and diffusion of oxygen through soils towards the volatile organic compound (VOC) source. Resistance to oxygen flow by a solid foundation or soil surface cover is neglected.

Input Value Estimation Methods: The user-specified concentration may be i) equal to the concentration of oxygen in atmospheric air, 21% v/v; ii) a site-specific measurement; or iii) an estimated value based on professional judgment. In cases (ii) and (iii), if the actual oxygen concentration is lower than the specified value, the model will yield non-conservative results. In case (i), if foundation resistance is not negligible, the model will yield non-conservative results.

b) Slab or Basement Foundation (e.g., specify airflow)

When this option is selected, maximum oxygen availability is limited by atmospheric oxygen concentration, and resistance to oxygen flow by both a building foundation and diffusion of oxygen from below the building foundation towards the VOC source.

Resistance to flow through a foundation (per unit area), is defined by the air flow through the foundation, Q_s, divided by the building foundation area. Since oxygen may also enter soils below a foundation through the building perimeter (without passing directly through the building envelope), the model specifies a limiting value for air flow below the foundation, Q_f, and recommends that Q_f is greater or equal to Q_s.

Input Value Estimation Methods: The user-specified air flow, Q_f, may be based on i) a value assumed to be equal to the rate of air flow through the building foundation (Q_s), or ii) estimated values based on professional judgment.

c) Specify Aerobic Depth Below Foundation

When options (a) constant concentration or (b) constant air flow are specified, the model calculates an aerobic depth from the entered parameters. Option (c) allows the user to directly specify the depth of the aerobic zone. Sufficient oxygen is assumed to be present within the specified aerobic zone.

Input Value Estimation Methods: The user-specified depth of the aerobic zone may be based on i) a site-specific oxygen vertical profile in the vadose zone or ii) an assumed value based on professional judgment.

2) Indoor Target Criteria

The ***BioVapor*** tool will present both forward (i.e., predicted concentrations in indoor air) and backward (i.e., source target concentrations) calculations. For the backward calculations, the user must choose to calculate the source target concentrations based on either i) the indoor risk / hazard target or ii) the specified indoor air target concentration. There is little practical difference between these two options because the risk limit (when combined with a chemical toxicity factor) yields a specific indoor air target concentration. However, the option to use either the risk limit or the target indoor air concentration provides the user with the ability to account for variations in regulatory requirements (i.e., specified risk limits or specified indoor air target concentrations).

For either option, the resulting source concentrations are calculated using a critical chemical approach rather than a cumulative risk approach. The critical chemical is the chemical in the user-specified mixture that has the greatest impact on indoor air quality relative to the specified indoor air concentration or target risk limit. Using the critical chemical approach, the back-calculated source concentration for the critical chemical is predicted to yield an indoor air concentration equal to the indoor air target concentration for that chemical. The back-calculated source concentrations for the remaining chemicals are determined from the user input source concentrations. For example, the user may enter a soil gas benzene source concentration of 10,000 ug/m^3 benzene and 20,000 ug/m^3 for toluene for the forward calculation. For this scenario, if benzene is the critical chemical for the backward calculation and the back-calculated benzene source concentration is 200,000 ug/m^3, then the back-calculated toluene source concentration would be 400,000 ug/m^3 (i.e., 200,000 x 20,000/10,000).

Default target indoor air concentrations in the chemical database have been set equal to the USEPA Unified Screening Values issued by the USEPA in September 2008. These values are based on a hazard quotient of 1 and a 10^{-6} excess cancer risk limit. The user can edit the target indoor air concentrations through the Chemical Database screen.

3) Exposure and Risk Factors

The user must enter exposure and risk factor values to be used for indoor risk calculations.

Input Value Estimation Methods: Default values (Tables 1 and 2) are provided for residential and commercial use scenarios based on values commonly used for risk assessments. The user can enter site-specific values in accordance with applicable regulatory guidance or site-specific conditions.

Table 1. Default Values for Exposure and Risk Factors: Residential

Parameter	Value	Units	Reference	Normal Range
Target Hazard Quotient For Individual Chemicals	1.0	(-)	USEPA 2003	0.1 - 1
Target Excess Individual Lifetime Cancer Risk	1.00E-06	(-)	USEPA 2003	1.00E-6 - 1.00E-04
Carcinogen Averaging Time	70	yrs	USEPA 2003	60 - 80
Non-Carcinogenic Averaging Time	30	yrs	USEPA 2003	6 - 80
Body Weight - Adult	70	kg	USEPA 2003	60 - 80
Exposure Duration	30	yrs	USEPA 2003	0.1 - 80
Exposure Frequency	350	days/yr	USEPA 2003	1 - 365
Indoor Inhalation Rate Correction Factor	1.0	(-)	None (Default value results in no adjustment)	0 - 1

Table 2. Default Values for Exposure and Risk Factors: Commercial

Parameter	Value	Units	Reference	Normal Range
Target Hazard Quotient For Individual Chemicals	1.0	(-)	USEPA 2003	0.1 - 1
Target Excess Individual Lifetime Cancer Risk	1.00E-06	(-)	USEPA 2003	1.00E-6 - 1.00E-04
Carcinogen Averaging Time	70	yrs	USEPA 2003	60 - 80
Non-Carcinogenic Averaging Time	25	yrs	ASTM 2000	6 - 80
Body Weight - Adult	70	kg	USEPA 2003	60 - 80
Exposure Duration	25	yrs	ASTM 2000	0.1 - 80
Exposure Frequency	250	days/yr	ASTM 2000	1 - 365
Indoor Inhalation Rate Exposure Adjustment	1.0	(-)	None (Default value results in no adjustment)	0 - 1

Indoor Inhalation Rate Exposure Adjustment: Inhalation toxicity factors (i.e., reference concentration for non-cancer toxicity and inhalation slope factor for cancer risk) are based on continuous (24 hr/day) inhalation exposure under conditions of typical physical activity. This exposure is assumed to correspond to a daily inhalation rate of 20 m^3-air/day for an adult (USEPA, 2003b). For exposure scenarios where the daily inhalation exposure in the receptor building will be significantly greater or less than 20 m^3-air/day, the Indoor Inhalation Rate Exposure Adjustment can be used to account for this difference in exposure. For example, an Indoor Inhalation Rate Exposure Adjustment of 0.33 can be used for an office building where the exposure would occur during 8 hr/day of typical physical activity.

4) Building Parameters

The user must enter building parameter values for use in simulating VOC transport into the building.

Input Value Estimation Methods: Default values (Tables 3 and 4) are provided for residential and commercial buildings based on values commonly used for risk assessments. The user can enter site-specific values consistent with applicable regulatory guidance or site-specific conditions.

Table 3. Default Values for Building Parameters: Residential (Single-Family House,Slab-On-Grade)

Parameter	Value	Units	Reference	Normal Range
Indoor Mixing Height	244	cm	USEPA 2003	(-)
Air Exchange Rate	6	1/day	USEPA 2003	Min: 1.3
Foundation Thickness	15	cm	USEPA 2003	(-)
Foundation Area	1.06E+06	cm^2	USEPA 2003	(-)
Foundation Crack Fraction	3.77E-04	cm^2-cracks/cm^2-total	USEPA 2003	0 - 1
Total Porosity (Soil-filled Cracks)	1.00E+00	cm^3-void/cm^3-soil	USEPA 2003	0 - 1
Water Filled Porosity (Soil-filled Cracks)	0.00E+00	cm^3-void/cm^3-soil	USEPA 2003	0 - 1
Airflow Through Basement Foundation	83	cm^3-air/sec	USEPA 2003	Min: 0

Table 4. Default Values for Building Parameters: Commercial (Small Office or Retail Building, Slab-On-Grade)

Parameter	Value	Units	Reference	Normal Range
Indoor Mixing Height	300	cm	ASTM 2000	(-)
Air Exchange Rate	12	1/day	ASHRE 2004	Min: 1.3
Foundation Thickness	15	cm	USEPA 2003	(-)
Foundation Area	1.06E+06	cm^2	USEPA 2003	(-)
Foundation Crack Fraction	3.77E-04	cm^2-cracks/cm^2-total	USEPA 2003	0 - 1
Total Porosity (Soil-filled Cracks)	1.00E+00	cm^3-void/cm^3-soil	USEPA 2003	0 - 1
Water Filled Porosity (Soil-filled Cracks)	0.00E+00	cm^3-void/cm^3-soil	USEPA 2003	0 - 1
Airflow Through Basement Foundation (Q_s)	83	cm^3-air/sec	USEPA 2003	Min: 0

5) Vadose Zone Parameters

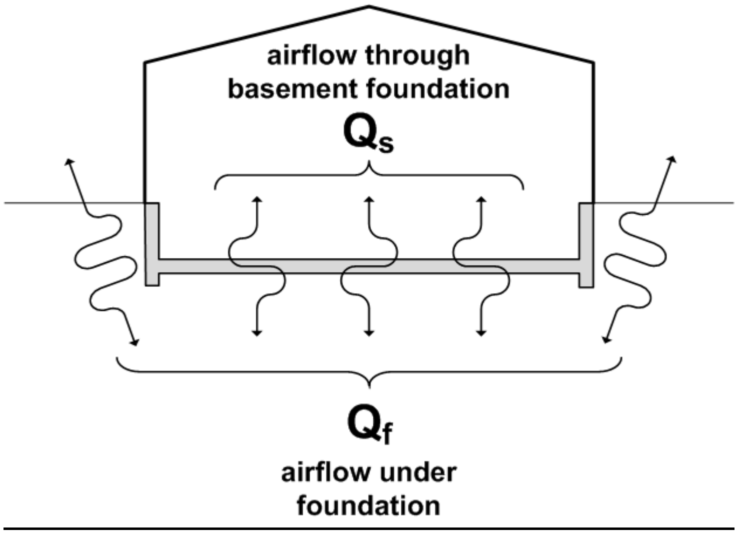
The user must enter vadose zone parameter values for use in simulating VOC fate and transport through the vadose zone.

Input Value Estimation Methods: The default values (Table 5) provided are based on values commonly used for risk assessments. The user can enter site-specific values in accordance with applicable regulatory guidance or site-specific conditions.

Table 5: Default Values for Vadose Zone Parameters: Residential and Commercial

3) Vadose Zone Parameters (Sandy Soil)	**Value**	**Units**	**Reference**	**Normal Range**
Soil Porosity	0.375	cm^3-void/cm^3-soil	USEPA 2003	0.1 – 0.5
Soil Water Content	0.054	cm^3-water/cm^3-soil	USEPA 2003	0 – 0.5
Soil Organic Carbon Fraction	0.005	cm^3/cm^3-soil	Recommended by George DeVaull	0.0001 – 0.1
Soil Density - Bulk	1.7	g-soil/cm^3-soil	ASTM 2000	1.5 – 2
Airflow Under Foundation	83	cm^3-air/sec	Matched to Qsoil	(-)
Depth of Aerobic Zone Under Foundation (Qf)	(-)	cm	No Default Provided	≥ Qs
O_2 Concentration Under Foundation	(-)	%	No Default Provided	0 – 21
Annual Median Soil Temperature	10	°C	USEPA 2003	0 – 30
Baseline Soil Oxygen Respiration Rate	1.95602E-07	mg-$_{O2}$ / g-soil - sec	Fxn of foc per DeVaull, 2007	Min: 0
Depth to Source (from bottom of foundation)	300	cm	None	(-)

The difference between Q_s (Airflow Through Basement Foundation) and Q_f (Airflow Under Foundation) is illustrated in the figure below. Q_f should be greater than or equal to Q_s.



Baseline Soil Oxygen Respiration Rate: This parameter is used to account for the oxygen demand from the soil that occurs even in the absence of degradable hydrocarbons. The user may directly specify this value or have the software calculate a value based on the soil organic carbon level (f_{oc}). For this purpose, the software uses the following relationship (DeVaull, 2007):

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

Since the user will rarely (if ever) have a site-specific basis for estimating the baseline soil oxygen respiration rate, use of the f_{oc} relationship is recommended.

6) Commands and Options

- ***Paste:*** Inserts selected default values (residential or commercial) into input parameter cells.

- ***Print:*** Performs the same action as choosing “Print” from Excel’s “File” menu or pressing Ctrl+P.

- ***Home:*** Returns the user to the Home screen.

- ***Next:*** Advances the user to the Chemical Selection screen.

CHEMICALS

This screen is used to select the individual chemicals and surrogates to be modeled. When either *constant concentration* or *constant air flow* is selected as the oxygen boundary condition on the Environmental Factors screen, it is important for the user to identify all biodegradable vapor phase hydrocarbons present in the source area. For these two boundary conditions, the model uses an oxygen mass balance (demand versus availability) to determine the depth of the aerobic zone. Therefore, if the user does not identify all volatile chemicals that exert an oxygen demand, then the model will over-estimate the depth of the aerobic zone and over-predict the effect of biodegradation. When “*directly specify the depth of aerobic zone*” is selected as the oxygen boundary condition, then no oxygen mass balance is performed and the model results for individual chemicals will not be affected by the total hydrocarbon concentration.

The user can select 1) potential risk drivers, 2) other hydrocarbons, and/or 3) hydrocarbon surrogates. “Potential risk drivers” represents the individual hydrocarbons most likely to contribute to the vapor intrusion risk based on volatility and toxicity. “Other hydrocarbons” represents volatile hydrocarbons that may be present in the source but are less likely to significantly contribute to the health risk potentially associated with vapor intrusion. “Hydrocarbon surrogates” represents groups of other hydrocarbons with similar fate and transport characteristics. Potential risk drivers are included in the evaluation of risk and oxygen demand, while other hydrocarbons and hydrocarbon surrogates are included only in the evaluation of oxygen demand. Guidance on chemical selection is provided below.

1) Source Type

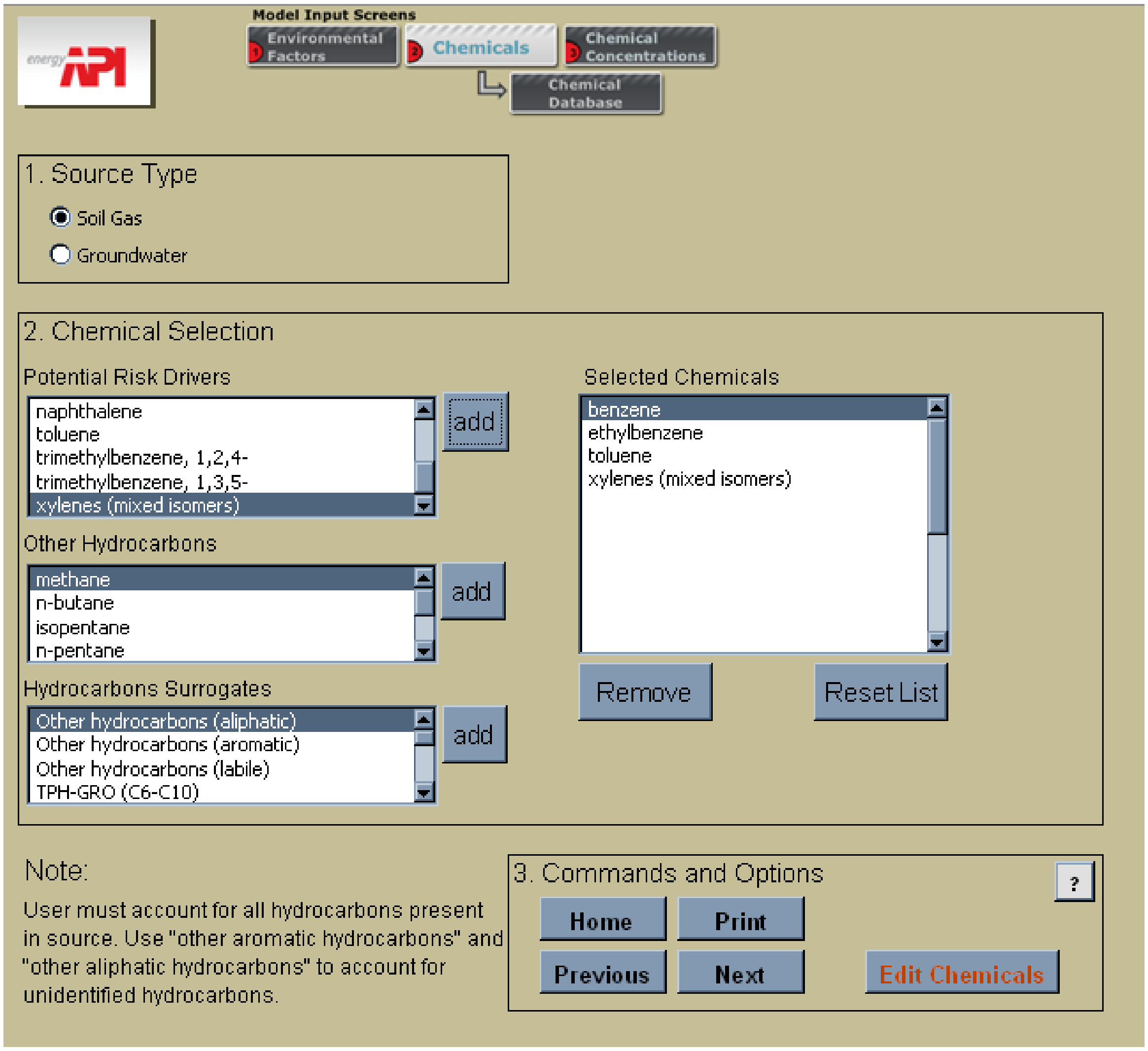
Select the source type as either “Soil Gas” or “Groundwater”. This selection defines the source matrix (i.e., soil gas or groundwater) used in the model. If the user selects “Groundwater”, then the model will estimate soil gas concentrations based on the user-specified hydrocarbon concentrations in groundwater (see CHEMICAL CONCENTRATIONS, below).

The user should choose “Soil Gas” when soil gas source concentration data are available. The user should choose “Groundwater” when groundwater, but not soil gas source concentration data are available. When neither soil gas nor groundwater source concentration data are available, the user should choose “Soil Gas”. In this case, the user will have to estimate the soil gas source hydrocarbon concentrations.

2) Chemical Selection

Select chemicals by clicking on the chemical and then clicking “*add*”. Note that ***BioVapor*** supports the simultaneous evaluation of up to 20 chemicals and surrogates.

If the desired chemical is not shown on any of the three chemical lists, the user can add the chemical to the database by clicking on the “Edit Chemicals” button under “Commands and Options.” Similarly, to include an “other hydrocarbon” or “hydrocarbon surrogate” as a “potential risk driver,” click on “Edit Chemicals” and add the chemical or surrogate to the “potential risk drivers” portion of the database. After adding all chemical data, it is necessary to go to the Chemicals screen and click the “Reset List” button. This will add the new chemical(s) into the Chemical Selection windows.



1. Source Type

● Soil Gas
○ Groundwater

2. Chemical Selection

Potential Risk Drivers
- naphthalene
- toluene
- trimethylbenzene, 1,2,4-
- trimethylbenzene, 1,3,5-
- xylenes (mixed isomers)

Other Hydrocarbons
- methane
- n-butane
- isopentane
- n-pentane

Hydrocarbons Surrogates
- Other hydrocarbons (aliphatic)
- Other hydrocarbons (aromatic)
- Other hydrocarbons (labile)
- TPH-GRO (C6-C10)

Selected Chemicals
- benzene
- ethylbenzene
- toluene
- xylenes (mixed isomers)

Note:

User must account for all hydrocarbons present in source. Use "other aromatic hydrocarbons" and "other aliphatic hydrocarbons" to account for unidentified hydrocarbons.

3. Commands and Options

Figure 3: Chemical Selection Screen

Selecting the Appropriate Chemicals: All biodegradable hydrocarbons present in the vapor-phase source must be represented through the selection of potential risk drivers, other hydrocarbons, and/or hydrocarbon surrogates.

For dissolved sources, benzene, toluene, ethyl benzene, and xylenes are likely to be the only COCs because these are the only gasoline constituents that have both relatively high solubility and relatively high volatility such that they can migrate away from the source area in groundwater and then volatilize into the soil gas.

For soil or NAPL sources, the hydrocarbon composition may be identified by i) laboratory analysis of the source area hydrocarbon vapors or ii) estimation of hydrocarbon composition based on other knowledge of the type of hydrocarbon mixture present (e.g., fresh gasoline, weathered gasoline, etc.). Laboratory analysis may include quantification of all individual hydrocarbons present in the sample or may rely on a combination of Total Petroleum Hydrocarbon (TPH) measurement and quantification of selected individual hydrocarbons.

Table 6 provides typical hydrocarbon vapor compositions for fresh gasoline. As shown in the table, only 14 hydrocarbons account for over 90% of the hydrocarbon mass in the vapor phase. The simplest approach for modeling these chemicals using ***BioVapor*** is to select a limited number of risk drivers (e.g., benzene and toluene) and to represent the remaining chemicals using hydrocarbon surrogates. Recommendations for estimating source concentrations for these chemicals are provided in the “Chemical Concentrations” section.

Table 6. Typical Vapor Composition For Fresh Reformulated Gasoline Containing Ethanol

	Vapor mass (wt %)		
Compound	**Regular**	**Mid-Grade**	**Premium**
Isopentane (C5)	24.1	24.8	26.0
n-pentane (C5)	14.2	12.6	9.3
2-methylpentane (C6)	9.3	9.8	10.4
Ethanol (C2)	7.6	8.7	10.0
n-butane (C4)	7.4	6.9	6.3
3-methylpentane (C6)	5.3	5.6	6.0
2,2-dimethylpentane (C6)	4.9	5.5	6.5
n-hexane (C6)	4.3	3.7	2.3
2,3-dimethylbutane (C6)	3.4	3.8	4.4
2,2,4-trimethylpentane (isooctane, C8)	2.7	2.8	3.3
Methylcyclopentane (C6)	2.7	2.6	2.6
Toluene (C7)	1.9	1.8	2.0
Cyclopentane (C5)	1.4	1.4	1.4
Benzene[1] (C6)	1.0	1.0	1.0
Total (14 compounds)	90.2	91.0	91.5

References:

1) Harley et al. 2000. *ES&T*, 34, 4088-4094.

Hydrocarbon Surrogates: Hydrocarbon surrogates can be used to represent one or more individual hydrocarbons. “Other hydrocarbons (aliphatic)” can be used to represent aliphatic hydrocarbons not modeled as individual chemicals and “Other hydrocarbons (aromatic)” can be used to represent aromatic hydrocarbons not modeled as individual chemicals. “Other hydrocarbons (labile)” has a very rapid biodegradation rate and can therefore be used as a conservative surrogate for any hydrocarbons that are not risk drivers. The rapid biodegradation rate will result in a conservative over-estimation of oxygen demand associated with these hydrocarbons. “TPH-GRO” and “TPH-DRO” can be used to represent hydrocarbons quantified through TPH-GRO and TPH-DRO laboratory analyses. The remaining surrogates (e.g., C5 Aliphatic) can be used to represent chemicals with the specified carbon number. Note that the chemical properties for the TPH fractions are most representative of NAPL sources and may not be appropriate for dissolved sources of TPH.

- ***Remove:*** Allows the user to select a single chemical and remove it from the list.

- ***Reset List:*** Allows the user to remove all chemicals from the list.

2) Commands and Options

- ***Edit Chemicals:*** Forwards the user to the chemical database where the user can add additional chemicals and edit parameter values for existing chemicals.

- ***Print:*** Performs the same action as choosing “Print” from Excel’s “File” menu or pressing Ctrl+P.

- ***Home:*** Returns the user to the Main screen.

- ***Next:*** Advances the user to the Chemical Concentrations screen.

- ***Previous:*** Returns the user to the Environmental Factors screen.

CHEMICAL DATABASE

This series of three screens is used to add chemicals to the chemical database and to edit chemical parameter values.

1) Adding and Editing Chemicals

To add a new chemical, select the appropriate chemical category (i.e., potential risk drivers, other hydrocarbons, or hydrocarbon surrogates) under “Commands and Options”. Next, enter the chemical name and parameter values into the first empty row below the existing chemicals. To edit parameters for existing chemicals, select the appropriate cell and enter the new value. After adding all chemical data, the chemicals are added to the appropriate list by navigating back to the “Chemical Selection” screen.

Default Biodegradation Rates: Documentation concerning selection of the default biodegradation rates provided in the chemical data is provided in Appendix C of this guide.

2) Commands and Options

- ***Chemical Concentrations:*** Returns the user to the Chemical Concentrations screen.

- ***Risk Drivers:*** Takes the user to the “Potential Risk Drivers” portion of the database.

- ***Other Hydrocarbons:*** Takes the user to the “Other Hydrocarbons” portion of the database.

- ***Hydrocarbon Surrogates:*** Takes the user to the "Hydrocarbon Surrogates" portion of the database.

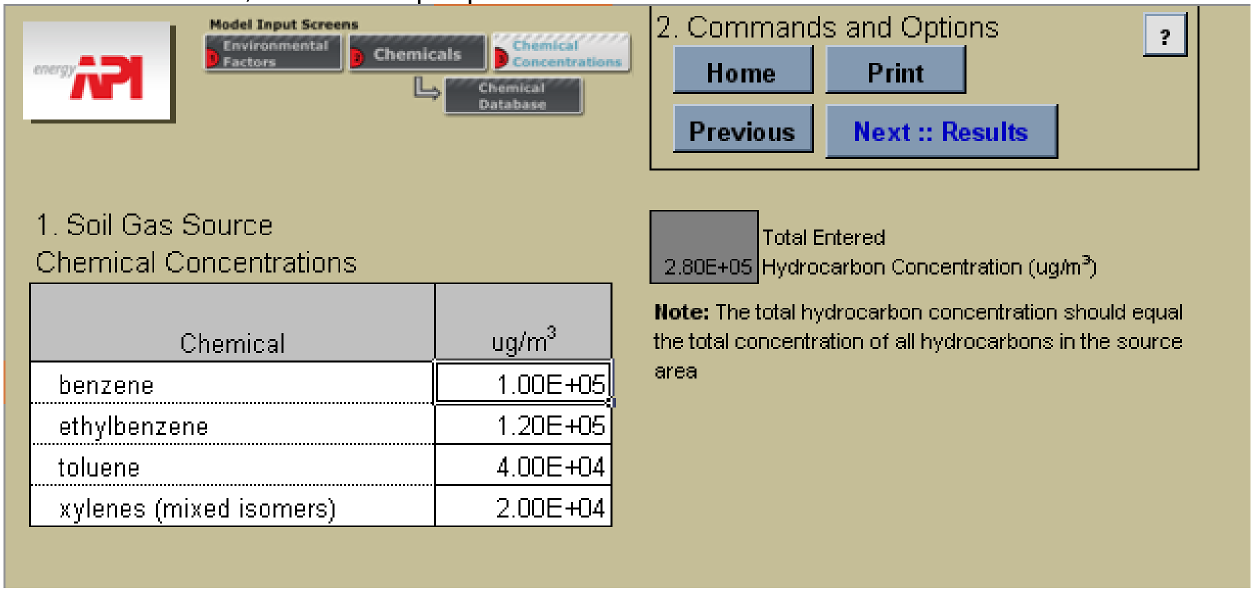
- ***Help:*** Displays on-line help for this screen.

CHEMICAL CONCENTRATIONS

This screen is used to specify the vapor phase or groundwater concentration of each hydrocarbon in the source zone. When either "*constant oxygen concentration below building"* or "*constant air flow below building"* is selected as the oxygen boundary condition on the Environmental Factors screen, it is important for the sum of hydrocarbon concentrations entered be equal to the total hydrocarbon concentration in the source area. For these two boundary conditions, the model uses an oxygen mass balance to determine the depth of the aerobic zone. Therefore, if the user does not specify an accurate total hydrocarbon concentration, then the model will not accurately determine the depth of the aerobic zone. When "*directly specify the depth of aerobic zone*" is selected as the oxygen boundary condition, then no oxygen mass balance is performed, and the model results for individual chemicals will not be affected by the total hydrocarbon concentration.

1) Soil Gas Source Chemical Concentrations

This screen is displayed if the user chose "Soil Gas" as the source type on the prior screen. For each chemical, enter the vapor phase concentration of the chemical in the source area.



1. Soil Gas Source Chemical Concentrations

Chemical	ug/m^3
benzene	1.00E+05
ethylbenzene	1.20E+05
toluene	4.00E+04
xylenes (mixed isomers)	2.00E+04

2.80E+05 Total Entered Hydrocarbon Concentration (ug/m^3)

Note: The total hydrocarbon concentration should equal the total concentration of all hydrocarbons in the source area

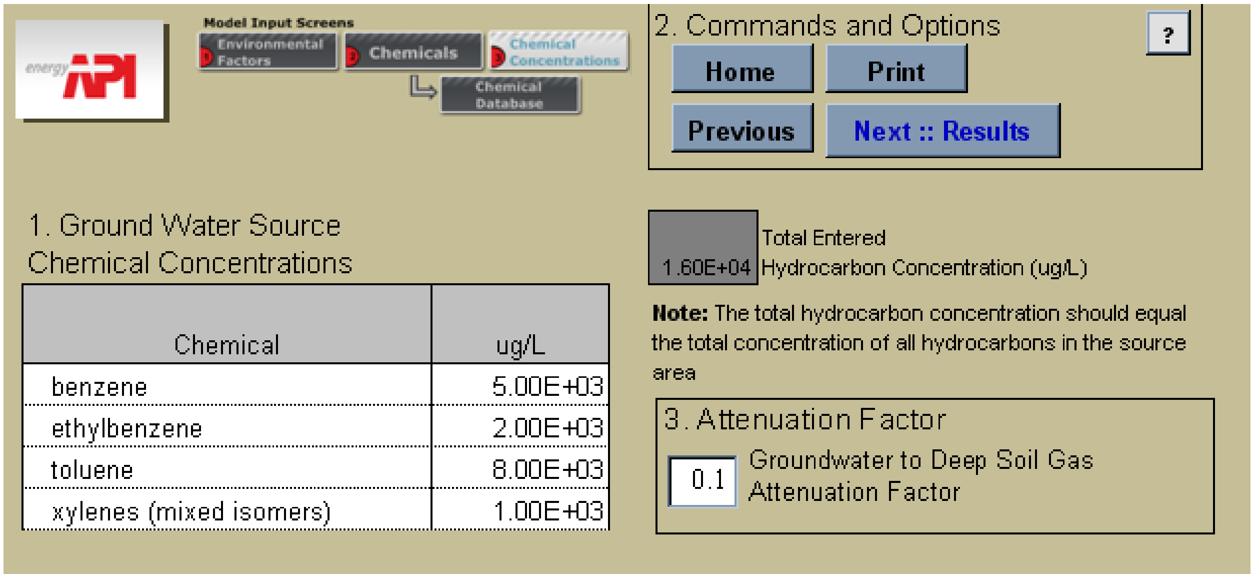
Figure 4: Soil Gas Source Chemical Concentrations Screen

<u>Input Value Estimation Methods</u>: The vapor phase concentration of hydrocarbons in the source area may be identified by i) laboratory analysis of the source area hydrocarbon vapors or ii) estimation of hydrocarbon concentrations based on other knowledge of the type of hydrocarbon mixture present (e.g., fresh gasoline, weathered gasoline, etc.). Laboratory analysis may include quantification of all individual hydrocarbons present in the sample or may rely on a combination of Total Petroleum Hydrocarbons (TPH) measurement and quantification of

selected individual hydrocarbons. Methods for estimating the source concentrations are provided in Appendix A.

1) Groundwater Source Chemical Concentrations

This screen is displayed if the user chose “Groundwater” as the source type on the prior screen. For each chemical, enter the concentration of the chemical in groundwater the source area.



1. Ground Water Source Chemical Concentrations

Chemical	ug/L
benzene	5.00E+03
ethylbenzene	2.00E+03
toluene	8.00E+03
xylenes (mixed isomers)	1.00E+03

1.60E+04 Total Entered Hydrocarbon Concentration (ug/L)

Note: The total hydrocarbon concentration should equal the total concentration of all hydrocarbons in the source area

3. Attenuation Factor

0.1 Groundwater to Deep Soil Gas Attenuation Factor

Figure 5: Groundwater Source Chemical Concentrations Screen

Input Value Estimation Methods: The “Groundwater” source type option should be selected only when the user has data concerning the concentrations of dissolved hydrocarbons in groundwater in the source area.

2) Groundwater to Deep Soil Gas Attenuation Factor ($AF_{GW\text{-}SG}$)

The model will estimate soil gas concentrations based on the user-specified hydrocarbon concentrations in groundwater and the $AF_{GW\text{-}SG}$ as follows:

$$C_{SG} = C_{GW} \times H' \times AF_{GW\text{-}SG} \times 1{,}000\ \mathrm{L/m^3}$$

Where:

C_{SG} = Chemical concentration in soil gas (ug/m^3)
C_{GW} = Chemical concentration in groundwater (ug/L)
H’ = Henry’s law constant (dim)
$AF_{GW\text{-}SG}$ = Groundwater to deep soil gas attenuation factor (dim)
1,000 L/m^3 = Units conversion factor

The user must specify a value for $AF_{GW\text{-}SG}$.

Attenuation Factor Value Selection: At sites with groundwater source concentrations data but not soil gas source concentration data, a site-specific value for $AF_{GW\text{-}SG}$ is typically not available. ***BioVapor*** uses a default $AF_{GW\text{-}SG}$ value of 0.1 based on the following considerations:

- A number of researchers have reported that VOC concentrations in deep soil gas are lower than would be predicted by equilibrium partitioning (e.g., McHugh and McAlary, 2009; Fitzpatrick and Fitzgerald, 1996).
- Although the USEPA vapor intrusion guidance does not specify a default groundwater to deep soil gas attenuation factor, the various subsurface to indoor air attenuation factors imply a default groundwater to deep soil gas attenuation factor of 0.1 (USEPA, 2002).

The user should modify the default value for $AF_{GW\text{-}SG}$ when appropriate based on site-specific considerations. Site-specific factors that might support use of an $AF_{GW\text{-}SG}$ of less than 0.1 include: the presence of a confining layer, a clean water lens, or other physical barriers that would limit the migration of VOCs from groundwater to deep soil gas. An $AF_{GW\text{-}SG}$ of one implies equilibrium partitioning between groundwater and deep soil gas. $AF_{GW\text{-}SG}$ cannot be greater than one.

Commands and Options

- ***Print:*** Performs the same action as choosing “Print” from Excel’s “File” menu or pressing Ctrl+P.
- ***Help:*** Displays on-line help for this screen.
- ***Home:*** Returns user to Main screen.
- ***Next-Results:*** Takes user to the Vapor Intrusion Risk Results screen.
- ***Previous:*** Takes user to the Environmental Factors screen.

OUTPUT SCREENS

VAPOR INTRUSION RISK RESULTS

This screen is used to present the risk results. Risk results are presented only for Risk Driver chemicals.

Forward Risk Calculations

Source Concentration: The values entered by the user.

Source to Indoor Air Attenuation Factor: The concentration ratio $C_{Indoor\ air}/C_{source}$.

Predicted Indoor Air Concentration: The predicted chemical concentration in the receptor building (ug/m^3).

Hazard Quotient: The predicted hazard quotient for non-cancer toxicity due to exposure to the chemical in indoor air. This value is calculated using the Reference Concentration for the chemical in the ***BioVapor*** chemical database. This toxicity value can be edited by accessing the Chemical Database screen.

Risk Level: The predicted excess lifetime cancer risk due to exposure to the chemical in indoor air. This value is calculated using the Inhalation Slope Factor for the chemical in the ***BioVapor*** chemical database. This toxicity value can be edited by accessing the Chemical Database screen.

Backward Risk Calculations

Critical Chemical: The source concentrations are calculated using a critical chemical approach rather than a cumulative risk approach. The critical chemical is the chemical in the user-specified mixture that has the greatest impact on indoor air quality relative to the specified indoor air concentration or target risk limit. Using the critical chemical approach, the back-calculated source concentration for the critical chemical is predicted to yield an indoor air concentration equal to the indoor air target concentration for that chemical. The back-calculated source concentrations for the remaining chemicals are determined from the user input source concentrations. For example, the user may enter a soil gas benzene source concentration of 10,000 ug/m^3 benzene and 20,000 ug/m^3 for toluene for the forward calculation. For this scenario, if benzene is the critical chemical for the backward calculation and the back-calculated benzene source concentration is 200,000 ug/m^3, then the back-calculated toluene source concentration would be 400,000 ug/m^3 (i.e., 200,000 x 20,000/10,000).

Target Hazard Quotient/Cancer Risk: The values entered by the user on the Environmental Factors input screen.

Target Indoor Air Concentration: The indoor air concentration limit from the ***BioVapor*** chemical database. Default target indoor air concentrations in the chemical database have been set equal to the USEPA Unified Screening Values issued by the USEPA in September 2008. These values are based on a hazard quotient of 1 and a 10^{-6} excess cancer risk limit.

The user can edit the target indoor air concentrations through the Chemical Database screen. The Chemical Database screen can be accessed through the Chemical Concentrations screen or the Home screen.

Soil Gas Source Concentration: The predicted soil gas source concentration that would result in an indoor air concentration equal to the target concentration or risk limit.

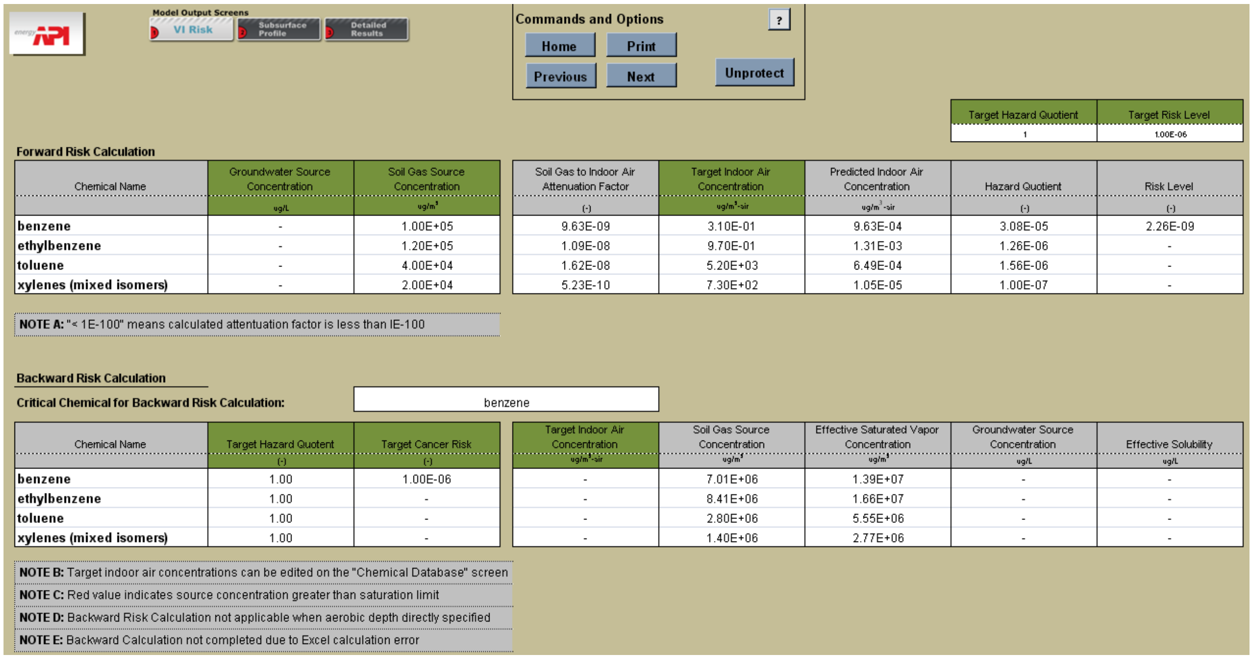
Effective Saturation Limit: Theoretically, the maximum possible concentration in soil gas (calculated using Raoult's Law to estimate the vapor pressure of each chemical in the mixture; see Appendix B.10).

Groundwater Source Concentration: The predicted groundwater source concentration that would result in an indoor air concentration equal to the target concentration or risk limit. The groundwater source concentration is calculated from the soil gas source concentration as:

$$C_{GW} = C_{SC}/(H' \times AF_{GW\text{-}SG} \times 1{,}000\ L/m^3)$$

See the CHEMICAL CONCENTRATIONS section of this guide for parameter definitions.

Effective Solubility: Theoretically, the maximum possible dissolved concentration in groundwater (calculated using the effective solubility relationship to estimate effect of the other VOCs on solubility; see Appendix B.10).



Target Hazard Quotient	Target Risk Level
1	1.00E-06

Forward Risk Calculation

Chemical Name	Groundwater Source Concentration ug/L	Soil Gas Source Concentration ug/m³	Soil Gas to Indoor Air Attenuation Factor (-)	Target Indoor Air Concentration ug/m³-air	Predicted Indoor Air Concentration ug/m³-air	Hazard Quotient (-)	Risk Level (-)
benzene	-	1.00E+05	9.63E-09	3.10E-01	9.63E-04	3.08E-05	2.26E-09
ethylbenzene	-	1.20E+05	1.09E-08	9.70E-01	1.31E-03	1.26E-06	-
toluene	-	4.00E+04	1.62E-08	5.20E+03	6.49E-04	1.56E-06	-
xylenes (mixed isomers)	-	2.00E+04	5.23E-10	7.30E+02	1.05E-05	1.00E-07	-

NOTE A: "< 1E-100" means calculated attentuation factor is less than IE-100

Backward Risk Calculation

Critical Chemical for Backward Risk Calculation: benzene

Chemical Name	Target Hazard Quotent (-)	Target Cancer Risk (-)	Target Indoor Air Concentration ug/m³-air	Soil Gas Source Concentration ug/m³	Effective Saturated Vapor Concentration ug/m³	Groundwater Source Concentration ug/L	Effective Solubility ug/L
benzene	1.00	1.00E-06	-	7.01E+06	1.39E+07	-	-
ethylbenzene	1.00	-	-	8.41E+06	1.66E+07	-	-
toluene	1.00	-	-	2.80E+06	5.55E+06	-	-
xylenes (mixed isomers)	1.00	-	-	1.40E+06	2.77E+06	-	-

NOTE B: Target indoor air concentrations can be edited on the "Chemical Database" screen

NOTE C: Red value indicates source concentration greater than saturation limit

NOTE D: Backward Risk Calculation not applicable when aerobic depth directly specified

NOTE E: Backward Calculation not completed due to Excel calculation error

Figure 6: Vapor Intrusion Risk Results Screen

Commands and Options

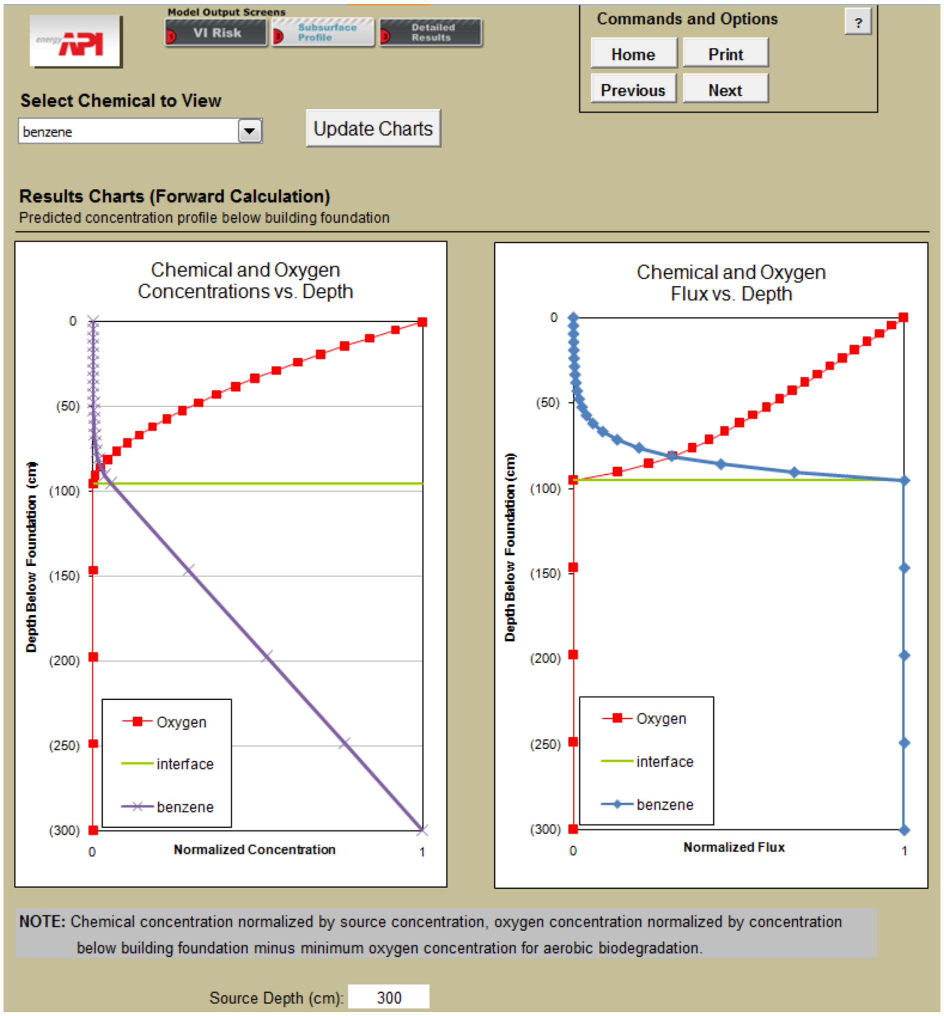
- ***Print:*** Performs the same action as choosing "Print" from Excel's "File" menu or pressing Ctrl+P.

- ***Help:*** Displays on-line help for this screen.

- ***Home:*** Returns user to Main screen.
- ***Next:*** Takes user to the Subsurface Profile screen.
- ***Previous:*** Takes user to the Chemical Concentrations screen.

SUBSURFACE PROFILE

This screen is used to present the predicted subsurface oxygen and hydrocarbon concentration and flux profiles. To view profiles for specific chemicals, choose the chemical from the dropdown menu and click “Update Charts.” If available, measured vertical profile data can be used to calibrate the chemical-specific biodegradation rates in the model so that the predicted profiles match the measured profiles. The user can edit the biodegradation rates through the Chemical Database screen.



Select Chemical to View: benzene

Results Charts (Forward Calculation)
Predicted concentration profile below building foundation

NOTE: Chemical concentration normalized by source concentration, oxygen concentration normalized by concentration below building foundation minus minimum oxygen concentration for aerobic biodegradation.

Source Depth (cm): 300

Figure 7: Subsurface Profile Screen

Select a Chemical to View

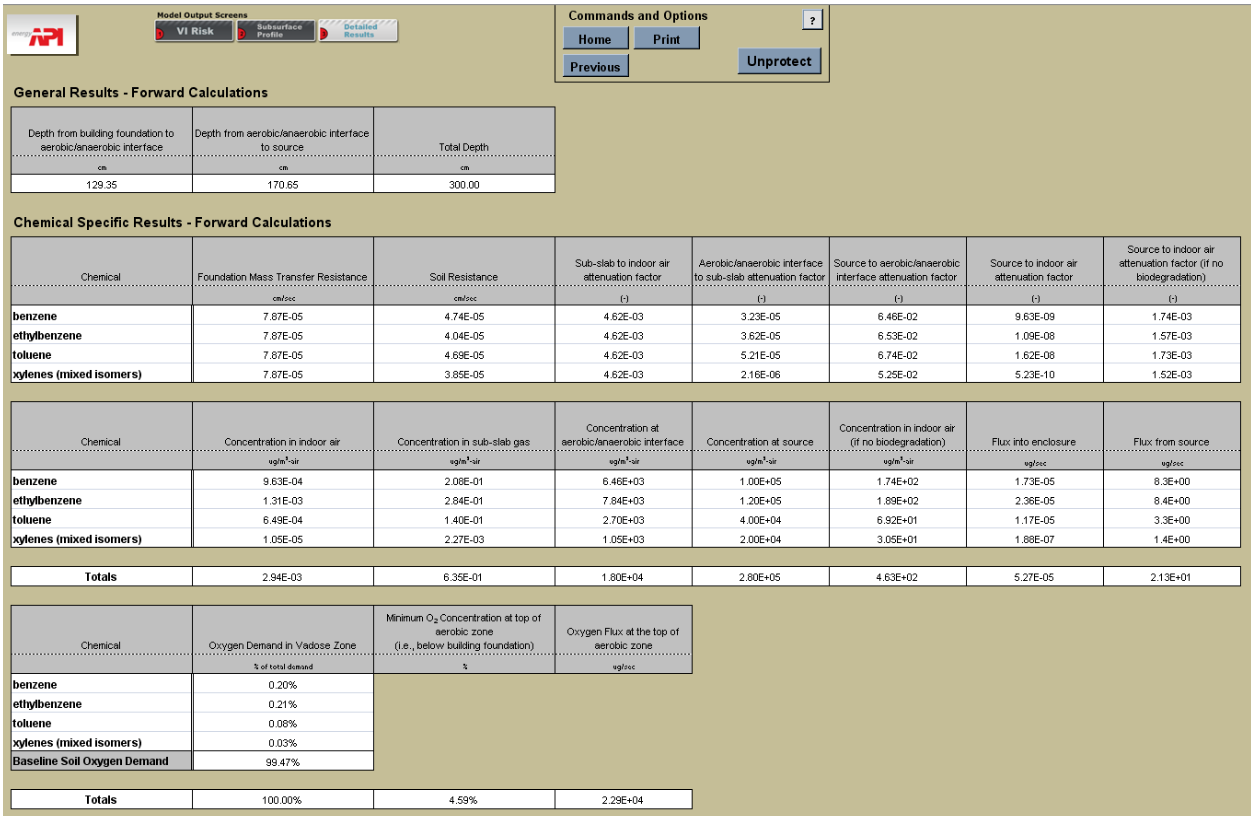
Allows the user to review each chemical. Select a chemical from the drop down and choose “update charts” to see that chemical’s subsurface profile.

Commands and Options

- ***Print:*** Performs the same action as choosing "Print" from Excel's "File" menu or pressing Ctrl+P.
- ***Help:*** Displays on-line help for this screen.
- ***Home:*** Returns user to the Main screen.
- ***Previous:*** Takes user to the Subsurface Profile screen.

DETAILED RESULTS

This screen is used to present the detailed results from the ***BioVapor*** model. These detailed results can be used to obtain a better understanding of which model input parameters are most important for the overall risk results.



General Results - Forward Calculations

Depth from building foundation to aerobic/anaerobic interface	Depth from aerobic/anaerobic interface to source	Total Depth
cm	cm	cm
129.35	170.65	300.00

Chemical Specific Results - Forward Calculations

Chemical	Foundation Mass Transfer Resistance	Soil Resistance	Sub-slab to indoor air attenuation factor	Aerobic/anaerobic interface to sub-slab attenuation factor	Source to aerobic/anaerobic interface attenuation factor	Source to indoor air attenuation factor	Source to indoor air attenuation factor (if no biodegradation)
	cm/sec	cm/sec	(-)	(-)	(-)	(-)	(-)
benzene	7.87E-05	4.74E-05	4.62E-03	3.23E-05	6.46E-02	9.63E-09	1.74E-03
ethylbenzene	7.87E-05	4.04E-05	4.62E-03	3.62E-05	6.53E-02	1.09E-08	1.57E-03
toluene	7.87E-05	4.69E-05	4.62E-03	5.21E-05	6.74E-02	1.62E-08	1.73E-03
xylenes (mixed isomers)	7.87E-05	3.85E-05	4.62E-03	2.16E-06	5.25E-02	5.23E-10	1.52E-03

Chemical	Concentration in indoor air	Concentration in sub-slab gas	Concentration at aerobic/anaerobic interface	Concentration at source	Concentration in indoor air (if no biodegradation)	Flux into enclosure	Flux from source
	ug/m^3-air	ug/m^3-air	ug/m^3-air	ug/m^3-air	ug/m^3-air	ug/sec	ug/sec
benzene	9.63E-04	2.08E-01	6.46E+03	1.00E+05	1.74E+02	1.73E-05	8.3E+00
ethylbenzene	1.31E-03	2.84E-01	7.84E+03	1.20E+05	1.89E+02	2.36E-05	8.4E+00
toluene	6.49E-04	1.40E-01	2.70E+03	4.00E+04	6.92E+01	1.17E-05	3.3E+00
xylenes (mixed isomers)	1.05E-05	2.27E-03	1.05E+03	2.00E+04	3.05E+01	1.88E-07	1.4E+00
Totals	2.94E-03	6.35E-01	1.80E+04	2.80E+05	4.63E+02	5.27E-05	2.13E+01

Chemical	Oxygen Demand in Vadose Zone	Minimum O_2 Concentration at top of aerobic zone (i.e., below building foundation)	Oxygen Flux at the top of aerobic zone
	% of total demand	%	ug/sec
benzene	0.20%		
ethylbenzene	0.21%		
toluene	0.08%		
xylenes (mixed isomers)	0.03%		
Baseline Soil Oxygen Demand	99.47%		
Totals	100.00%	4.59%	2.29E+04

Figure 8: Detailed Results Screen

Commands and Options

- ***Print:*** Performs the same action as choosing “Print” from Excel’s “File” menu or pressing Ctrl+P.
- ***Help:*** Displays on-line help for this screen.
- ***Home:*** Returns user to the Main screen.
- ***Previous:*** Takes user to the Subsurface Profile screen.

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VERSION 2.1 CHANGES

BioVapor 2.1 is a minor update of BioVapor 2.0. The following changes have been made for Version 2.1:

1) Environmental Factors, f_{oc}: The acceptable range of input values for fraction of organic carbon (f_{oc}) has been modified to include zero. Previously, the user would be shown an error message unless f_{oc} was greater than zero. Also, the units shown for f_{oc} were corrected from "cm3-void/cm3-soil" to "g-oc/g-soil"
2) Environmental Factors, Soil Oxygen Respiration Rate: An error associated with user-specified soil oxygen respiration rate has been corrected. Version 2.0 worked correctly when the user selected the option to have the soil respiration rate calculated from f_{oc}. However, when the user elected to directly enter the soil oxygen respiration rate, the software did not correctly apply the user-specified value.
3) Chemical Database: The water diffusion coefficient values have been corrected for ethanol, methane, TPH-GRO, TPH C4 to C5 Aliphatic, TPH C5 to C6 Aliphatic, TPH C6 to C7 Aliphatic, TPH C7 to C8 Aliphatic, TPH C8 to C9 Aliphatic.

APPENDIX A

Methods to Estimate Petroleum Vapor Composition in NAPL Source Area

The vapor phase concentration of hydrocarbons in the NAPL source area may be identified by i) laboratory analysis of the source area hydrocarbon vapors or ii) estimation of hydrocarbon concentrations based on knowledge of the type of hydrocarbon mixture present (e.g., fresh gasoline, weathered gasoline, etc.). Laboratory analysis may include quantification of all individual hydrocarbons present in the sample or may rely on a combination of Total Petroleum Hydrocarbons (TPH) measurement and quantification of selected individual hydrocarbons. A summary of estimation methods is provided in Table A.1 below.

Table A.1. Estimation Methods For Vapor Composition In NAPL Source Area.

Available Data for Vapor Phase Source	Chemicals to be Included in *BioVapor*	Method to Estimate Concentration
1) Concentration data for individual hydrocarbons C4 to C10	Select individual chemicals from the Risk Driver and Other Hydrocarbons lists. Use Hydrocarbon Surrogates to represent any hydrocarbons not on the chemical lists.	Enter the measured source concentrations for each selected chemical.
2) Concentration data for benzene and other selected risk drivers but not other hydrocarbons or TPH	Select the individual chemicals from the Risk Driver for which data is available. Select “Other Hydrocarbons (aromatic)” and “Other Hydrocarbons (aliphatic)” to represent the other (unmeasured) hydrocarbons in the source.	Enter the measured source concentrations for each individual chemical. Estimate the concentrations of “Other Hydrocarbons (aromatic)” and “Other Hydrocarbons (aliphatic)” using the composition relationships developed for the hydrocarbon source. See examples below.
3) Concentration data for TPH but not individual chemicals	Select benzene, toluene, ethylbenzene, and xylenes from the Risk Drivers list. Select “Other Hydrocarbons (aromatic)” and “Other Hydrocarbons (aliphatic)” to represent the other (unmeasured) hydrocarbons in the source.	Estimate the concentrations of benzene, toluene, ethylbenzene, xylenes, “Other Hydrocarbons (aromatic)” and “Other Hydrocarbons (aliphatic)” using composition relationships developed for the hydrocarbon source. See examples below.

The choice of estimation method depends upon the type of data available for the site. The methods basically fall into three groups."

1) Vapor-phase concentration data available for individual hydrocarbons C4 to C10

Concentration data from laboratory analysis for individual hydrocarbons can be entered directly into ***BioVapor***. This method is applicable to both NAPL and dissolved source areas. For NAPL source areas, it is important to include analysis of C4 and C5 hydrocarbons that are commonly not included in TO-15 analysis.

2) Vapor-phase concentration data available for benzene and other individual chemicals

If the concentration of only selected individual hydrocarbons have been measured, it is possible to estimate the vapor composition based on the typical vapor-phase hydrocarbon composition of common petroleum products.

Estimation Methods for Fresh Gasoline NAPL Source:

1) In the **BioVapor** software, select each individual chemical for which source concentration data is available. In addition, choose "Other Hydrocarbons (aromatic)" and "Other Hydrocarbons (aliphatic)".

2) Enter the source concentration for each individual hydrocarbon.

3a) If the total BTEX concentration is known (measured), then calculate the other hydrocarbon concentrations as follows:

Other Hydrocarbons (aromatic) = Total BTEX * 0.15

Other Hydrocarbons (aliphatic) = Total BTEX * 99

For this calculation, concentrations should be in units of ug/m^3 or other mass per volume units. If any other individual hydrocarbon concentrations have been entered into ***BioVapor***, then subtract these values from the calculated "Other Hydrocarbons (aromatic)" and "Other Hydrocarbons (aliphatic)" concentrations. Enter the resulting values into the ***BioVapor*** software.

3b) If benzene (but not total BTEX) concentration is known (measured), then calculate the other hydrocarbon concentrations as follows:

Other Hydrocarbons (aromatic) = Benzene * 0.65

Other Hydrocarbons (aliphatic) = Total BTEX * 430

For this calculation, concentrations should be in units of ug/m^3 or other mass per volume units. If any other individual hydrocarbon concentrations have been entered into ***BioVapor***, then subtract these values from the calculated "Other Hydrocarbons (aromatic)" and "Other Hydrocarbons (aliphatic)" concentrations. Enter the resulting values into the ***BioVapor*** software.

See Tables A.2 and A.3 for derivation of the other hydrocarbon concentration relationships

Estimation Methods for Weathered Gasoline NAPL Source:

1) In the ***BioVapor*** software, select each individual chemical for which source concentration data is available. In addition, choose “Other Hydrocarbons (aromatic)” and “Other Hydrocarbons (aliphatic).”

2) Enter the source concentration for each individual hydrocarbon.

3a) If the total BTEX concentration is known (measured), then calculate the other hydrocarbon concentrations as follows:

Other Hydrocarbons (aromatic) = Total BTEX * 0.09

Other Hydrocarbons (aliphatic) = Total BTEX * 11

For this calculation, concentrations should be in units of ug/m^3 or other mass per volume units. If any other individual hydrocarbon concentrations have been entered into ***BioVapor***, then subtract these values from the calculated “Other Hydrocarbons (aromatic)” and “Other Hydrocarbons (aliphatic)” concentrations. Enter the resulting values into the ***BioVapor*** software.

3b) If benzene (but not total BTEX) concentration is known (measured), then calculate the other hydrocarbon concentrations as follows:

Other Hydrocarbons (aromatic) = Benzene * 0.47

Other Hydrocarbons (aliphatic) = Total BTEX * 57

For this calculation, concentrations should be in units of ug/m^3 or other mass per volume units. If any other individual hydrocarbon concentrations have been entered into ***BioVapor***, then subtract these values from the calculated “Other Hydrocarbons (aromatic)” and “Other Hydrocarbons (aliphatic)” concentrations. Enter the resulting values into the ***BioVapor*** software.

See Tables A.4 and A.5 for derivation of the other hydrocarbon concentration relationships

3) Vapor-phase concentration data available for total TPH but not for individual hydrocarbons

If the concentration of total TPH has been measured, it is possible to estimate the vapor composition based on the typical vapor-phase hydrocarbon composition of common petroleum products.

Estimation Methods for Fresh Gasoline NAPL Source:

1) In the **BioVapor** software, select benzene, “Other Hydrocarbons (aromatic)”, and “Other Hydrocarbons (aliphatic)”.

2) Calculate the hydrocarbon concentrations as follows:

Benzene = Total TPH * 0.0023

Other Hydrocarbons (aromatic) = Total TPH * 0.0089

Other Hydrocarbons (aliphatic) = Total TPH * 0.99

For this calculation, concentrations should be in units of ug/m^3 or other mass per volume units. If any other individual hydrocarbon concentrations have been entered into ***BioVapor***, then subtract these values from the calculated “Other Hydrocarbons (aromatic)” and “Other Hydrocarbons (aliphatic)” concentrations. Enter the resulting values into the ***BioVapor*** software.

See Tables A.2 and A.3 for derivation of the other hydrocarbon concentration relationships

Estimation Methods for Weathered Gasoline NAPL Source:

1) In the ***BioVapor*** software, select benzene, "Other Hydrocarbons (aromatic)," and "Other Hydrocarbons (aliphatic)."

2) Calculate the hydrocarbon concentrations as follows:

   Benzene = Total TPH * 0.016

   Other Hydrocarbons (aromatic) = Total TPH * 0.074

   Other Hydrocarbons (aliphatic) = Total TPH * 0.91

   For this calculation, concentrations should be in units of ug/m^3 or other mass per volume units. If any other individual hydrocarbon concentrations have been entered into ***BioVapor***, then subtract these values from the calculated "Other Hydrocarbons (aromatic)" and "Other Hydrocarbons (aliphatic)" concentrations. Enter the resulting values into the ***BioVapor*** software.

See Tables A.4 and A.5 for derivation of the other hydrocarbon concentration relationships

Table A.2 NAPL and Vapor-Phase Composition of Fresh Gasoline

Hydrocarbon Source Composition				Associated Vapor Composition					
Component (1)	Molecular Weight (g) (1)	Vapor Pressure (20c, atm) (1)	Mole Fraction (1)	Class	Activity Coeff	Partial Pressure (2)	Mole Fraction	Mass	Mass Fraction
1. propane	44.1	8.5	0	Alkane	1.7	0.00289	0.0035483	0.1564821	0.0023913
2. isobutene	58.1	2.93	0.0666	Alkane	1.7	0.0995702	0.1222524	7.1028666	0.1085412
3. n-butane	58.1	2.11	0	Alkane	1.7	0.3698197	0.4540652	26.381189	0.4031394
4. trans-2-butene	56.1	1.97	0.0325	Alkene	1.5	0.003546	0.0043538	0.2442473	0.0037324
5. cis-2-butene	56.1	1.79	0.0169	Alkene	1.5	0	0	0	0
6. 3 methyl-1-butene	70.1	0.96	0.0249	Alkene	1.5	0.001152	0.0014144	0.0991514	0.0015152
7. isopentane	72.2	0.78	0.0218	Alkane	1.7	0.1835184	0.2253242	16.268406	0.2486027
8. 1-pentene	70.1	0.7	0.0094	Alkene	1.5	0	0	0	0
9. 2-methyl-1 -butene	70.1	0.67	0.0091	Alkene	1.5	0	0	0	0
10. 2-methyl-1, 3-butadiene	68.1	0.65	0.026	Alkene	1.5	0	0	0	0
11. n-pentane	72.2	0.57	0.0129	Alkane	1.7	0.0749037	0.0919669	6.6400088	0.1014681
12. trans-2-pentene	70.1	0.53	0.0033	Alkene	1.5	0	0	0	0
13. 2-methyl-2-butene	70.1	0.51	0	Alkene	1.5	0.00459	0.0056356	0.3950562	0.006037
14. 3-methyl-1, 2-butadiene	68.1	0.46	0.0015	Alkene	1.5	0	0	0	0
15. 3, 3-dimethyl-1-butene	84.2	0.47	0	Alkene	1.5	0.0038775	0.0047608	0.4008594	0.0061257
16. cyclopentane	70.1	0.35	0.0666	Cycloalkane	1.6	0	0	0	0
17. 3-methyl-1-pentene	84.2	0.29	0	Alkene	1.5	0	0	0	0
18. 2, 3-dimethylbutane	86.2	0.26	0.0325	Alkane	1.7	0.0356694	0.0437949	3.7751243	0.0576889
19. 2-methylpentane	86.2	0.21	0.0169	Alkane	1.7	0.0107814	0.0132374	1.1410656	0.017437
20. 3-methylpentane	86.2	0.2	0.0249	Alkane	1.7	0	0	0	0
21. n-hexane	86.2	0.16	0.0218	Alkane	1.7	0.0085136	0.010453	0.9010496	0.0137692
22. methylcyclopentane	84.2	0.15	0.0094	Cycloalkane	1.6	0	0	0	0
23. 2, 2-dimethylpentane	100.2	0.11	0.0091	Alkane	1.7	0.0017391	0.0021353	0.213954	0.0032695
24. benzene	78.1	0.1	0.026	Aromatic	1.7	0.001581	0.0019412	0.1516042	0.0023167
25. cyclohexane	84.2	0.1	0.0129	Cycloalkane	1.6	0	0	0	0
26. 2, 3-dimethylpentane	100.2	0.072	0.0033	Alkane	1.7	0.004541	0.0055755	0.5586647	0.0085371
27. 3-methylhexane	100.2	0.064	0	Alkane	1.7	0	0	0	0
28. 3-ethylpentane	100.2	0.06	0.0015	Alkane	1.7	0	0	0	0
29. 2, 2, 4-trimethylpentane	114.2	0.051	0	Alkane	1.7	0.0008757	0.0010751	0.122782	0.0018763
30. n-heptane	100.2	0.046	0.0666	Alkane	1.7	0.0004692	0.0005761	0.0577237	0.0008821
31. methylcyclohexane	98.2	0.048	0	Cycloalkane	1.6	0	0	0	0
32. 2, 2-dimethylhexane	114.2	0.035	0.0325	Alkane	1.7	0.0002737	0.000336	0.0383768	0.0005864
33. toluene	92.1	0.029	0.0169	Aromatic	1.7	0.0028002	0.0034381	0.3166526	0.0048389
34. 2, 3, 4-trimethylpentane	114.2	0.028	0.0249	Alkane	1.7	0.0004808	0.0005903	0.0674097	0.0010301
35. 2-methylheptane	114.2	0.021	0.0218	Alkane	1.7	0.0004605	0.0005654	0.0645732	0.0009868
36. 3-methylheptane	114.2	0.02	0.0094	Alkane	1.7	0	0	0	0
37. n-octane	114.2	0.014	0.0091	Alkane	1.7	2.618E-05	3.214E-05	0.0036708	5.61E-05

APPENDIX A: PETROLEUM VAPOR COMPOSITION

Hydrocarbon Source Composition				Associated Vapor Composition					
Component (1)	Molecular Weight (g) (1)	Vapor Pressure (20c, atm) (1)	Mole Fraction (1)	Class	Activity Coeff	Partial Pressure (2)	Mole Fraction	Mass	Mass Fraction
38. 2, 4, 4-trimethylhexane	128.3	0.013	0.026	Alkane	1.7	0.0001437	0.0001764	0.0226287	0.0003458
39. 2, 2-dimethylheptane	128.3	0.011	0.0129	Alkane	1.7	0	0	0	0
40. p-xylene	106.2	0.0086	0.0033	Aromatic	1.7	0.0012544	0.0015401	0.1635639	0.0024995
41. m-xylene	106.2	0.008	0	Aromatic	1.7	0	0	0	0
42. 3, 3, 4-trimethylhexane	128.3	0.0073	0.0015	Alkane	1.7	0.0002594	0.0003185	0.0408576	0.0006244
43. o-xylene	106.2	0.0066	0	Aromatic	1.7	0	0	0	0
44. 2, 2, 4-trimethylheptane	142.3	0.0053	0.0666	Alkane	1.7	6.307E-05	7.744E-05	0.0110193	0.0001684
45. 3, 3, 5-trimethylheptane	142.3	0.0037	0	Alkane	1.7	0	0	0	0
46. n-propylbenzene	120.2	0.0033	0.0325	Aromatic	1.7	0.0003736	0.0004587	0.0551404	0.0008426
47. 2, 3, 4-trimethylheptane	142.3	0.0031	0.0169	Alkane	1.7	0	0	0	0
48. 1, 3, 5-trimethylbenzene	120.2	0.0024	0.0249	Aromatic	1.7	0.0001326	0.0001628	0.0195693	0.000299
49. 1, 2, 4-trimethylbenzene	120.2	0.0019	0.0218	Aromatic	1.7	5.459E-05	6.702E-05	0.008056	0.0001231
50. methylpropylbenzene	134.2	0.001	0.0094	Aromatic	1.7	4.233E-05	5.197E-05	0.0069748	0.0001066
51. dimethylethylbenzene	134.2	0.0007	0.0091	Aromatic	1.7	2.594E-05	3.185E-05	0.0042745	6.532E-05
52. 1, 2, 4, 5-tetramethylbenzene	134.2	0.00046	0.026	Aromatic	1.7	7.351E-06	9.025E-06	0.0012112	1.851E-05
53. 1, 2, 3, 4-tetramethylbenzene	134.2	0.00033	0.0129	Aromatic	1.7	5.105E-06	6.268E-06	0.0008412	1.285E-05
54. 1, 2, 4-trimethyl-5-ethylbenzene	148.2	0.00029	0.0033	Aromatic	1.7	1.282E-05	1.574E-05	0.0023324	3.564E-05
55. n-dodecane	170.3	0.0004	0	Alkane	1.7	8.772E-06	1.077E-05	0.0018342	2.803E-05
56. naphthalene	128.2	0.00014	0.0015	Aromatic	1.7	7.854E-07	9.643E-07	0.0001236	1.889E-06
57. n-hexylbenzene	162.3	0.0001	0	Aromatic	1.7	0	0	0	0
58. methylnaphthalene	142.2	0.000054	0.0666	Aromatic	1.7	1.377E-07	1.691E-07	2.404E-05	3.674E-07
					TOTAL:	**0.8144638**	**1**	**65.439369**	**1**

Notes:

1) Composition of gasoline from Johnson, P.C.,M.W. Kemblowski, and J.D.Colthart. 1990. Quantitative Analysis of Cleanup of Hydrocarbon-Contaminated Soils by In-Situ Soil Venting. Ground Water, Vol. 28, No. 3. May - June, 1990, pp 413-429.

2) Harley et al, 2000, Relating Liquid Fuel and Headspace Vapor Composition for California Reformulated Gasoline Samples Containing Ethanol. Formula 2.

Table A.3 Summary Vapor Phase Composition of Fresh Gasoline

Component	Vapor Phase Mass Fractions
Benzene	0.0023
Total BTEX	0.0097
Other Aromatics	0.0015
Aliphatics	0.9888

Table A.4 NAPL and Vapor-Phase Composition of Weathered Gasoline

Hydrocarbon Source Composition				Associated Vapor Composition					
Component (1)	Molecular Weight (g) (1)	Vapor Pressure (20c, atm) (1)	Mole Fraction (1)	Class	Activity Coeff	Partial Pressure (2)	Mole Fraction	Mass	Mass Fraction
1. propane	44.1	8.5	0	Alkane	1.7	0	0	0	0
2. isobutene	58.1	2.93	0	Alkane	1.7	0	0	0	0
3. n-butane	58.1	2.11	0	Alkane	1.7	0	0	0	0
4. trans-2-butene	56.1	1.97	0	Alkene	1.5	0	0	0	0
5. cis-2-butene	56.1	1.79	0	Alkene	1.5	0	0	0	0
6. 3 methyl-1-butene	70.1	0.96	0	Alkene	1.5	0	0	0	0
7. isopentane	72.2	0.78	0.0296	Alkane	1.7	0.0392496	0.2907473	2.8338211	0.2505066
8. 1-pentene	70.1	0.7	0	Alkene	1.5	0	0	0	0
9. 2-methyl-1 -butene	70.1	0.67	0	Alkene	1.5	0	0	0	0
10. 2-methyl-1, 3-butadiene	68.1	0.65	0	Alkene	1.5	0	0	0	0
11. n-pentane	72.2	0.57	0.0169	Alkane	1.7	0.0163761	0.1213084	1.1823544	0.1045188
12. trans-2-pentene	70.1	0.53	0	Alkene	1.5	0	0	0	0
13. 2-methyl-2-butene	70.1	0.51	0	Alkene	1.5	0	0	0	0
14. 3-methyl-1, 2-butadiene	68.1	0.46	0	Alkene	1.5	0	0	0	0
15. 3, 3-dimethyl-1-butene	84.2	0.47	0	Alkene	1.5	0	0	0	0
16. cyclopentane	70.1	0.35	0	Cycloalkane	1.6	0	0	0	0
17. 3-methyl-1-pentene	84.2	0.29	0	Alkene	1.5	0	0	0	0
18. 2, 3-dimethylbutane	86.2	0.26	0.0744	Alkane	1.7	0.0328848	0.2435991	2.8346698	0.2505816
19. 2-methylpentane	86.2	0.21	0	Alkane	1.7	0	0	0	0
20. 3-methylpentane	86.2	0.2	0	Alkane	1.7	0	0	0	0
21. n-hexane	86.2	0.16	0.0459	Alkane	1.7	0.0124848	0.092483	1.0761898	0.095134
22. methylcyclopentane	84.2	0.15	0	Cycloalkane	1.6	0	0	0	0
23. 2, 2-dimethylpentane	100.2	0.11	0	Alkane	1.7	0	0	0	0
24. benzene	78.1	0.1	0.0137	Aromatic	1.7	0.002329	0.0172524	0.1818949	0.0160793
25. cyclohexane	84.2	0.1	0	Cycloalkane	1.6	0	0	0	0
26. 2, 3-dimethylpentane	100.2	0.072	0.1088	Alkane	1.7	0.0133171	0.0986485	1.3343754	0.1179573
27. 3-methylhexane	100.2	0.064	0	Alkane	1.7	0	0	0	0
28. 3-ethylpentane	100.2	0.06	0	Alkane	1.7	0	0	0	0
29. 2, 2, 4-trimethylpentane	114.2	0.051	0	Alkane	1.7	0	0	0	0
30. n-heptane	100.2	0.046	0.0853	Alkane	1.7	0.0066705	0.0494124	0.6683801	0.059084
31. methylcyclohexane	98.2	0.048	0	Cycloalkane	1.6	0	0	0	0
32. 2, 2-dimethylhexane	114.2	0.035	0	Alkane	1.7	0	0	0	0
33. toluene	92.1	0.029	0.1216	Aromatic	1.7	0.0059949	0.044408	0.5521284	0.0488075

APPENDIX A: PETROLEUM VAPOR COMPOSITION

Hydrocarbon Source Composition				Associated Vapor Composition					
Component (1)	Molecular Weight (g) (1)	Vapor Pressure (20c, atm) (1)	Mole Fraction (1)	Class	Activity Coeff	Partial Pressure (2)	Mole Fraction	Mass	Mass Fraction
34. 2, 3, 4-trimethylpentane	114.2	0.028	0	Alkane	1.7	0	0	0	0
35. 2-methylheptane	114.2	0.021	0.0468	Alkane	1.7	0.0016708	0.0123764	0.1908008	0.0168666
36. 3-methylheptane	114.2	0.02	0	Alkane	1.7	0	0	0	0
37. n-octane	114.2	0.014	0.0468	Alkane	1.7	0.0011138	0.0082509	0.1272005	0.0112444
38. 2, 4, 4-trimethylhexane	128.3	0.013	0	Alkane	1.7	0	0	0	0
39. 2, 2-dimethylheptane	128.3	0.011	0	Alkane	1.7	0	0	0	0
40. p-xylene	106.2	0.0086	0.1247	Aromatic	1.7	0.0018231	0.013505	0.1936147	0.0171153
41. m-xylene	106.2	0.008	0	Aromatic	1.7	0	0	0	0
42. 3, 3, 4-trimethylhexane	128.3	0.0073	0.0208	Alkane	1.7	0.0002581	0.0019121	0.0331178	0.0029276
43. o-xylene	106.2	0.0066	0	Aromatic	1.7	0	0	0	0
44. 2, 2, 4-trimethylheptane	142.3	0.0053	0	Alkane	1.7	0	0	0	0
45. 3, 3, 5-trimethylheptane	142.3	0.0037	0.0188	Alkane	1.7	0.0001183	0.000876	0.0168273	0.0014875
46. n-propylbenzene	120.2	0.0033	0.0737	Aromatic	1.7	0.0004135	0.0030627	0.0496975	0.0043932
47. 2, 3, 4-trimethylheptane	142.3	0.0031	0	Alkane	1.7	0	0	0	0
48. 1, 3, 5-trimethylbenzene	120.2	0.0024	0.0222	Aromatic	1.7	9.058E-05	0.000671	0.0108872	0.0009624
49. 1, 2, 4-trimethylbenzene	120.2	0.0019	0.0222	Aromatic	1.7	7.171E-05	0.0005312	0.0086191	0.0007619
50. methylpropylbenzene	134.2	0.001	0.0297	Aromatic	1.7	5.049E-05	0.000374	0.0067758	0.000599
51. dimethylethylbenzene	134.2	0.0007	0.0319	Aromatic	1.7	3.796E-05	0.0002812	0.0050944	0.0004503
52. 1, 2, 4, 5-tetramethylbenzene	134.2	0.00046	0.0319	Aromatic	1.7	2.495E-05	0.0001848	0.0033477	0.0002959
53. 1, 2, 3, 4-tetramethylbenzene	134.2	0.00033	0	Aromatic	1.7	0	0	0	0
54. 1, 2, 4-trimethyl-5-ethylbenzene	148.2	0.00029	0	Aromatic	1.7	0	0	0	0
55. n-dodecane	170.3	0.0004	0.0181	Alkane	1.7	1.231E-05	9.117E-05	0.0020961	0.0001853
56. naphthalene	128.2	0.00014	0.0083	Aromatic	1.7	1.975E-06	1.463E-05	0.0002532	2.239E-05
57. n-hexylbenzene	162.3	0.0001	0.0078	Aromatic	1.7	1.326E-06	9.823E-06	0.0002152	1.902E-05
58. methylnaphthalene	142.2	0.000054	0	Aromatic	1.7	0	0	0	0
					TOTAL:	**1.35E-01**	**1**	**1.13E-01**	**1**

Notes:

1) Composition of gasoline from P.C. Johnson, M.W. Kemblowski, and J.D.Colthart. 1990. *Quantitative Analysis of Cleanup of Hydrocarbon-Contaminated Soils by In-Situ Soil Venting*. Ground Water, Vol. 28, No. 3. , pp. 413-429.

2) Harley et al, 2000, *Relating Liquid Fuel and Headspace Vapor Composition for California Reformulated Gasoline Samples Containing Ethanol*. Formula 2.

Table A.5 Summary Vapor Phase Composition of Weathered Gasoline

Component	Total Mass Fractions
Benzene	0.016
Total BTEX	0.082
Other Aromatics	0.0075
Aliphatics	0.91

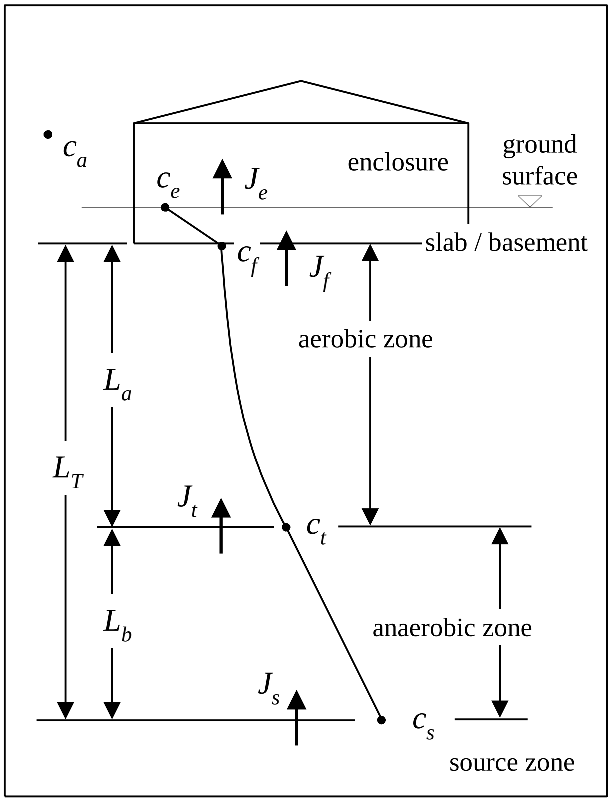
APPENDIX B: BIOVAPOR MODEL EQUATIONS

George DeVaull
Shell Global Solutions US Inc.
3333 Highway Six South
Houston, Texas, USA
george.devaull@shell.com
7 May 2009

Contents

B.1. Introduction

This Appendix is documentation of the **BioVapor** model equations, assumptions, and parameters. **BioVapor** is a one-dimensional subsurface soil to indoor air chemical vapor intrusion model that includes oxygen-limited biodegradation for a multi-component chemical source. A shallow aerobic layer, L_a, with biodegradation, and a deeper anaerobic layer, L_b, without biodegradation are included, as in Figure 1, and $L_T = L_a + L_b$. Chemical vapor concentrations are indicated in the source zone, c_s, at an anaerobic - aerobic interface, c_t, just below the building foundation, c_f, and within the indoor building enclosure air, c_e. Chemical fluxes, J, are similarly defined, positive (+) upward. Algebraic relations for chemical concentration across each layer, that is, c_e / c_f across the building foundation, c_f / c_t across the aerobic soil layer, and c_t / c_s across the anaerobic soil layer are included. The overall indoor air to source concentration ratio, c_e / c_s, is the product of these terms.



Steady state conditions are presumed for vapor transport in soil, with constant chemical source concentrations, homogeneous soil properties, and diffusion-dominated soil vapor transport. No immiscible chemical phase is presumed within the soil layer L_T.

Chemical-specific subscripts, *i*, (for multiple chemicals) are omitted in Sections B.2 and B.3 but are included in discussion of summed chemical concentrations and fluxes.

Oxygen availability in subsurface soils is limited in the model both by downward diffusion of atmospheric oxygen from the soil surface, and by a specified maximum advective airflow rate below a building foundation.

Two equation sets are included in this model and are documented in this appendix:

[1] Diffusion and reaction of chemicals and oxygen in soils defined by a coupled set of algebraic conservation equations. Finite aerobic biodegradation rates are applied for the chemical components. Solution of a coupled set of algebraic equation is required. This approach requires a specified chemical-specific source composition.

[2] The aerobic depth, L_a, is calculated presuming fast biodegradation relative to soil diffusion. This assumption allows an explicit solution for L_a. The result is applied in estimating chemical degradation across the aerobic layer L_a using finite biodegradation rates for the chemicals of interest. This approach minimally requires a total source vapor concentration, and source vapor concentrations (or fractions) for the chemicals of interest. With all other parameters equal it yields answers that are either equal to or over predict indoor concentrations calculated using [1].

Detailed model development for [1] is shown in DeVaull (2007). The fast reaction model [2] is presented in Patterson and Davis (2009) and Roggemans (2001) in relating aerobic depth to concentration data, but extended here to include zero-order aerobic soil respiration in the aerobic zone and oxygen flux-limited degradation, as well as applying finite degradation rates to estimate chemical flux in the aerobic layer.

B.2 Building and Foundation

For negligible ambient air concentrations, a ratio between enclosure and sub-foundation concentrations is:

$$\left(\frac{c_e}{c_f}\right) = \frac{\dfrac{1}{L_{mix} \cdot ER}}{\left(\dfrac{1}{L_{mix} \cdot ER} + \dfrac{1}{h}\right)} \qquad \text{[B.2.1]}$$

The value *h* is a chemical mass transfer coefficient across a building foundation. It is defined empirically, or from available models. The value L_{mix} is a building mixing height; *ER* is building air exchange rate.

B.3 Chemicals in Soil

Chemical Concentrations: The governing equation for chemical vapor transport in a homogeneous soil layer, including diffusion and first-order chemical degradation in one dimension, at steady-state, is:

$$D_{eff} \cdot \frac{\partial^2 c_v}{\partial z^2} = \frac{\theta_w}{H} \cdot k_w \cdot c_v \qquad \text{[B.3.1]}$$

Diffusive chemical flux, *J*, in a vertical coordinate direction, *z*, through the soil layer is:

$$J = -D_{eff} \cdot \frac{\partial c_v}{\partial z} \qquad [B.3.2]$$

In these equations, c_v is soil vapor concentration, θ_w is soil moisture, H is (dimensionless) Henry's law coefficient, and k_w is an empirical aerobic water-phase (pseudo) first-order degradation rate.

The model is based on solution to Eqs. B.3.1 and B.3.2 with constant specified flux and concentration boundary conditions. This is implemented as an algebraic solution in two homogeneous soil layers, a shallow aerobic soil layer of depth L_a with degradation and a deeper anaerobic soil layer of depth L_b without degradation. Total soil layer depth is $L_T = L_a + L_b$. In the shallow aerobic soil layer of depth L_a, the ratio of concentration from below a foundation, c_f, to an aerobic-anaerobic transition point, c_t, is:

$$\left(\frac{c_f}{c_t}\right) = \left(\frac{\left(\frac{1}{L_{mix} \cdot ER} + \frac{1}{h}\right)}{A \cdot \left(\frac{1}{L_{mix} \cdot ER} + \frac{1}{h}\right) + B \cdot \frac{L_a}{D_{eff}}}\right) \qquad [B.3.3]$$

The value D_{eff} is the effective diffusion coefficient of chemical in the soil. In the deeper anaerobic soil layer of depth L_b, the ratio of concentration from the aerobic-anaerobic transition point, c_t, to the chemical source, c_s, is:

$$\left(\frac{c_t}{c_s}\right) = \frac{\left(A \cdot \left(\frac{1}{L_{mix} \cdot ER} + \frac{1}{h}\right) + B \cdot \frac{L_a}{D_{eff}}\right)}{\left(A + \frac{L_b}{L_a}\frac{\left(A^2 - 1\right)}{B}\right) \cdot \left(\frac{1}{L_{mix} \cdot ER} + \frac{1}{h}\right) + \frac{\left(B \cdot L_a + A \cdot L_b\right)}{D_{eff}}} \qquad [B.3.4]$$

Defined terms in Eqs. B.3.3 and B.3.4 include:

$$A = \left(\frac{exp(-\alpha_a) + exp(\alpha_a)}{2}\right) = cosh(\alpha_a) \qquad [B.3.5]$$

$$B = \left(\frac{exp(\alpha_a) - exp(-\alpha_a)}{2 \cdot \alpha_a}\right) = \frac{1}{\alpha_a} sinh(\alpha_a) \qquad [B.3.6]$$

with

$$\alpha_a = \frac{L_a}{L_R} \quad \text{and} \quad L_R = \sqrt{\frac{D_{eff} \cdot H}{k_w \cdot \theta_w}}$$

The defined functions include hyperbolic cosine (*cosh*), hyperbolic sine (*sinh*), and the exponential function (*exp*). For $\alpha_a > 0$, as $\alpha_a \rightarrow 0$, $A \rightarrow 1$. From L'Hospital's rule, as $\alpha_a \rightarrow 0$, $B \rightarrow 1$. The ratio of chemical concentration from the building enclosure to the source is the product of Eqs. B.2.1, B.3.3, and B.3.4.

$$\left(\frac{c_f}{c_s}\right) = \left(\frac{c_f}{c_t}\right) \cdot \left(\frac{c_t}{c_s}\right) \quad \text{and} \quad \left(\frac{c_e}{c_s}\right) = \left(\frac{c_e}{c_f}\right) \cdot \left(\frac{c_f}{c_t}\right) \cdot \left(\frac{c_t}{c_s}\right) \qquad [B.3.7]$$

Eqs. 3.3 and 3.4 can result in software-dependent errors for very large values of $exp(\alpha_a)$. Approximations for very large values of α_a are:

$$\left(\frac{c_f}{c_t}\right)=\left(\frac{\left(\frac{1}{L_{mix}\cdot ER}+\frac{1}{h}\right)}{\left(\frac{1}{L_{mix}\cdot ER}+\frac{1}{h}\right)+\frac{L_R}{D_{eff}}}\right)\cdot 2\cdot exp(-\alpha_a) \qquad \alpha_a > 0$$ [B.3.3a]

$$\left(\frac{c_t}{c_s}\right)=\frac{\left(\left(\frac{1}{L_{mix}\cdot ER}+\frac{1}{h}\right)+\frac{L_R}{D_{eff}}\right)}{\left(1+\frac{L_b}{L_R}\right)\cdot\left(\frac{1}{L_{mix}\cdot ER}+\frac{1}{h}\right)+\frac{L_R}{D_{eff}}+\frac{L_b}{D_{eff}}} \qquad \alpha_a > 0$$ [B.3.4a]

Chemical Flux: The change in chemical flux across the aerobic soil layer from solution of Eqs. B.3.1 and B.3.2 is

$$(J_f - J_t) = -\frac{D_{eff}}{L_a}\cdot\frac{(A-1)}{B}\cdot(c_t + c_f) \qquad \alpha_a > 0$$ [B.3.8]

Through the building envelope, $J_f = J_e$, and in the anaerobic soil layer with no chemical degradation, $J_t = J_s$. The chemical flux across the building foundation is

$$J_f = h\cdot\left(c_f - c_e\right)$$ [B.3.9]

B.4 Oxygen in Soil – Coupled Solution

Diffusion and transport of oxygen in the soil layer depends on the summed oxygen demand from multiple degrading chemicals and soil respiration.

Oxygen Flux: For chemicals and oxygen, mass conservation requires:

$$\vec{\nabla}\cdot\vec{J}_i = \rho_s\cdot\Lambda_i$$ [B.4.1]

$$\vec{\nabla}\cdot\vec{J}_{O_2} = \rho_s\cdot\Lambda_{O_2}$$ [B.4.2]

Soil density is ρ_s. Oxygen respiration, Λ_{O_2}, is specified as a sum of oxygen demand in biodegradation of N individual chemicals, i, at rates Λ_i, plus a zero-order baseline soil oxygen respiration term, Λ_{base,O_2}

$$\Lambda_{O_2} = \sum_{i=1}^{N}\Lambda_i/\varphi_i + \Lambda_{base,O_2}$$ [B.4.3]

The value φ_i is a chemical-specific mass ratio of oxygen to chemical consumption. Multiply Eq. [B.4.1] by $1/\varphi_i$, sum over N chemicals, and subtract from Eq. [B.4.2]

$$\vec{\nabla}\cdot\left(\vec{J}_{O_2} - \sum_{i=1}^{N}\frac{1}{\varphi_i}\cdot\vec{J}_i\right) = \rho_s\cdot\left(\Lambda_{O_2} - \sum_{i=1}^{N}\frac{1}{\varphi_i}\cdot\Lambda_i\right) = \rho_s\cdot\Lambda_{base,O_2}$$ [B.4.4]

In one dimension (z),

$$\frac{d}{dz}\left(J_{O_2} - \sum_{i=1}^{N}\frac{1}{\varphi_i}\cdot J_i\right) = \rho_s\cdot\Lambda_{base,O_2}$$ [B.4.5]

Eq. B.4.5 integrated across the aerobic soil layer, L_a, is

$$J_{f,O_2} - J_{t,O_2} = \sum_{i=1}^{N} \frac{1}{\varphi_i} \cdot (J_{f,i} - J_{t,i}) + \rho_s \cdot L_a \cdot \Lambda_{base,O_2} \qquad \text{[B.4.6]}$$

Oxygen availability below a building foundation may be constrained by advective airflow below and through the building foundation. With downward oxygen flux negative

$$J_{f,O_2} \geq -\frac{Q_f}{A_b} \cdot (c_{O_2-atm} - c_{O_2-\min}) \qquad \text{[B.4.7]}$$

The value A_b is the foundation area in contact with soil; Q_f is the volumetric advective airflow below the building foundation. Oxygen flux at the aerobic to anaerobic interface is zero at a minimum, $J_{t,O_2} = 0$. Advective airflow under a building is a positive value that includes air passing under a building without entering the building and air flowing through the building foundation, Q_s.

<u>Oxygen Concentrations</u>: From Eq. B.4.5 with diffusive flux only, as in Eq B.3.2

$$\frac{d}{dz}\left(- D_{eff} \cdot \frac{\partial c_{O_2}}{\partial z} + \sum_{i=1}^{N} \frac{D_{eff}}{\varphi_i} \cdot \frac{\partial c_v}{\partial z} \right) = \rho_s \cdot \Lambda_{O_2} \qquad \text{[B.4.8]}$$

Integration of Eq. B.4.8 across the aerobic soil layer,

$$c_{f,O_2} - c_{t,O_2} = \sum_{i=1}^{N} \frac{1}{\varphi_i} \cdot \frac{D_{eff,i}}{D_{eff,O_2}} \cdot \left[c_{f,i} - c_{t,i} \right] - \frac{\rho_s \cdot \Lambda_{base,O_2}}{D_{eff,O_2}} \cdot \frac{L_a^2}{2} + \frac{L_a}{D_{eff,O_2}} \sum_{i=1}^{N} \frac{1}{\varphi_i} \cdot J_{t,i} \qquad \text{[B.4.9]}$$

An oxygen concentration constraint is imposed.

$$(c_{f,O_2} - c_{t,O_2}) \leq (c_{O_2-atm} - c_{O_2-\min}) \qquad \text{[B.4.10]}$$

Atmospheric oxygen concentration is c_{O_2-atm} and the minimum oxygen concentration at which aerobic degradation is supported is $c_{O_2-\min}$.

<u>Solution of the Coupled Equation Set</u>: A solution to the coupled equations for chemicals and oxygen is found in a search for L_a within the range 0 ≤ L_a ≤□L_T to meet either or both the oxygen constraints imposed by: [1] a maximum oxygen flux (downward, into the soil layer, below a building foundation), J_{f,O_2}; and [2] maximum oxygen concentration, as $\left(c_{f,O_2} - c_{t,O_2}\right)$. The soil layer L_T will be completely aerobic if oxygen flux calculated with Eq. B.4.6 and oxygen concentration calculated with Eq. B.4.9 meets the criteria of Eqs. B.4.7 and B.4.10, respectively, when $L_a = L_T$ is presumed.

A monotonic relation exists between L_a, J_{f,O_2}, and c_{f,O_2}. That is, J_{f,O_2}, and $\left(c_{f,O_2} - c_{t,O_2}\right)$ are a minimum for L_a = 0, and are a maximum for $L_a = L_T$.

B.5 Oxygen in Soil – Fast Reaction

A simplified solution is available for aerobic depth if reaction rates are presumed fast relative to diffusion rates. This approximation requires less chemical-specific information, and allows explicit calculation of L_a.

For fast chemical reactions, relative to diffusion, chemical concentration is zero, $c_i = 0$ in the aerobic zone, and oxygen concentration is zero, $c_{O_2} - c_{O_2,min} = 0$ in the anaerobic zone. Chemical and oxygen concentrations in the soil layer are continuous. Therefore $c_i = 0$ and $c_{O_2} - c_{O_2,min} = 0$ at the anaerobic - aerobic interface.

With zero-order baseline soil respiration included in the aerobic soil zone, oxygen flux at the foundation-soil interface is:

$$J_{f,O_2} = -D_{eff,O_2} \cdot \left(\frac{c_{O_2,f} - c_{O_2,t}}{L_a} \right) - \frac{1}{2} \cdot \rho_s \cdot \Lambda_{O_2} \cdot L_a \tag{B.5.1}$$

At the aerobic-anaerobic interface, oxygen flux is:

$$J_{t,O_2} = -D_{eff,O_2} \cdot \left(\frac{c_{O_2,f} - c_{O_2,t}}{L_a} \right) + \frac{1}{2} \cdot \rho_s \cdot \Lambda_{O_2} \cdot L_a \tag{B.5.2}$$

Subtracting Eq. B.5.1 from B.5.2 shows the change in oxygen flux across the aerobic layer is equal to the oxygen consumed in the aerobic zone due to baseline soil respiration.

$$J_{t,O_2} - J_{f,O_2} = \rho_s \cdot L_a \cdot \Lambda_{base,O_2} \tag{B.5.3}$$

With no reaction in the anaerobic zone, chemical flux is

$$J_{T,s} = J_{T,t} = J_T = \sum_{i=1}^{N} J_i = \sum_{i=1}^{N} D_{eff,i} \cdot \left(\frac{c_{i,s} - c_{i,t}}{L_b} \right) \tag{B.5.4}$$

At the reaction front (the anaerobic – aerobic interface) chemical and oxygen disappear (instantaneously) at stoichiometric ratios.

$$J_{O_2,t} + \sum_{i=1}^{N} \frac{1}{\varphi_i} \cdot J_i = 0 \tag{B.5.5}$$

Oxygen Flux Specified: For oxygen flux specified below the building foundation, substituting Eqs. B.5.3 and A5.4 into Eq. B.5.5

$$J_{f,O_2} + \rho_s \cdot L_a \cdot \Lambda_{base,O_2} + \sum_{i=1}^{N} \left(\frac{D_{eff,i} \cdot \left(c_{i,s} - c_{i,t} \right)}{\varphi_i \cdot L_b} \right) = 0 \tag{B.5.6}$$

Substituting $L_T = L_a + L_b$ into B.5.6 yields:

$$-\left(\frac{\rho_s \cdot \Lambda_{base,O_2} \cdot L_T}{J_{f,O_2}} \right) \cdot \left(\frac{L_a}{L_T} \right)^2 + \left(\frac{\rho_s \cdot \Lambda_{base,O_2} \cdot L_T}{J_{f,O_2}} - 1 \right) \cdot \left(\frac{L_a}{L_T} \right) + 1 + \sum_{i=1}^{N} \left(\frac{D_{eff,i} \cdot \left(c_{i,s} - c_{i,t} \right)}{J_{f,O_2} \cdot \varphi_i \cdot L_T} \right) = 0 \tag{B.5.7}$$

Eq. B.5.7 is solved for (L_a / L_T) with the quadratic equation. The aerobic-anaerobic interface is within the soil layer for real solution(s) to Eq. B.5.7 in the range of $0 < L_a / L_T < 1$. From Eq. B.5.7 with no soil respiration ($\Lambda_{base,O_2} = 0$)

$$\left(\frac{L_a}{L_T} \right) = 1 + \sum_{i=1}^{N} \left(\frac{D_{eff,i} \cdot \left(c_{i,s} - c_{i,t} \right)}{J_{f,O_2} \cdot \varphi_i \cdot L_T} \right) \tag{B.5.8}$$

A physical solution ($0 < L_a / L_T < 1$) to Eq B.5.7 requires

$$-1 \le \sum_{i=1}^{N}\left(\frac{D_{eff,i}\cdot\left(c_{i,s}-c_{i,t}\right)}{J_{f,O_2}\cdot\varphi_i\cdot L_T}\right)\le 0 \qquad \text{[B.5.9]}$$

Eq. B.5.9 shows a ratio of the minimum oxygen demand from summed total chemical diffusion through the soil depth, L_T, divided by the maximum available oxygen flux. If the magnitude of this ratio is less than one, no aerobic zone is present, and no chemical degradation occurs.

For: $$\left|\sum_{i=1}^{N}\frac{D_{eff,i}\cdot\left(c_{i,s}-c_{i,t}\right)}{J_{f,O_2}\cdot\varphi_i\cdot L_T}\right|\ge 1, \qquad L_a = 0$$

Solution to Eq. B.5.7 is based on specified oxygen flux at the foundation, J_{f,O_2}. From Eqs. B.4.10 and B.5.1, a test on whether sufficient oxygen concentration is available to deliver this flux is:

$$\frac{J_{f,O_2}+\frac{1}{2}\cdot\rho_s\cdot\Lambda_{O_2}\cdot L_a}{-(D_{eff,O_2}/L_a)\cdot(c_{O_2-atm}-c_{O_2-min})}=\frac{(c_{O_2,f}-c_{O_2,t})}{(c_{O_2-atm}-c_{O_2-min})}\le 1 \qquad \text{[B.5.10]}$$

If Eq. B.5.10 is not met, an oxygen concentration constraint (and not the oxygen flux constraint) will be limiting.

<u>Oxygen Concentration Specified</u>: Substituting Eqs. B.5.3 and B.5.4 into Eq. B.5.5

$$-\frac{D_{eff,O_2}}{L_a}\cdot\left(c_{O_2,f}-c_{O_2,t}\right)+\frac{\rho_s\cdot\Lambda_{O_2}\cdot L_a}{2}+\sum_{i=1}^{N}\frac{1}{\varphi_i}\cdot\left(\frac{D_{eff,i}}{L_b}\right)\cdot\left(c_{i,s}-c_{i,t}\right)=0 \qquad \text{[B.5.10]}$$

Substituting $L_T = L_a + L_b$ into Eq. B.5.10, with $c_{i,t} = 0$ yields:

$$\left[1+\sum_{i=1}^{N}\left(\frac{D_{eff,i}\cdot c_{i,s}}{D_{eff,O_2}\cdot c_{O_2,f}\cdot\varphi_i}\right)\right]\cdot\left(\frac{L_a}{L_T}\right)+\left[\frac{\rho_s\cdot\Lambda_{O_2}\cdot L_T^{2}}{2\cdot D_{eff,O_2}\cdot c_{O_2,f}}\right]\cdot\left(\frac{L_a}{L_T}\right)^2+\left[-\frac{\rho_s\cdot\Lambda_{O_2}\cdot L_T^{2}}{2\cdot D_{eff,O_2}\cdot c_{O_2,f}}\right]\cdot\left(\frac{L_a}{L_T}\right)^3=1 \qquad \text{[B.5.11]}$$

Eq. B.5.11 is solved for L_a/L_T with the cubic equation. Potentially viable solutions must be real and fall in the range of $0 < L_a / L_T < 1$. With no soil respiration, $\Lambda_{O_2} = 0$:

$$\left(\frac{L_a}{L_T}\right)=\frac{1}{\left[1+\sum_{i=1}^{N}\left(\frac{D_{eff,i}\cdot c_{i,s}}{D_{eff,O_2}\cdot c_{O_2,f}\cdot\varphi_i}\right)\right]} \qquad \text{[B.5.12]}$$

<u>Fast Reaction – Application of Equations</u>: Oxygen flux calculated with Eq. B.4.6 and oxygen concentration calculated with Eq. B.4.9, with $L_a = L_T$ presumed, are checked against the criteria of Eqs. B.4.7 and B.4.10, respectively. This explicit test determines if the soil layer L_T is completely aerobic.

If the soil layer is at least partially anaerobic, L_a is calculated using either Eq. B.5.7 (and related constraints) or B.5.11. The minimum applicable result for L_a is applied in Eqs. B.3.3 to B.3.7 (with finite degradation rates) to estimate chemical-specific concentrations.

<u>Fast Reaction – Bias</u>: The fast reaction assumption, when applied with all assumptions and model parameters matched, yields results for aerobic depth, L_a, which are always less than or

equal to L_a calculated with finite reaction rates, as discussed in Sections 3 and 4. Indoor air concentration estimates, c_e, calculated with the fast reaction assumption are always equal to or greater than those estimated with a finite reaction rate assumption.

The maximum bias between the two assumptions occurs when the fast reaction model indicates the soil layer is nearly or completely anaerobic, but the calculation of maximum oxygen demand with finite reaction rates indicates the soil layer is completely aerobic. This bias can be significant when degradation of the chemical of interest is contributing significantly to oxygen demand and L_a is approximately equal to L_R.

B.6 Foundation Mass Transfer Coefficient

Mass Transfer Coefficient from Model: From Johnson and Ettinger (1991), a nominal estimate of the mass transfer coefficient h can be based on building and foundation physical characteristics.

$$h = \left(\frac{\eta \cdot D_{crk}}{L_{crk}} \right) \qquad Q_s = 0 \qquad \text{[B.6.1]}$$

$$h = \frac{L_{mix} \cdot ER}{\left(\frac{1}{\exp(\xi)} \right) + \left(\frac{L_{mix} \cdot ER \cdot A_b}{Q_s} \right) \cdot \frac{(\exp(\xi) - 1)}{\exp(\xi)} - 1} \qquad Q_s > 0 \qquad \text{[B.6.2]}$$

Eq. B.6.1 applies for diffusion-dominated vapor flow through cracks in a foundation of thickness L_{crk}. The cracks cover an areal fraction, h, of the foundation area in contact with soil, A_b. Eq. B.6.2 applies with convective volumetric airflow, Q_s, entering the building through foundation cracks. Within Eq. B.6.2, ξ is

$$\xi = \frac{Q_s \cdot L_{crk}}{A_b \cdot D_{crk} \cdot \eta} \qquad \text{[B.6.3]}$$

Eq. B.6.2 can result in calculated errors for very large values of exp(ξ), depending on computers and software. An approximation for very large ξ is:

$$h = \frac{1}{\frac{A_b}{Q_s} - \frac{1}{L_{mix} \cdot ER}} \qquad \text{[B.6.2a]}$$

Mass Transfer Coefficient From Measured Data: Values of the foundation mass transfer coefficient h may also be estimated from measured data. AF_{VI} is defined as an attenuation factor across a foundation with background influences considered.

$$AF_{VI} = \frac{(c_e - c_{bkgnd})}{(c_f - c_{bkgnd})} = \frac{\frac{1}{L_{mix} \cdot ER}}{\left(\frac{1}{L_{mix} \cdot ER} + \frac{1}{h} \right)} \qquad \text{[B.6.4]}$$

The background concentration, c_{bkgnd}, includes contributions from outdoor air, c_a, and chemical mass emissions within the enclosure as a source, $\dot{m}_e$, (+) or sink (-).

$$c_{bkgnd} = c_a + \frac{\dot{m}_e}{A_b \cdot L_{mix} \cdot ER} \qquad \text{[B.6.5]}$$

Eq. B.6.5 simplifies to Eq. B.2.1 when c_{bkgnd} is negligible. Since there are a considerable number of chemical datasets of potential interest for which c_{bkgnd} is not negligible, an estimate of the bias error on h due to background concentrations is shown. With a defined empirical attenuation factor $AF_{EMP} = c_e / c_f$, from Eq. B.6.4,

$$AF_{EMP} = AF_{VI} \cdot (1 - c_{bkgnd} / c_f) + c_{bkgnd} / c_f \qquad \text{[B.6.6]}$$

A foundation mass transfer coefficient h_{VI}, with background considered is:

$$h_{VI} = \frac{L_{mix} \cdot ER}{\left(\dfrac{1}{AF_{VI}} - 1 \right)} = \frac{L_{mix} \cdot ER}{\left(\dfrac{1 - c_{bkgnd} / c_f}{AF_{EMP} - c_{bkgnd} / c_f} - 1 \right)} \qquad \text{[B.6.7]}$$

An empirical foundation mass transfer coefficient derived from AF_{EMP} without consideration of background is:

$$h_{EMP} = \frac{L_{mix} \cdot ER}{\left(\dfrac{1}{AF_{EMP}} - 1 \right)} \qquad \text{[B.6.8]}$$

Bias error in the estimated mass transfer coefficient, h, due to background influence is found from the ratio of Eqs. B.6.7 and B.6.8.

$$\left(\frac{h_{EMP} - h_{VI}}{h_{VI}} \right) = \left(\frac{c_{bkgnd} / c_f}{AF_{EMP} - c_{bkgnd} / c_f} \right) = \left(\frac{c_{bkgnd}}{c_e - c_{bkgnd}} \right) \qquad \text{[B.6.9]}$$

Minimal bias error in the estimated mass transfer coefficient requires larger differences between measured values of c_e and c_{bkgnd}. For example, limiting the bias error in mass transfer coefficient to approximately less than 0.1 due to background concentration would require enclosure concentrations approximately ten times greater than background concentrations.

B.7 Concentration And Flux Profiles Through The Soil Layer

Chemical Flux: Chemical flux through the aerobic soil layer for $0 \le z_a \le L_a$ ($\alpha_{a,i} > 0$) is:

$$\frac{J_i(z_a)}{J_{t,i}} = \frac{\left(\exp(-\alpha_{a,i}) - \beta_{a,i}\right) \cdot \exp(\alpha_{a,i} \cdot z_a / L_a) - \left(\beta_{a,i} - \exp(\alpha_{a,i})\right) \cdot \exp(-\alpha_{a,i} \cdot z_a / L_a)}{\exp(-\alpha_{a,i}) + \exp(\alpha_{a,i}) - 2 \cdot \beta_{a,i}} \qquad \text{[B.7.1]}$$

$$\frac{J_i(z_a)}{J_{t,i}} = 1 \qquad \alpha_{a,i} = 0 \qquad \text{[B.7.2]}$$

Chemical flux through the anaerobic soil layer for $0 \le z_b \le L_b$ is constant

$$\frac{J_i(z_b)}{J_{t,i}} = \frac{J_i(z_b)}{J_{s,i}} = 1 \qquad \text{[B.7.3]}$$

Oxygen Flux: Oxygen flux through the aerobic soil layer for $0 \le z_a \le L_a$ is:

$$J_{O_2}(z_a) - J_{t,O_2} = \sum_{i=1}^{N} \frac{1}{\varphi_i} \cdot (J_i(z_a) - J_{t,i}) + \rho_s \cdot z_a \cdot \Lambda_{base,O_2} \quad \text{[B.7.4]}$$

$J_{t,O_2} = 0$ is applied at $z_a = 0$, and $J_{t,O_2}(z_b) = 0$ for $0 \leq z_b \leq L_b$.

Chemical Concentration Profile: Chemical concentration through the aerobic soil layer, $0 \leq z_a \leq L_a$ is:

$$\left(\frac{c_i(z_a)}{c_{t,i}}\right) = \frac{\left(\exp(-\alpha_{a,i}) - \beta_{a,i}\right) \cdot \exp(\alpha_{a,i} \cdot z_a / L_a) + \left(\beta_{a,i} - \exp(\alpha_{a,i})\right) \cdot \exp(-\alpha_{a,i} \cdot z_a / L_a)}{\exp(-\alpha_{a,i}) - \exp(\alpha_{a,i})} \qquad \alpha_{a,i} > 0 \quad \text{[B.7.5]}$$

$$\left(\frac{c_i(z_a)}{c_{t,i}}\right) = 1 - \left(\frac{z_a}{L_a}\right) \cdot (1 - \beta_{a,i}) \qquad \alpha_{a,i} = 0 \quad \text{[B.7.6]}$$

with $\alpha_{a,i} = L_a / L_{R,i}$ and $b_{a,i} = c_{f,i} / c_{t,i}$. Chemical concentration through the anaerobic soil layer, $0 \leq z_b \leq L_b$ is:

$$\left(\frac{c_i(z_b)}{c_{t,i}}\right) = 1 - \left(\frac{z_b}{L_b}\right) \cdot (1 - \beta_{b,i}) \quad \text{[B.7.7]}$$

with $\beta_{b,i} = c_{t,i} / c_{s,i}$.

Oxygen Concentration Profile: Oxygen concentration through the aerobic soil layer is:

$$c_{O_2}(z_a) - c_{t,O_2} = \left(\sum_{i=1}^{N} \left(\frac{D_{eff,i}}{D_{eff,O_2} \cdot \varphi_i} \cdot \left[c_i(z_a) - c_{t,i}\right] + \frac{z_a}{D_{eff,O_2} \cdot \varphi_i} \cdot J_{t,i} \right) - \frac{\rho_s \cdot \Lambda_{base,O_2}}{D_{eff,O_2}} \cdot \frac{z_a^2}{2} \right) \quad \text{[B.7.8]}$$

Chemical Degradation Rate: Specific chemical degradation rate (per unit volume soil), is:

$$\Lambda(z_a) = \frac{\theta_w}{H} \cdot k_w \cdot c_v(z_a) \qquad \alpha_{a,i} > 0 \quad \text{[B.7.9]}$$

$$\Lambda(z_a) = 0 \qquad \alpha_{a,i} = 0 \quad \text{[B.7.10]}$$

Oxygen Degradation Rate: Specific oxygen degradation rate (per unit volume soil), is:

$$\Lambda_{O_2}(z_a) = \sum_{i=1}^{N} \Lambda_i(z_a) / \varphi_i + \Lambda_{base,O_2} \quad \text{[B.7.11]}$$

B.8 Source Concentration Screening Levels

The model as presented may be applied in estimating indoor air concentrations with source vapor concentrations specified. It may also be applied in estimating source concentrations, when indoor air target criteria are specified.

Bounding Attenuation Factors: Solving the equation set with biodegradation included requires a bounded range of possible source concentrations. Given a specified scenario, minimum and maximum ranges of possible source concentration to indoor air ratios (c_e/c_s) are estimated with Eq. B.3.3 for a no degradation ($\alpha_a = 0$) and a completely aerobic soil layer ($\alpha_a = L_T / L_R$) assumption. The completely aerobic soil layer assumption may yield unrealistically high source concentrations; therefore, in application, the maximum possibly source concentration in the search range is capped (at an arbitrarily and unrealistically high 10^{10} mg/m^3-air per chemical).

Indoor Air Target Concentrations and Source Concentrations: For individual chemicals, target indoor air vapor concentrations (*RBSL*) for a specified hazard quotient, *HQ* or risk level, *TR*, are calculated as:

$$RBSL_{e,i}(HQ_i) = \frac{HQ_i \cdot RfC_i \cdot IR_{in} \cdot 365\ day/year}{EF \cdot IR_{out}} \qquad [B.8.1]$$

$$RBSL_{e,i}(TR_i) = \frac{TR_i \cdot BW \cdot AT_c \cdot 365 dy/yr}{SF_i \cdot IR_{indoor} \cdot ED \cdot EF} \qquad [B.8.2]$$

For one or more (summed) selected chemicals, estimates of total source vapor concentrations that meet a specified total indoor air hazard index, *HI*, or risk, *TR*, are:

$$c_{s,T} = \frac{HI}{\sum_{i=1}^{N}\left(\frac{HQ_i}{RBSL_{e,i}(HQ_i)}\right)\cdot\left(\frac{c_{e,i}}{c_{s,i}}\right)\cdot\left(\frac{c_{s,i}}{c_{s,T}}\right)} \qquad [B.8.3]$$

$$c_{s,T} = \frac{TR}{\sum_{i=1}^{N}\left(\frac{TR_i}{RBSL_{e,i}(TR_i)}\right)\cdot\left(\frac{c_{e,i}}{c_{s,i}}\right)\cdot\left(\frac{c_{s,i}}{c_{s,T}}\right)} \qquad [B.8.4]$$

In Eqs. B.8.3 and B.8.4, (c_e/c_s) are chemical-specific source concentration to indoor air ratios, ($c_{s,i}$ / $c_{s,T}$) is the mass fraction of chemical i in source vapor, and the total source vapor concentration is:

$$c_{s,T} = \sum_{i=1}^{N} c_{s,i} \qquad [B.8.5]$$

For the no biodegradation case, solution of Eqs. B.8.3 and B.8.4 is explicit. With biodegradation included, the relevant possible ranges of source concentrations are optimized to meet the indoor air criteria.

B.9. Soil and Water Concentrations

Source vapor concentrations, c_s, are specified in the model calculations. Chemical vapor concentrations are used throughout the vapor transport model calculations, with linear three-phase equilibrium partitioning presumed between soil, soil vapor, and soil pore water in the soil zone.

Pore water concentration is $c_w = c_v / H$. *H* is dimensionless Henry's law coefficient (cm^3-water/cm^3-air) and

$$H = \frac{H'}{R \cdot T_{amb}} \cdot 10^3 \cdot \frac{L}{m^3} \qquad [B.9.1]$$

with *H'*, Henry's law coefficient (atm-m^3/mol); *R*, ideal gas constant (0.08206 atm-L/g-mol-K); and T_{amb}, ambient temperature (K).

Soil concentration is estimated in three-phase partitioning between soil and soil pore water, as $c_{soil} = K_{sw} \cdot c_w$ with c_{soil}, soil concentration, and K_{sw} (cm^3-water/g-soil) is a partition coefficient between soil concentration and pore water concentration.

$$K_{sw} = \frac{\theta_w + K_{oc} \cdot f_{oc} \cdot \rho_s + H \cdot (\theta_T - \theta_w)}{\rho_s} \qquad [B.9.2]$$

The value θ_w is soil moisture (cm^3-water/cm^3-soil), θ_T is soil porosity (cm^3-void/cm^3-soil), f_{oc} is soil organic carbon (g-oc/g-soil), ρ_s is soil bulk density (g/cm^3), and K_{oc} is the chemical-specific partition coefficient between organic carbon and pore water (cm^3-water/g-oc).

B.10 Saturated Vapor Limits for a Chemical Mixture

Linear partitioning between soil pore vapor, soil pore water, and soil concentrations is only valid up to a saturated vapor concentration limit. A separate calculation (Brost and Devaull, 2000; Mariner, 1997; Mott, 1995; Johnson et al., 1995) is included in the model to check whether the specified or inverse-calculated source vapor concentrations exceed a saturated vapor concentration for the chemical mixture.

Parameter limits are applied for chemicals that are miscible in water (ethanol, for example), or may be gases at ambient temperatures (methane, for example). For chemicals with pure chemical vapor pressure, P_{vap}, greater than the total ambient atmospheric pressure, P_{amb}, a maximum pure chemical volume concentration is:

$c_{sat,vap} = 1000000$ ppmv if $P_{vap} > P_{amb}$ or

$c_{sat,vap} = 1000000 \cdot (P_{vap} / P_{amb})$ if $P_{vap} > P_{amb}$ or $P_{vap} = P_{amb}$ [B.10.1]

Volume to mass concentration of chemicals are related as

c_v [ppmv] = c_v [mg/m^3] $\cdot R \cdot T_{amb} / MW$ [B.10.2]

with R, ideal gas constant (0.08206 atm-L/g-mol-K); T_{amb}, ambient temperature (K), and MW, molecular weight (g/g-mol).

For miscible chemicals in water, a maximum pure chemical aqueous solubility is:

$S = (c_{sat,vap} / 1000000) \cdot MW / H'$ [B.10.3]

The value of S in Eq. B.10.3 may be limited by either the chemical vapor pressure or atmospheric pressure.

For ideal chemicals which are partially miscible in water, the pure chemical aqueous solubility limit in water, S (mg/L) and pure chemical vapor pressure, P_{vap} (mmHg) are related as:

$$H' = \frac{P_v \cdot MW}{S} \cdot \frac{atm}{760 mmHg} \cdot \frac{mg}{g} \cdot \frac{m^3}{L} \qquad [B.10.4]$$

Variation from this relationship may occur, or may be evident in empirical data, especially for very low measured values of aqueous solubility, S, or vapor pressure, P_v. Therefore, saturation limits are estimated and checked in the model using both vapor pressure and aqueous solubility.

An estimate of whether a vapor mixture concentration is above, below, or equal to a saturated vapor concentration limit is:

For: mixture vapor concentrations are:

$$\sum_{i=1}^{N}\frac{c_{v,i}}{c_{v,sat,i}}>1$$ above the saturation limit

$$\sum_{i=1}^{N}\frac{c_{v,i}}{c_{v,sat,i}}=1$$ at the saturation limit

$$\sum_{i=1}^{N}\frac{c_{v,i}}{c_{v,sat,i}}<1$$ below the saturation limit [B.10.5]

$c_{v,i}$ is the specified component vapor concentration in a chemical mixture of N chemicals, and $c_{v,sat,i}$ is the pure chemical saturated vapor concentration. Saturated vapor concentrations occur when the equality of Eq. B.10.5 holds.

$$\sum_{i=1}^{N}\frac{c_{v,sat,eff,i}}{c_{v,sat,i}}=1$$ [B.10.6]

Component effective saturated vapor concentrations, $c_{v,sat,eff,i}$, in the mixture are:

$$c_{v,sat,eff,i}=\frac{c_{v,i}}{\sum_{i=1}^{N}\frac{c_{v,i}}{c_{v,sat,i}}} \quad \text{or} \quad c_{v,sat,eff,i}=c_{v,sat,i}\cdot\frac{\left(c_{v,i}/c_{v,sat,i}\right)}{\sum_{i=1}^{N}\frac{c_{v,i}}{c_{v,sat,i}}}$$ [B.10.7]

As indicated previously, empirical chemical-specific pure chemical solubility and vapor pressure values may not be entirely consistent due to variability in measured or estimated chemical property values. An estimate of whether a water-phase mixture is above, below, or equal to an aqueous saturated concentration limit is:

For: mixture aqueous concentrations are:

$$\sum_{i=1}^{N}\frac{c_{w,i}}{S_i}>1$$ above the saturation limit

$$\sum_{i=1}^{N}\frac{c_{w,i}}{S_i}=1$$ at the saturation limit

$$\sum_{i=1}^{N}\frac{c_{w,i}}{S_i}<1$$ below the saturation limit [B.10.8]

$c_{w,i}$ is the calculated component water-phase concentration of a chemical mixture of N chemicals, and S_i is the pure chemical aqueous solubility limit. Saturation occurs when the equality holds.

$$\sum_{i=1}^{N} \frac{S_{eff,i}}{S_i} = 1 \quad \text{[B.10.9]}$$

Component effective saturated water concentrations, $S_{eff,i}$, in the mixture are:

$$S_{eff,i} = \frac{c_{w,i}}{\sum_{i=1}^{N} \frac{c_{w,i}}{S_i}} \quad \text{or} \quad S_{eff,i} = S_i \cdot \frac{\left(c_{w,i} / S_i\right)}{\sum_{i=1}^{N} \frac{c_{w,i}}{S_i}} \quad \text{[B.10.10]}$$

In the model, a residual phase is indicated at the source if the tests of either Eq. B.10.5 or B.10.8 exceeds unity.

B.11. Dimensionless Form of the Henry's Law Constant

For some calculations, in order to correct for soil temperature, ***BioVapor*** utilizes the dimensionless form of the Henry's law constant. The equations used are those described in the EPA Fact Sheet "Correcting the Henry's Law Constant for Soil Temperature." The fact sheet is available at the following website:
http://www.epa.gov/swerrims/riskassessment/airmodel/johnson_ettinger.htm

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APPENDIX C: DERIVATION OF DEFAULT BIODEGRADATION RATES

George DeVaull
Shell Global Solutions US Inc.
3333 Highway Six South
Houston, Texas, USA
george.devaull@shell.com
7 May 2009

Contents

C.1 Introduction

This appendix is documentation of the biodegradation rates applied in the ***BioVapor*** model. Additional information is included in the references.

C.2. Petroleum Hydrocarbon Aerobic Biodegradation Rates

Water phase (pseudo) first-order aerobic biodegradation rates applied in the model are defined in DeVaull (2007). Values are based on a compilation of data from batch microcosms, diffusive columns, columns with advective flow, and measured field data. The included data are for a variety of soil type; the soils included no amendments (native soils only). ***BioVapor*** applies these rates only in the aerobic portion of the vadose zone.

C.2.1 BTEX and Alkylbenzenes

k_w = 0.73/hr

Median value. Based on an analysis of data sets for alkylbenzenes (benzene, toluene, ethylbenzene, xylenes, trimethylbenzene, and cumene). This value is consistent with the geometric mean value of 0.79 /hr in DeVaull (2007), and is based on the same data set.

C.2.2 Naphthalene

k_w = 19/hr

Median value. Based on a re-analysis of data in DeVaull (2007), specifically for naphthalene.

C.2.3 Short-chain (C3-C4) Branched- and Cyclo-aliphatic Hydrocarbons

k_w = 11/hr

Median value. Data for propane, butane, and C6-C9 branched and ring aliphatic chemicals. This is based on a re- analysis of data in DeVaull (2007), specifically for these aliphatic chemicals. The value is lower than the overall value for ‘aliphatics’ presented in DeVaull (2007).

C.2.4 Normal Alkanes (C5-C12)

k_w = 170/hr

Median value. Based on analysis of data for C5 to C12 normal paraffins. This is based on a re-analysis of data in DeVaull (2007), specifically for these straight-chain aliphatic chemicals. The value is higher than the overall value for ‘aliphatics’ presented in DeVaull (2007).

C.2.5 Mixed Normal Alkanes, Branched- and Cyclo-aliphatic Hyrocarbons

k_w = 71/hr

Geometric mean value. Based on data including C6-C12 -range normal paraffins and isomers of dimethylpentane, dimethylhexane, trimethylpentane, and trimethylhexane aliphatic hydrocarbons as in DeVaull (2007). This value is between those for the branched- and cyclo-aliphatic chemicals and normal alkanes as listed in this appendix and is appropriate for mixed aliphatic hydrocarbons.

C.2.6 Methane

k_w = 82/hr

Median value. This is from an analysis of data using methods in DeVaull (2007). Data is consolidated from information in: Einola (2007), Chanton (2004), Scheutz (2004), and Lundegard (2008).

C.3. Baseline Soil Respiration

A correlation for baseline oxygen respiration in soils is presented in the supplementary information for DeVaull (2007).

$$\Lambda_{base,O_2} = -\left(1.69\,\frac{mg-O_2}{g-oc\cdot day}\right)\cdot f_{oc}$$

with baseline respiration rate, Λ_{base,O_2} [mg-O_2/(g-soil · day)] and organic carbon fraction in soil f_{oc} (g-oc/g-soil). For the included range of data $0.0004 < f_{oc} < 0.4$, at this 95% confidence, errors in the oxygen respiration estimate are within a factor (×/÷) of approximately 10 of the correlation.

C.4 References

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