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United States
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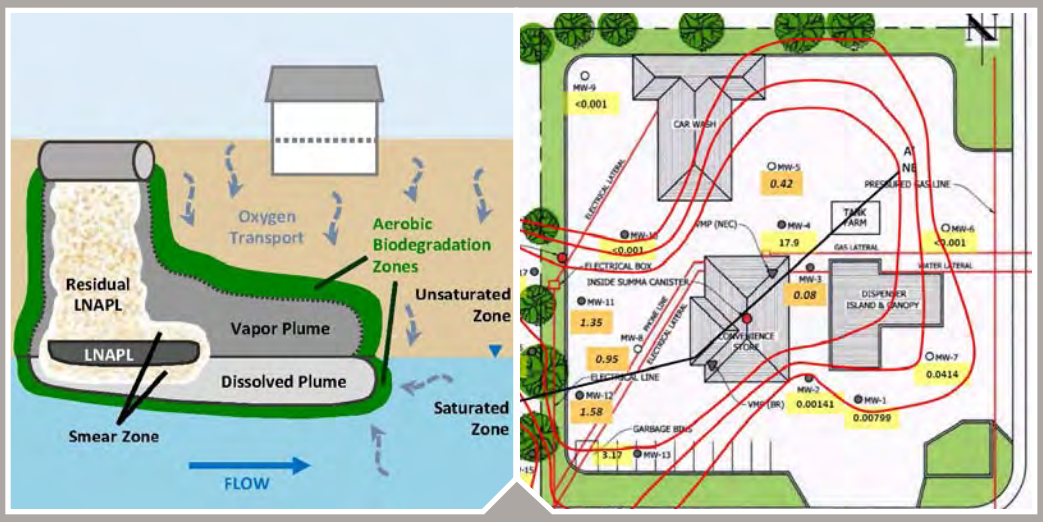
Agency

# Petroleum Vapor Intrusion Modeling Assessment with PVIScreen




Office of Research and Development
National Risk Management Research Laboratory | Groundwater, Watershed, and Ecosystem Restoration Division

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# Petroleum Vapor Intrusion Modeling Assessment with PVIScreen

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# Abstract

Vapor intrusion of petroleum compounds differs from that of chlorinated solvents because of the dominant effect of aerobic biodegradation on the concentration and distribution of petroleum vapors. To better understand the behavior of petroleum compounds, a model called PVIScreen was developed that applies the theory developed for the BioVapor model (DeVaull, 2007) to a lens of petroleum hydrocarbons in the subsurface that is capable of acting as a source of petroleum vapors. The PVIScreen model automatically conducts an uncertainty analysis using Monte Carlo simulations. The model is intended to make uncertainty analysis practical for application at petroleum vapor intrusion sites. The model can be run in either a batch mode, using Microsoft Excel files for both input and model outputs, and an interactive mode using a graphical user interface. Each of these is described, along with required inputs, example problems and the theoretical background of the model. Model simulations are in agreement with an EPA-sponsored analysis of field data that illustrate and document the attenuation of concentrations of petroleum compounds in soil gas with distance above the source of the vapors.

# Disclaimer

# 1. Background

## 1.1 Outline

This report describes the basis of the PVIScreen model, the procedure to run the model using the PVIScreen user interface, detailed description of input files, statistical inputs, example problems and the theoretical background of the model.

## 1.2 Environmental Models and Vapor Intrusion

Environmental models are based on the application of mass conservation principles to transport and transformation of chemicals in the environment. Generally, all environmental models are based on a two-part conceptualization: an empirically-determined principle relating chemical, physical and biological quantities, and empirical coefficients. Taken together these two components have the potential for representing transport and transformation of petroleum vapors in the vadose zone below a building.

Although models may represent important processes, the ability to determine definitively that there are no vapor impacts to buildings ("screen for PVI") also depends on application-related factors. These factors include the degree to which the site conceptual model matches the structure of the mathematical model, the inherent limitations imposed by the assumptions in the mathematical model, the values chosen for input parameters, and the ability to calibrate the mathematical model to site conditions. Many of these factors are difficult to address at leaking underground storage tank sites, so as will be noted below, model results should be viewed as one line of evidence in a site assessment.

Over ten years ago, vapor intrusion and its evaluation through modeling approaches were identified as a potential problem at subsurface contamination sites (Obamascik, 2002). Application of simplified models using mostly generic default parameters has contributed to confusion over appropriate assessment strategies for these sites. One of the primary models in use, the Johnson-Ettinger model (JEM) was presented as a heuristic screening model (Johnson and Ettinger, 1991). Essentially, the model consists of two completely-mixed compartments, one representing the interior of a building and the other the soil below. This conceptualization reflects the potential for both features of the building and the subsurface to contribute to indoor air contamination. In its original form, the model simply related the concentration in the soil gas to the concentration in indoor air. No biodegradation of the compound was included as the model conceptualization only related concentration between the two compartments. Later extension of the JEM included diffusive flux from a deeper source zone to the bottom of the foundation. Even though the JEM does not include biodegradation, the JEM could be a valid conceptualization for chlorinated solvents, because most of these compounds do not undergo aerobic biodegradation.

Petroleum hydrocarbons, however, are readily degraded under aerobic conditions so the JEM excludes a process with the potential for greatly affecting petroleum vapor intrusion (Figure 1). Chlorinated solvents are not degraded in the presence of oxygen, so dissolved contamination in the aquifer (saturated zone) almost always has the potential to contaminate indoor air (Figure 1, left). In contrast, petroleum hydrocarbons can be degraded under aerobic conditions, so the prospect for vapor intrusion is more limited, but also more dependent on the specific configuration of a source, presence of light non-aqueous phase liquid (LNAPL), and depth to water, among other factors (Figure 1, right).

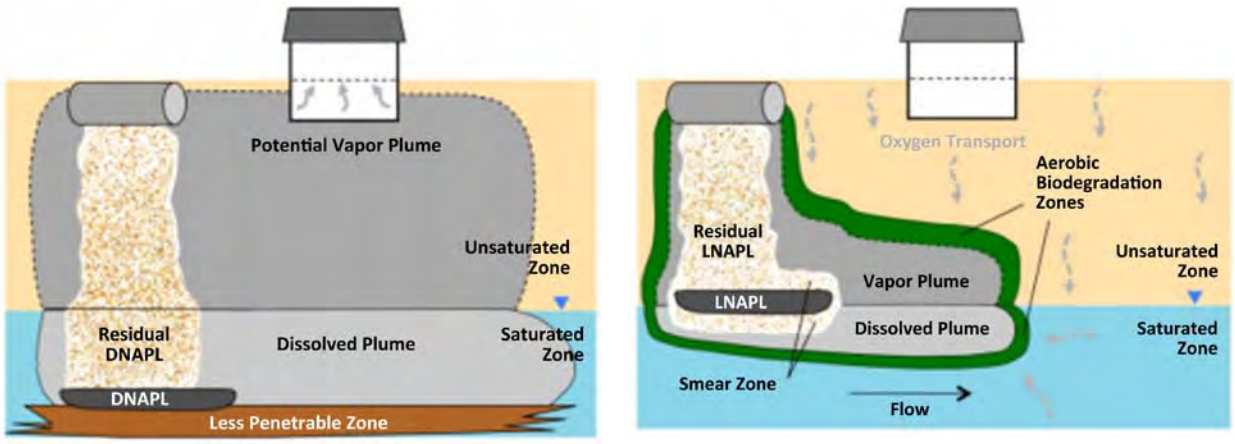


Figure 1. Comparison between the processes governing non-biodegrading solvent vapor intrusion (left) and petroleum vapor intrusion (right) (U.S. EPA, 2012).

## 1.3 Empirical Basis for Bioattenuation

In 2013, EPA published a report that evaluated a large set of empirical petroleum vapor data from the United States, Canada and Australia (USEPA 2013). This evaluation confirmed model simulation results, and that aerobic biodegradation of petroleum hydrocarbons is a well-documented, widespread and robust process that has been demonstrated under a wide range of environmental conditions. Important factors influencing aerobic biodegradation of petroleum vapors include:

- Vapor source concentration, flux, and composition;
- Minimal oxygen concentration is required to support aerobic biodegradation;
- Oxygen supply and demand;
- Distance between the vapor source and a building foundation;
- Soil type and properties (e.g., porosity and moisture); and
- Size and characteristics of the building and adjacent land surface.

The empirical data show that the capacity for biodegradation of petroleum hydrocarbons is high. In cases where uncontaminated soil overlies dissolved benzene and total petroleum hydrocarbon concentrations in ground water, vapors have been shown to be attenuated (Figure 2 and Figure 3). The thickness of clean soil associated with attenuation depends on the concentration in ground water as higher levels in ground water require greater thickness of clean soil. These data demonstrate the ability of the vadose zone to attenuated benzene and TPH vapor concentrations, and formed the basis for the EPA approach to screening sites that was published in 2015 (U.S EPA, 2015), which is discussed in section 1.5 “PVIScreen Use in the Context of a Petroleum Vapor Intrusion Assessment”.

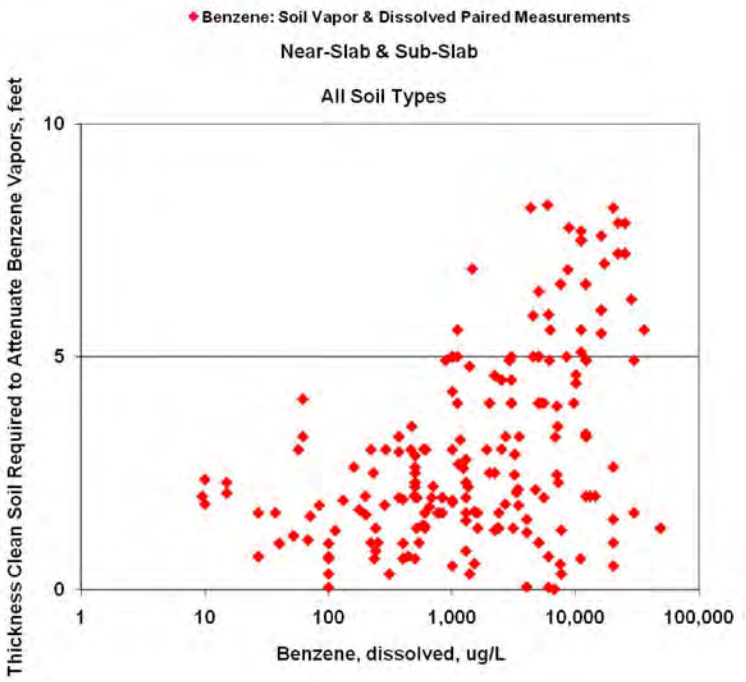


Figure 2. Thickness of clean soil associated with attenuation of benzene vapors (Davis, 2009).

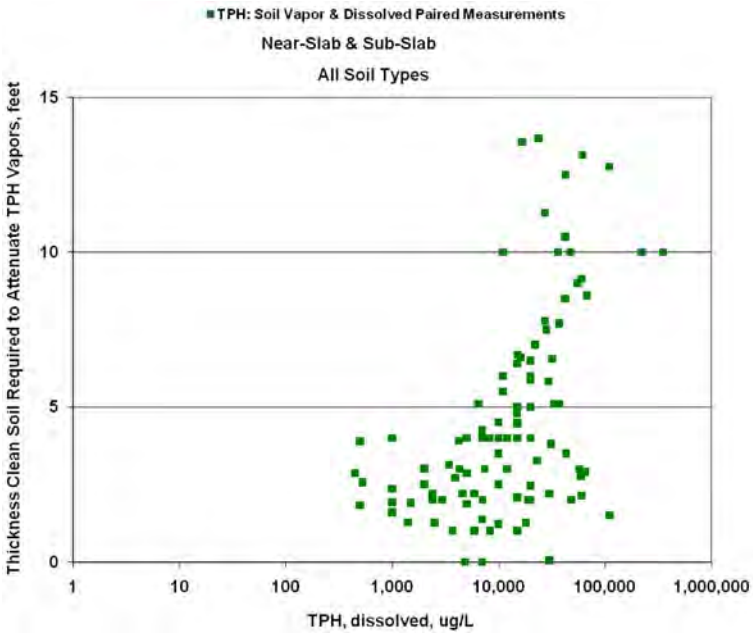


Figure 3. Thickness of clean soil associated with attenuation of TPH vapors (Davis, 2009).

## 1.4 The BioVapor Model

The BioVapor code was developed (DeVaull, 2007; API, 2010) to account for:

- aerobic biodegradation in the vadose zone,
- limits on oxygen supply imposed by the diffusive flux into the vadose zone,
- the oxygen demand of any number of compounds present in soil gas, and
- oxygen consumption by native soil respiration.

Conceptually, oxygen from the atmosphere (Figure 4) permeates the soil gas providing the electron acceptor needed for aerobic biodegradation of petroleum hydrocarbons. Because of the typical large flux of oxygen from the atmosphere, petroleum hydrocarbons react in a zone near their source and consequently their concentrations may be reduced relatively deeply in the vadose zone.

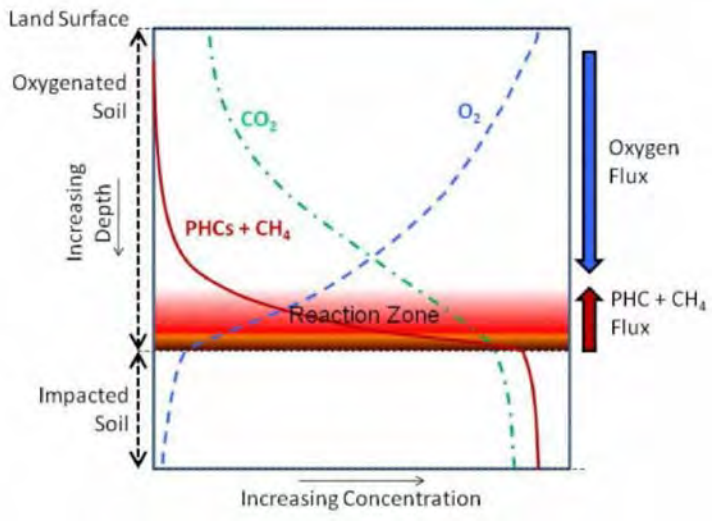


Figure 4. Schematic illustration of petroleum hydrocarbon (PHC) flux and distribution and oxygen flux and distribution (US EPA, 2012).

BioVapor was developed as a Microsoft Excel spreadsheet application. BioVapor balances the supply of oxygen from the atmosphere with the degradation-driven demand for oxygen in the soil gas. The outputs of the model include the depth of the aerobic zone, indoor air concentration for all chemicals included in the simulation, and the chemical concentrations at other points in the soil profile.

PVIScreen is an object-oriented petroleum vapor intrusion model, which extends the concepts of BioVapor by

- implementing an automated uncertainty analysis,
- linking directly to a fuel leaching model,
- providing the capability to use a flexible unit conversion system,
- displaying key outputs in an intuitive fashion.

In PVIScreen, the building, vadose zone and aquifer are defined in a layout which relates the bottom of the foundation to a zone of petroleum contamination. Input parameters describe the size and characteristics of each component in the model. Data on vadose zone contamination are needed to drive the simulation. These are expected to be soil gas (Figure 5) or ground water data (Figure 6).

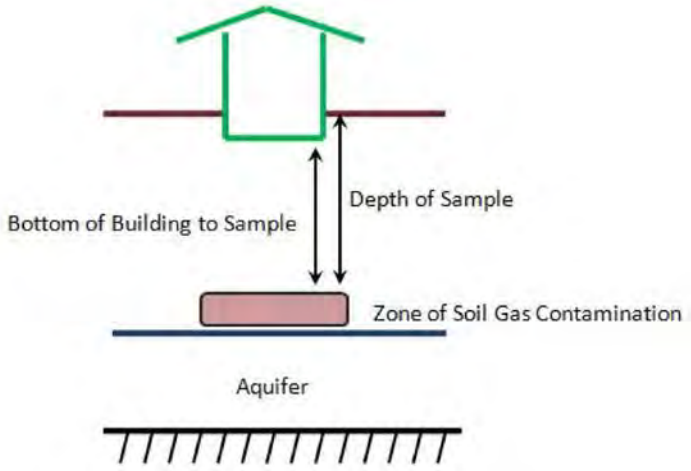


Figure 5. Building, vadose zone, ground water contamination layout used in PVIScreen for a **soil gas** source.

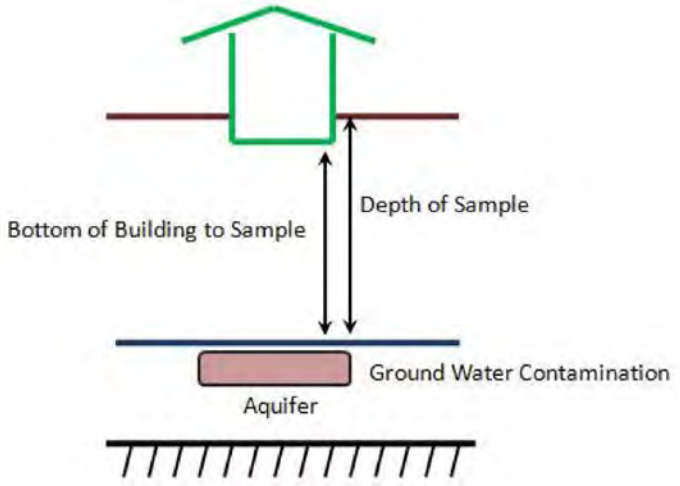


Figure 6. Building, vadose zone, petroleum (NAPL) contamination, and aquifer layout used in PVIScreen for a **ground water** source.

### *1.4.1 Uncertainty Analysis*

#### 1.4.1.1 The General Need for Uncertainty Analysis

Uncertainty analysis, as used here, uses the response of the model to changes in parameter values to assess the uncertainty in model output. The method used in PVIScreen is to presume that some or all parameters of the model are uncertain. The probability of a parameter taking on a value is governed by a cumulative probability curve. The graphical user interface allows for two choices: a constant parameter, and a parameter defined by a minimum and maximum value[1].

If the model is used in batch mode more options are available. These include entering sets of points defining the input probabilities. No assumptions of particular distributions (i.e., normal) are needed, although a normal distribution can be approximated empirically. (See Appendix Entry of Deterministic and Stochastic (Monte Carlo) Data").

#### 1.4.1.2 Uncertainty in Biodegradation Rates

The need for uncertainty analysis is illustrated by numerical model simulations by Abreu et al. (2009). The results were presented as attenuation factors, defined as the indoor air concentration ($C_{building}$) divided by the source concentration ($C_{source}$):

$$\alpha = AF = {C_{building}}/{C_{source}}$$

When this factor is low, the vapor concentration in the building is reduced over that in the subsurface, and the potential for vapor intrusion is low. Briefly summarizing the results, the attenuation factors are much lower when aerobic biodegradation is included as compared to the non-biodegradation case (TCE and other solvents). The literature shows that degradation rates, however, are not known with certainty; neither are they measured at typical field sites. Thus, the degradation rate is one that should be (and is) treated as uncertain in PVIScreen (Figure 7).

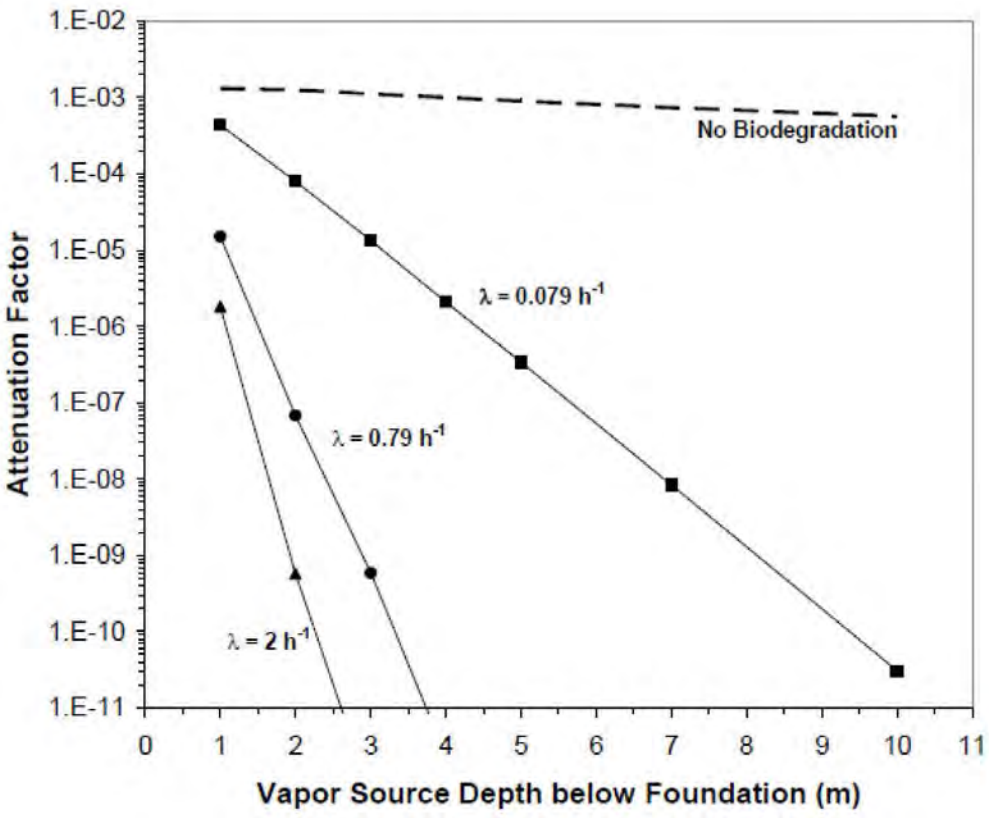


Figure 7. Vapor attenuation factors predicted by three-dimensional numerical model as a function of separation distance from a residential building foundation to an underlying petroleum contaminant vapor source concentration of 10 mg/L (10,000,000 ug/m$^3$), with various first-order biodegradation rates (Abreu and Johnson, 2005; Abreu et al., 2009).

[1]Use of the minimum and maximum values correspond to a uniform distribution where there is a straight-line (linear) relationship between the two specified values.

#### 1.4.1.3 Uncertainty Analysis in PVIScreen

In the Monte Carlo procedure, the model is run a specified number of times and the uncertain parameters are chosen randomly from the probability curves. A sampling technique called Latin Hypercube Sampling (LHS) is used to assure that parameter values are drawn from all parts of the probability distributions. LHS generally reduces the number of simulations required. After completing all required runs of the model, the results are processed into output probability curves and a summary table for each chemical specified in soil gas.

The main PVIScreen outputs are cumulative probability (or frequency) curves. As an illustrative example, 1000 runs of the model produced the aerobic zone thicknesses ranging from 10.88 cm to 120.86 cm (Figure 8). No result had an aerobic zone thickness less than 10.88 cm and no simulation had one that exceeded 120.86 cm. There was a 100% probability that the result was between these two values. The probability that the result was between 10.88 cm and 60 cm (vertical blue arrow on Figure 8) was 31% (horizontal blue arrow on Figure 8). The probability that the aerobic zone thickness was between 60 cm and 120.86 cm was 69%, as indicated by the upward-sloping, red-colored, cross hatching on Figure 8.

The main display of PVIScreen output is based on the cumulative probability curve (Figure 8). The probability that simulations exceed a risk-based concentration is displayed as output. This result is directly analogous to the cross-hatched area in Figure 8.

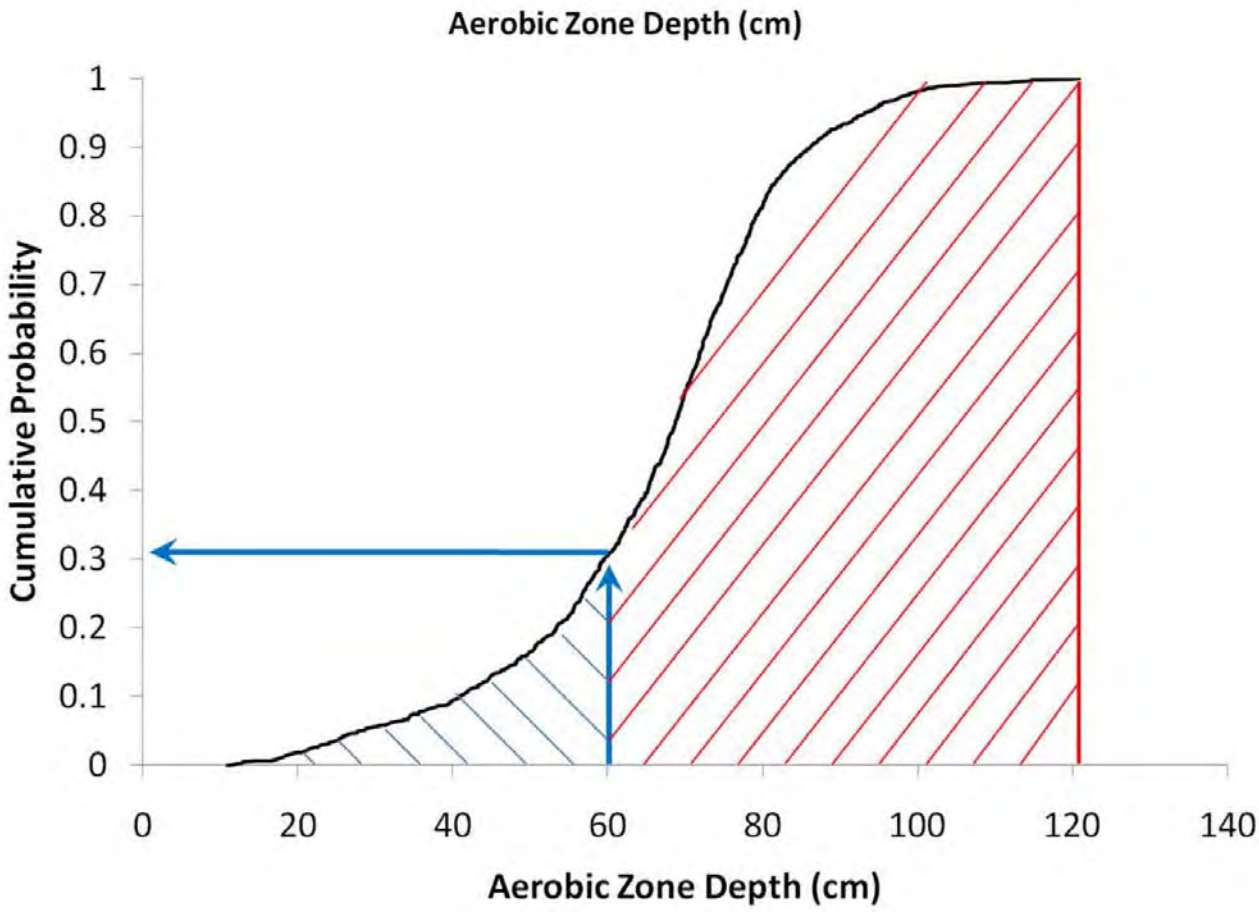


Figure 8. Example cumulative probability curve. The probability that the aerobic zone depth is 60 cm is 31%, while the probability that the aerobic zone thickness is greater than 60 cm is 69%.

## 1.5 PVIScreen Use in Context of a Petroleum Vapor Intrusion Assessment

The use of models in general, and PVIScreen specifically, should be integrated with site assessment. EPA's PVI guidance document outlined steps for an assessment. Because PVIScreen needs measured concentrations to represent the source of contamination, its use comes after sufficient characterization of the site and construction of a conceptual site model (Figure 9). Professional judgment is needed to determine when the characterization data is sufficient. Two possibilities for PVIScreen use follow:

An option is to use the model in parallel with determination of a vertical separation distance (box outlined with dashed line in Figure 9). For this scenario, the model provides an additional line of evidence to support site decision making. Because the model is essentially based on the same set of observations as the empirical database, these two lines of evidence should provide similar results. The model may, however, allow for unique site-specific factors to be incorporated, such as commercial rather than residential air exchange rates.

A second option is to use the model where the site fails the vertical separation zone criteria, or is a marginal case (the circled "NO" in Figure 9). Here the use of the model results may provide an additional line of evidence to support a site decision (which could be to conduct further sampling or which could be that no further investigation is needed).

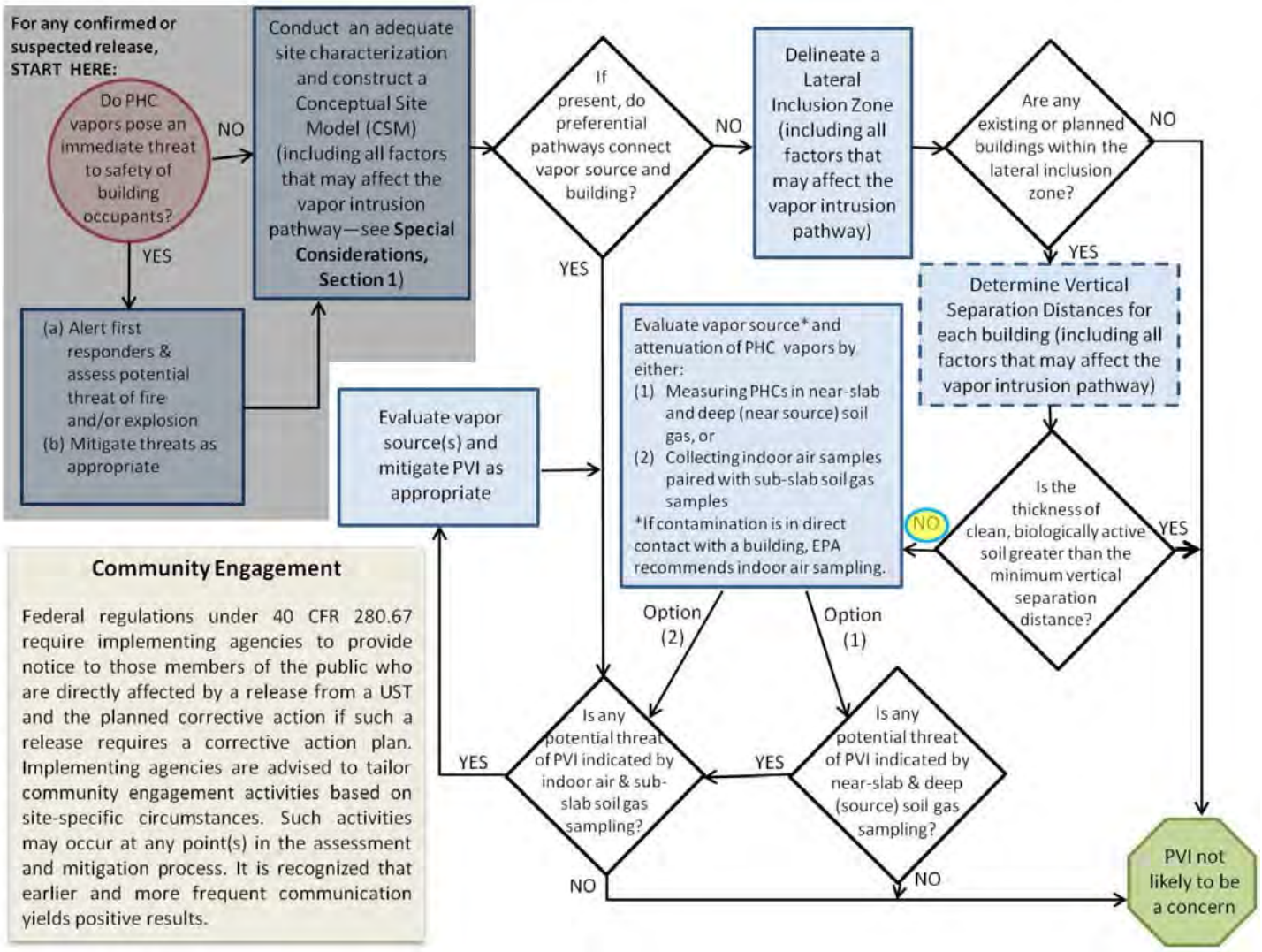


Figure 9. Petroleum vapor intrusion site assessment flow chart. PVIScreen could be used anytime after the site has been characterized and a conceptual site model constructed (outside dark gray box). One scenario is to use the model in parallel with determination of a vertical separation distance (box outlined with a dashed line). A second is to use the model when the vertical separation criteria fails or is marginal (circled "NO").

# 2. Getting Started

The PVIScreen distribution file (***PVIScreen.zip***) needs only to be copied to ***C:\MyDocuments\PVIScreen***, followed by extraction of all the files to this location. PVIScreen will open by double clicking on the ***PVIScreen.jar*** file[2]. All needed data files and examples will be available in the ***SRC \systemData and projects\examples*** directories.

# 3. Running the Model

## 3.1 PVIScreen User Interface

PVIScreen is incorporated into a user interface (UI) that facilitates preparing and editing input files, running the model and displaying the results[3]. The interface is designed so that the model options are selected from left to right. As more options become available, more of the buttons turn green (Figure 10).

### *3.1.1 File Selection*

PVIScreen ***must*** begin with an existing data file. There are two options:

1) For a new project, template files are provided for the common types of inputs. Template files are available for cases with soil gas sources and ground water sources, and residential and commercial buildings. These are found in the directory PVIScreen/projects/templates (Figure 11)[4].

After editing, these must be saved under new names in a project directory. A new directory is created by right-clicking on the directory pane and selecting "New", renaming to match project, and then saving input file in the new directory (Figure 12).

2) When later coming back to a project, the original input data can be accessed or previously-created results files can be accessed. The input file can be run again or the previous results displayed (Figure 13).

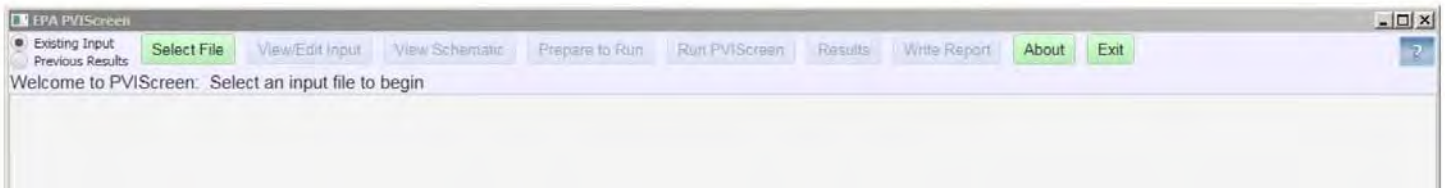


Figure 10. File selection in PVIScreen.

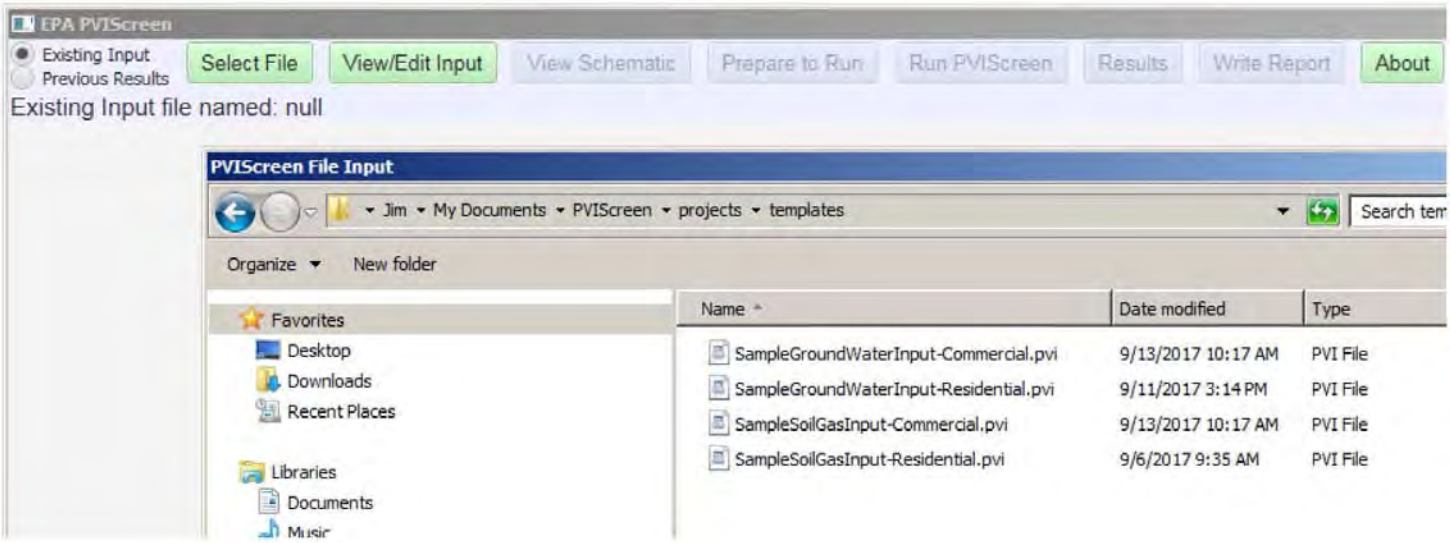


Figure 11. Opening a Template File in PVIScreen.

[2]If the model fails to execute, make sure that the Java runtime environment is in the computer's path. Check with your system administrator for guidance.

[3]PVIScreen can be run in a command line mode, which is described in Appendix A. Running PVIScreen in Command Line and Batch Mode.

[4]PVIScreen regenerates all the template files each time it is run. When template files are used, they must be renamed and/or moved to save data for future use.

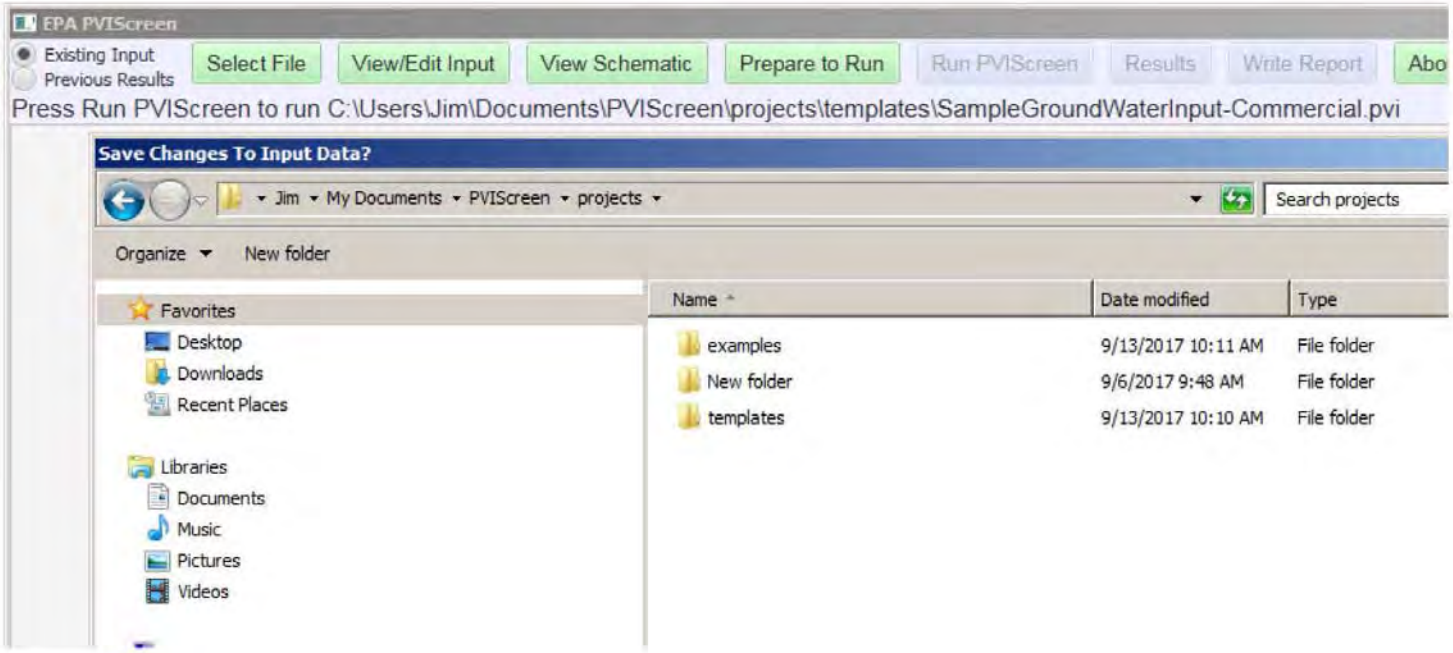


Figure 12. New folder created for a PVIScreen project.

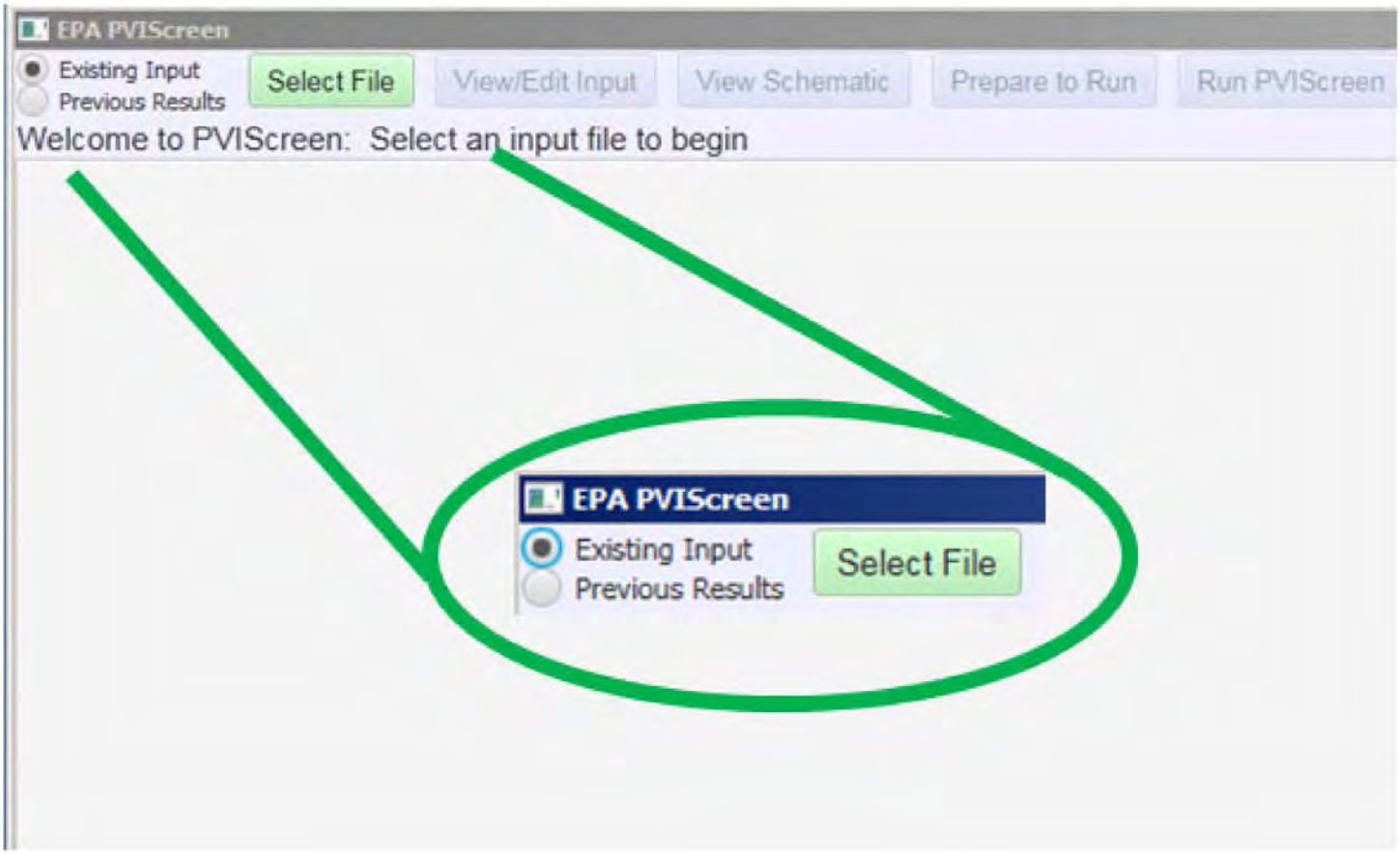


Figure 13. Selection of existing input or previous results.

PVIScreen uses Microsoft Excel spreadsheet files in a comma-separated-value format for both input and output (Appendix B. Microsoft Excel Comma Separated Value (.csv) Format). These are saved to the user's computer disk.

### 3.1.2 PVIScreen File Names

Several types of files are used in PVIScreen. An input file is named:

**SampleSoilGasInput.pvi**

The "pvi" extension is used to identify the file as a PVI Screen input file. The format of this file is the Microsoft Excel comma-separated-value. Thus the file can be opened and read by Microsoft Excel.

#### 3.1.2.1 PVIScreen Output Files

PVIScreen produces an output file for each run of the model with a file name related to the input file. For example, the input file:

**SampleSoilGasInput.pvi**

has a results file called:

**SampleSoilGasInput2016-May-31-16h-52m-13.0s.PVIScreen.Results.csv**

where the input file name is given a date/time stamp and *".PVIScreen.Results"* is added to the file name. The final *".cvs"* extension identifies the file as a comma-separated-value and allows its editing in Microsoft Excel and other spreadsheet software.

### 3.1.3 Editing an Existing Data Set

The first input screen lists general information on the simulation (Figure 14). This and each other tab of the input data screens can be edited in turn. Detailed examples follow in the soil gas and soil sample source examples below.

### 3.1.4 Editing the Data Screens

#### 3.1.4.1 Identification & Options

The Identification & Options screen (Figure 14) contains general information on the simulation and choices for cancer risk level, hazard quotient and oil distribution[5].

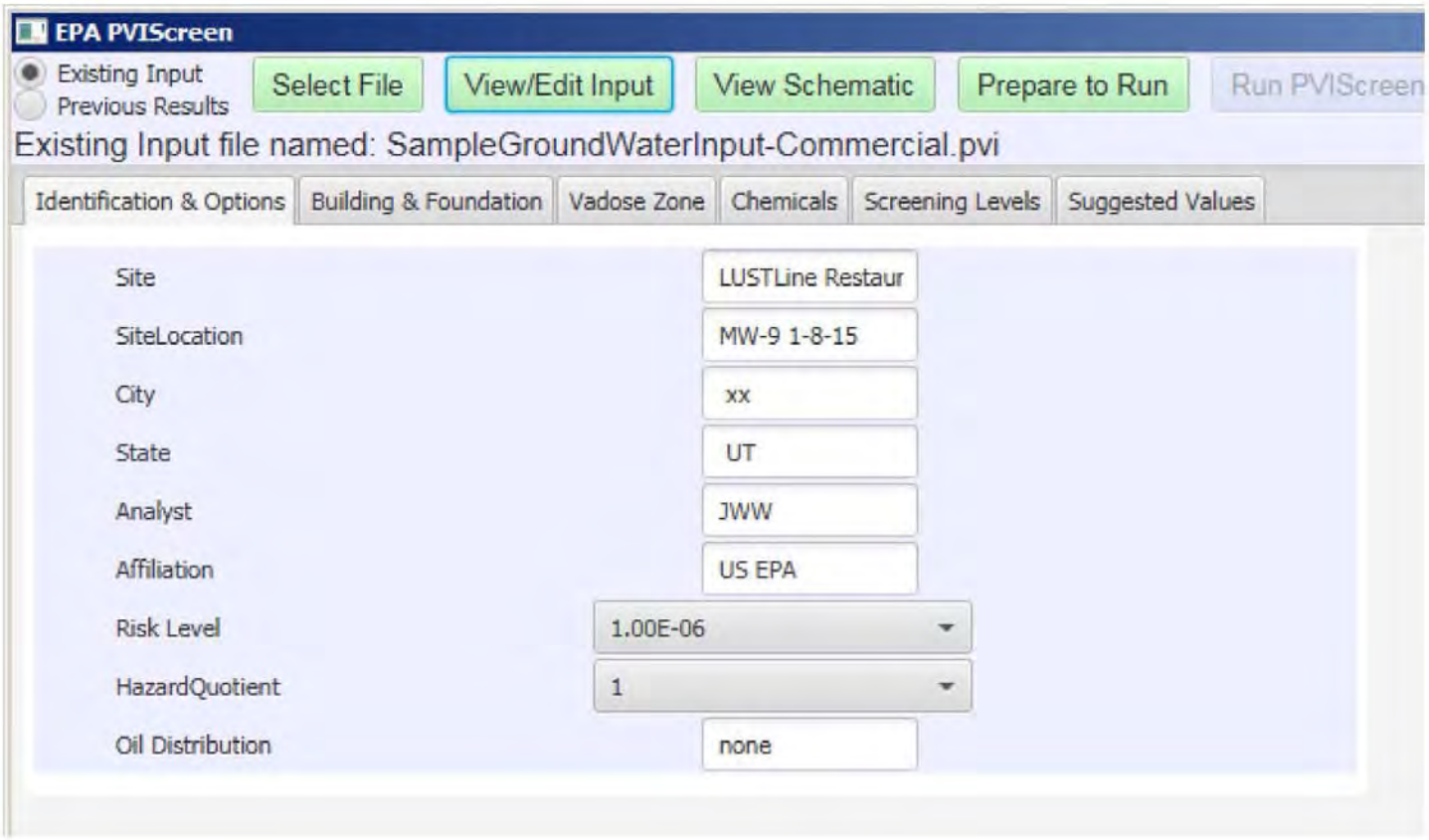


Figure 14. Identification & Options input screen.

[5]These are in the process of being removed as they are typically overridden elsewhere, especially through the use of predetermined screening levels.

### 3.1.4.2 General Input Parameter Information

Each numerical parameter of the model can be specified as constant or uniformly distributed (Figure 15). Constant parameters are chosen to be values that can be determined with a high degree of confidence. Typically, these include the building width, length and ceiling height. Other parameters are either unmeasured or unlikely to be estimated very precisely. For these, a uniform distribution is available, where a minimum and a maximum value are specified. Parameters likely to be in this category are crack width, air exchange rate, and porosity. More options including standard statistical and empirical distributions are available in the command line mode of running the model. See ***Appendix A Running PVIScreen in Command Line and Batch Mode***.


Figure 15. Illustration of input distribution choices.

### 3.1.4.3 Building & Foundation

The Building & Foundation screen contains the specification of building and foundation parameters (Figure 16).

**Dirt Floor:** yes or no.
Only buildings with a true dirt floor should answer "yes."[6]

**Width:** From measurement of building.

**Length:** From measurement of building.

**Ceiling Height:** The JEM and other models include a mixing zone height. Examination of example values show that these correspond to ceiling heights of 8 to 12 (US EPA, 2004). The mixing zone may not correspond exactly to ceiling height, but an independent evaluation of mixing zone height is not expected to be available.

**Foundation Depth Below Grade:** This is the depth of the bottom of the foundation below grade.

**Foundation Thickness:** Measurement of building.

**Crack Width:** US EPA (2003) lists crack widths from hairline (<0.1 mm) to 5 mm.

**Air Exchange Rate:** Values of 0.1 $hr^{-1}$ to 1.5 $hr^{-1}$ were developed by US EPA (2003) for residential buildings.

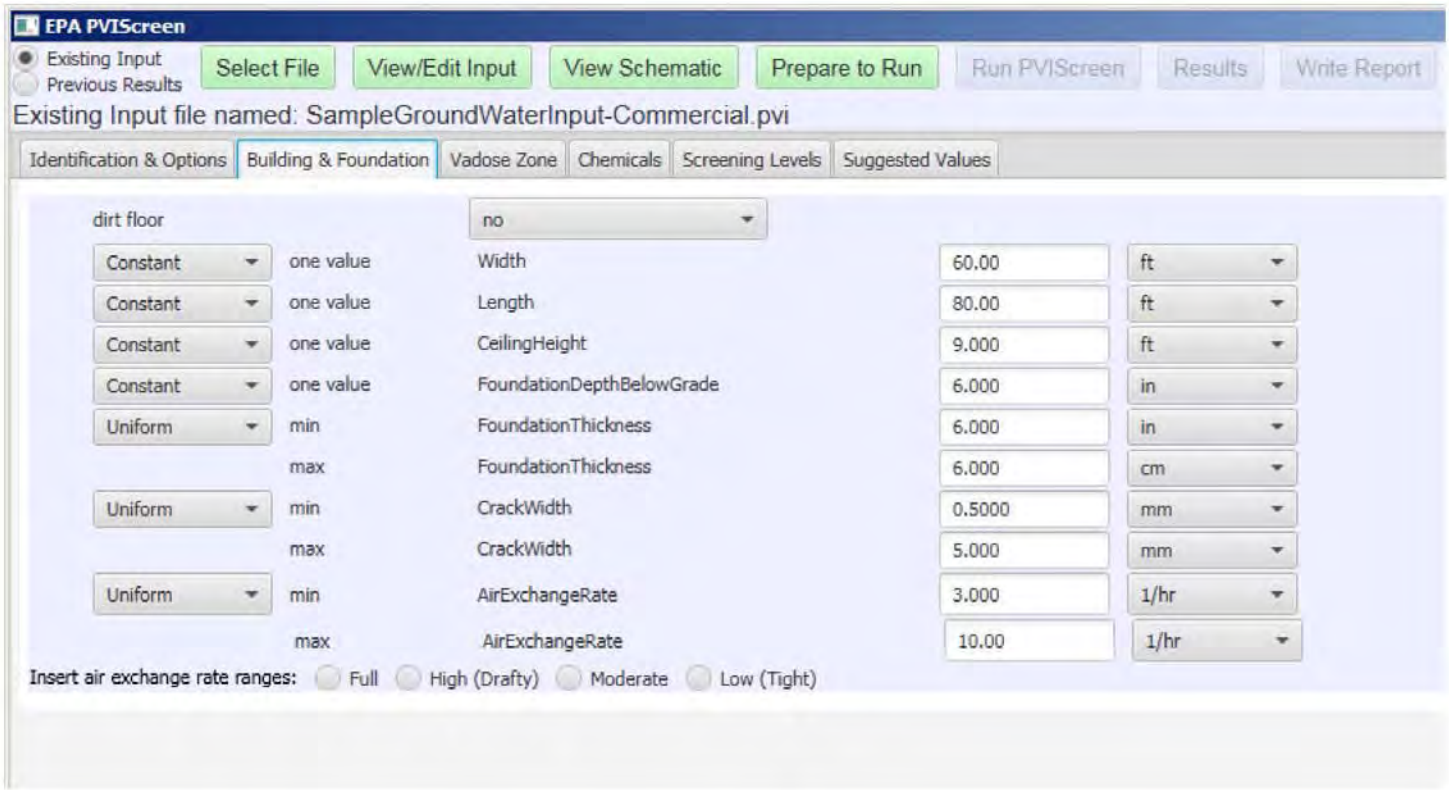


Figure 16. Building & Foundation input screen.

[6]The only current option is a concrete floor.

### 3.1.4.4 Chemicals

The Chemicals screen contains the specification of chemical parameters (Figure 17). Chemicals that appear in the PVIScreen database (Table 1) can be selected as a component of the contaminant source. In the example in Figure 17, BTEX and petroleum hydrocarbon equivalent carbon number fractions have been chosen. The source type given (Fuel Phase Concentration By Volume) is determined in the template for the input data set[7]. Templates are available for soil gas and water sample input files.

| Table 1. Chemicals in the PVIScreen database. |
|---|
| Benzene |
| Toluene |
| Ethylbenzene |
| xylenes |
| TPH-GRO |
| TPH-DRO |
| C8 To C9 Aromatic |
| C9 To C10 Aromatic |
| C10 To C11 Aromatic |
| Naphthalene |
| C5 To C6 Aliphatic |
| C6 To C7 Aliphatic |
| C7 To C8 Aliphatic |
| C8 To C9 Aliphatic |
| MTBE |
| EDB |

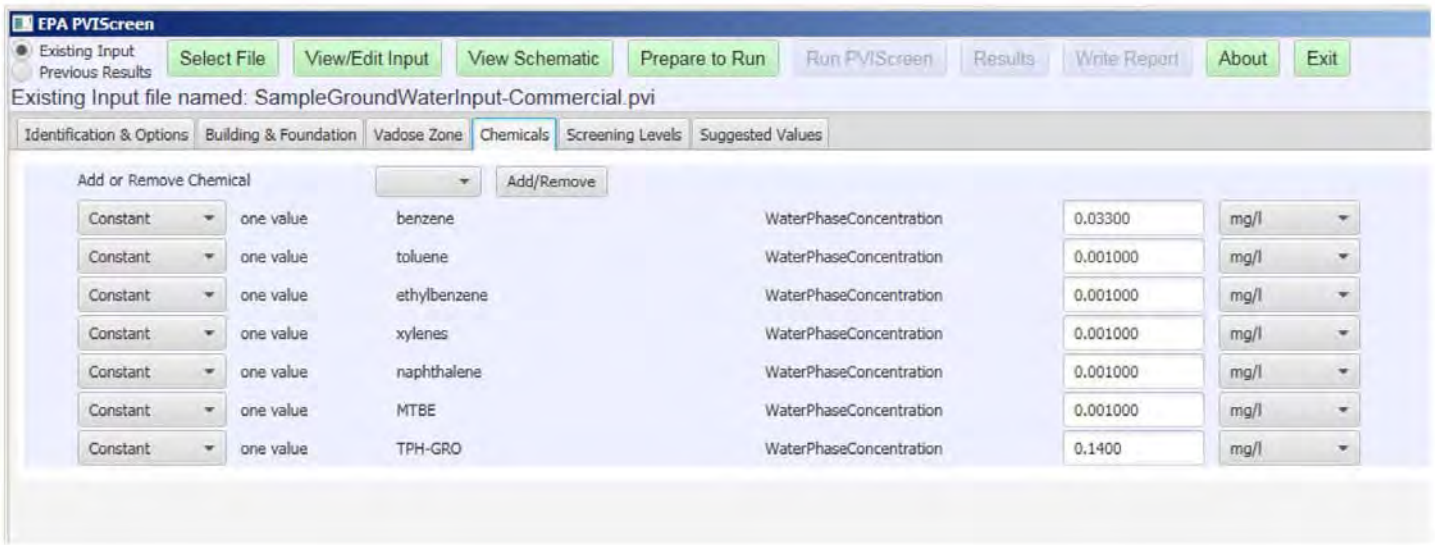


Figure 17. Chemicals input screen.

[7]In an updated version of the model these will be editable from the input data screen.

### 3.1.5 Treatment of Ground Water Samples

A soil sample is used as a direct input to PVIScreen, because soil gas is the media through which contaminants are transported in the vadose zone. No adjustments to the concentration are needed. For ground water samples, a paradigm is needed to simulate the transition between water and soil gas. Once in the soil gas, the calculation proceeds as for a soil gas sample. The following describes the approach used in PVIScreen.

Transport across the capillary fringe follows a complex process. Data from McCarthy and Johnson (1993) are used to develop a simplified water table paradigm for PVIScreen. Trichloroethene (TCE) in aqueous solution was used to generate a distribution of concentration through the capillary in a laboratory column. The concentrations in pore water were measured for both a rising and falling water table. Because TCE would not be subject to aerobic biodegradation in this experiment as in the case of chlorinated solvent vapor intrusion (Figure 1), it permits study of the mechanical aspects of transport, without additional impacts from biodegradation. For ground water flow in a moderate flow range (i.e., 0.1 m/d), McCarthy and Johnson (1993) found that the concentration of TCE in the capillary fringe was reduced by a factor of 10 at the top of the tension saturated zone (Figure 18 and Figure 19). The factor is included in the Suggested Value tab of PVIScreen, with the value set to 0.1.

Experimental results from McCarthy and Johnson demonstrate the reduction in water phase concentration occurring through the capillary fringe. By comparing the moisture content and relative concentration, these experiments showed a roughly 1/10-fold to 1/100-fold reduction in water phase concentration (Figure 18). These relationships held during both imbibition and drainage[8].

Although factors greater than 10 may be justified, the data from McCarthy and Johnson (1993) represent only one set of laboratory conditions. Ground water data, also, might have representational problems. A primary concern is a sample that is obtained from a depth below the water table. If that sample is drawn from a screen that crosses a contaminant plume so water with differing concentrations are mixed together, then the concentration is not representative of the concentration at the water table.

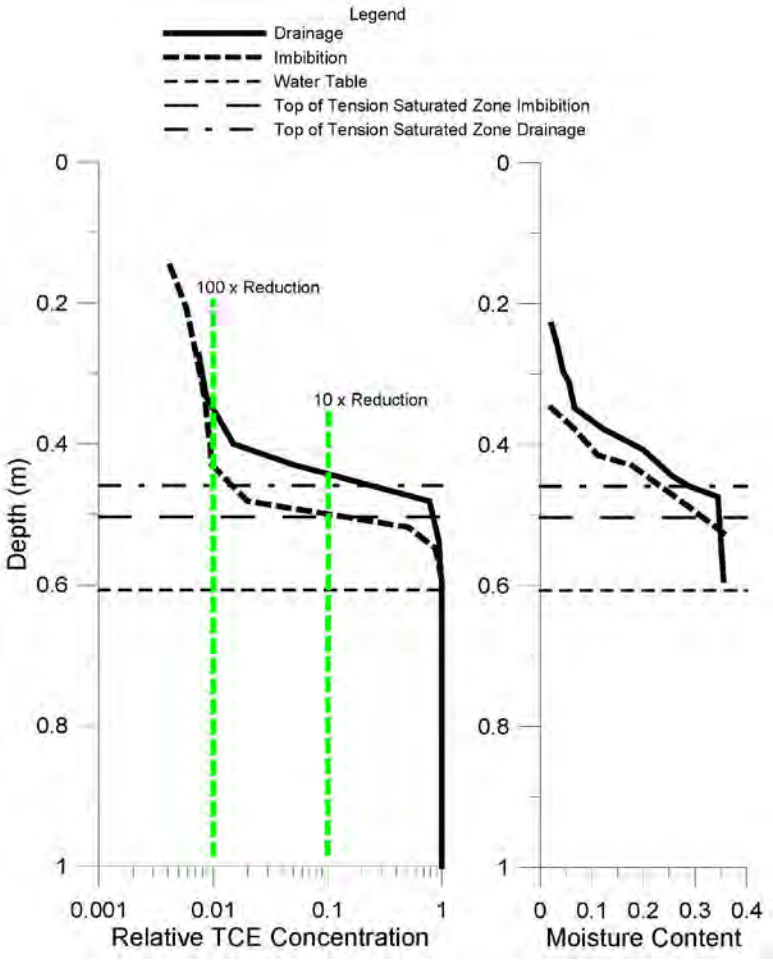


Figure 18. Reduction in water phase TCE concentration across the capillary fringe from a laboratory experiment (McCarthy and Johnson, 1993, used by permission, John Wiley and Sons).

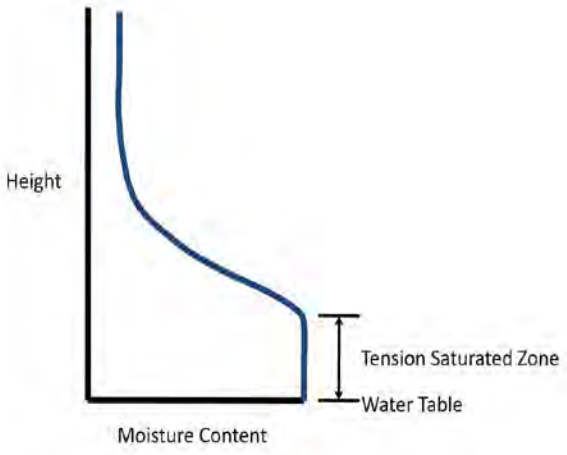


Figure 19. Schematic illustrating capillary rise and the tension saturated zone, which is an area above the water table where the water fills the pore space and is held by capillary suction. Air is admitted to the pore space above the tension saturated zone.

[8]Imbibition is defined as the replacement of a non-wetting fluid by a wetting fluid, and drainage is defined as the replacement of a wetting fluid by a non-wetting fluid.

### *3.1.6 Vadose Zone*

The Vadose Zone screen contains the specification of the vadose zone parameters (Figure 20).

**Depth To Sample:** Depth from the surface to the sample that is treated as the source of contamination.

**Depth To Water:** Depth from the surface to the water table.

**Depth To Historic Water Table:** Depth to the deepest water table depth (that contributed to a smear zone.)

**Depth To Bottom:** Depth from the surface to the bottom of the aquifer.

**Moisture Content:** Volumetric moisture content of soil must be less than the porosity.

**Porosity:** Fraction of void volume in vadose zone.

**Fraction Organic Carbon:** Typically below the root zone, the fraction organic carbon is 0.0001 to 0.001, but depends on soil type.

**Soil Temperature:** Historic ground water temperatures in the U.S. range from 3°C (37°F) to 25°C (77°F) and give a rough guide for soil temperatures (Figure 21).

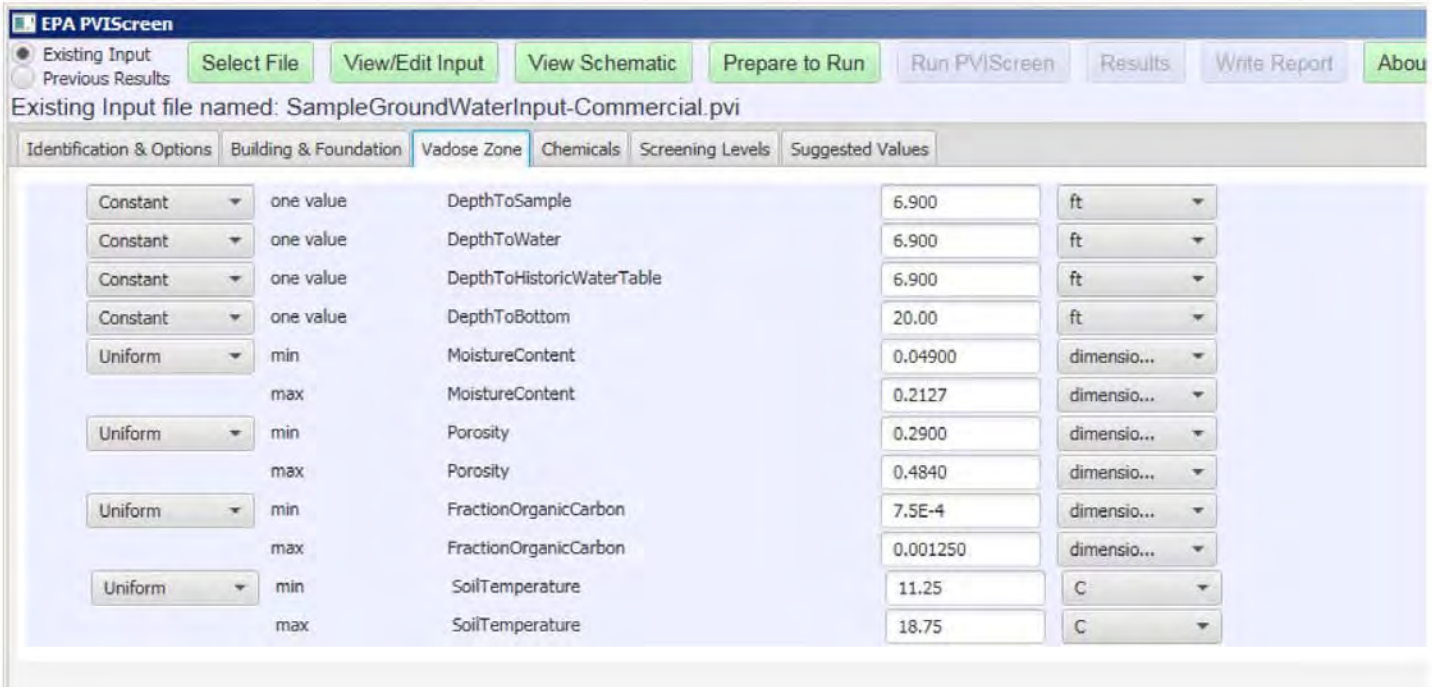


Figure 20. Vadose Zone input screen.

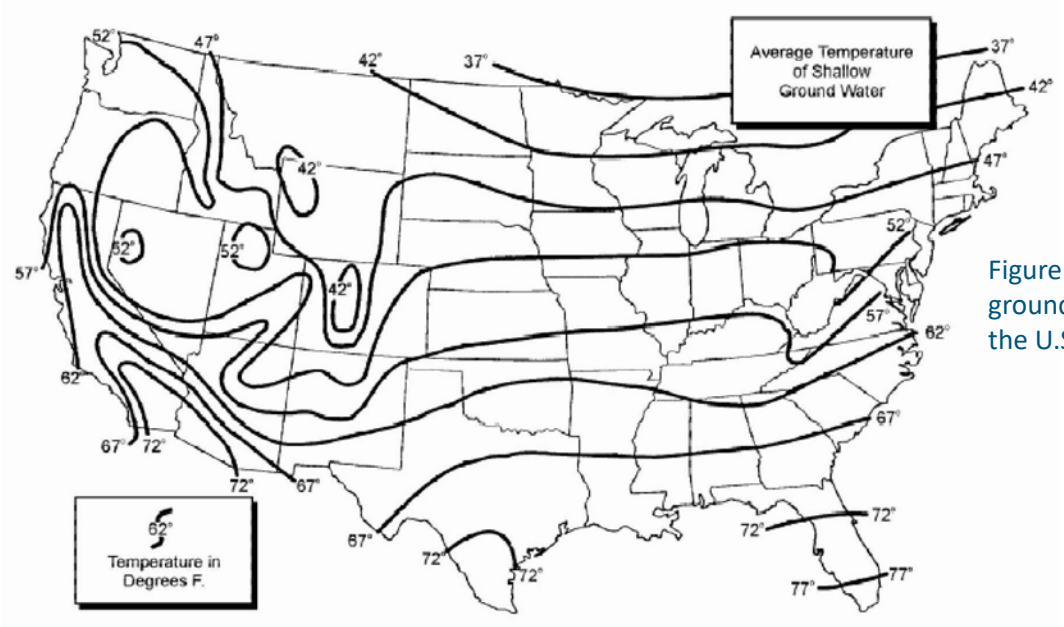


Figure 21. Average shallow ground water temperature in the U.S. (Collins, 1925).

#### 3.1.6.1 Suggested Values

Practitioners are unlikely to have ready access to some specialized parameters of the model, so suggested values are provided (Figure 22 through Figure 24).

#### 3.1.6.2 Suggested Values: Air Flow and Oxygen

On Figure 22:

**$Q_{soil}$:** US EPA (2003) gives a "typical" range for houses on coarse-grained soils is on the order of 1 to 10 L/min. In PVIScreen a second air flow parameter, the Air Flow Below Building, is set equal to $Q_{soil}$ based on the suggestion by API (2010).

**Soil Respiration Rate:** Estimated by DeVaull (2007) as 1.69 mg/g-d.

**Diffusion In Air:** The diffusion coefficient of oxygen in air, as estimated by the methods used in Lyman et al., 1982.

**Diffusion In Water:** The diffusion coefficient of oxygen in water, as estimated by the methods used in Lyman et al., 1982.

**Surface Concentration:** Value from atmospheric concentration of oxygen.

**Minimum Biodegradation Concentration:** The minimum concentration allowing biodegradation is taken as 1%.

#### 3.1.6.3 Suggested Values: Concentration Adjustment

The Suggested Values: Concentration Adjustment screen holds the value of the ground water concentration factor (Figure 23). This value is saved with the input data file and its selection is described in Section 3.1.5, "Treatment of Ground Water Samples".

#### 3.1.6.4 Suggested Values: Model Control

The Suggested Values: Model Control screen contains miscellaneous parameters which control the simulation and presentation of the results (Figure 24). Under normal circumstances, these should not be modified.

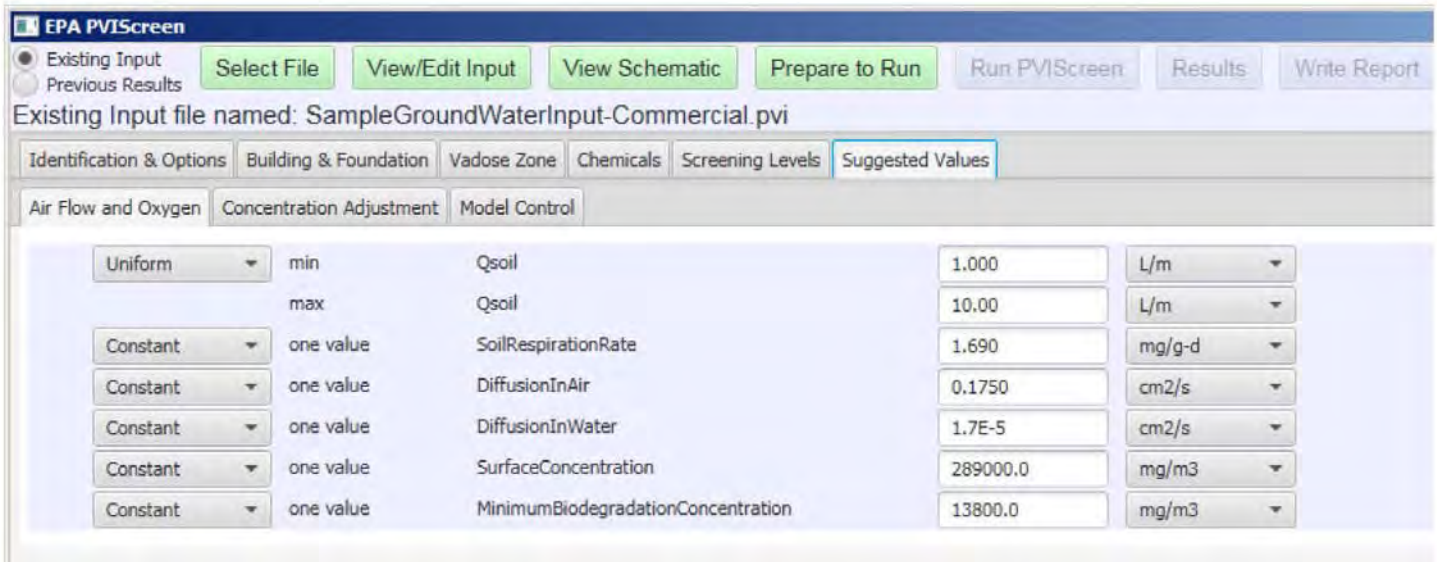


Figure 22. Suggested Values: Air Flow and Oxygen input screen.

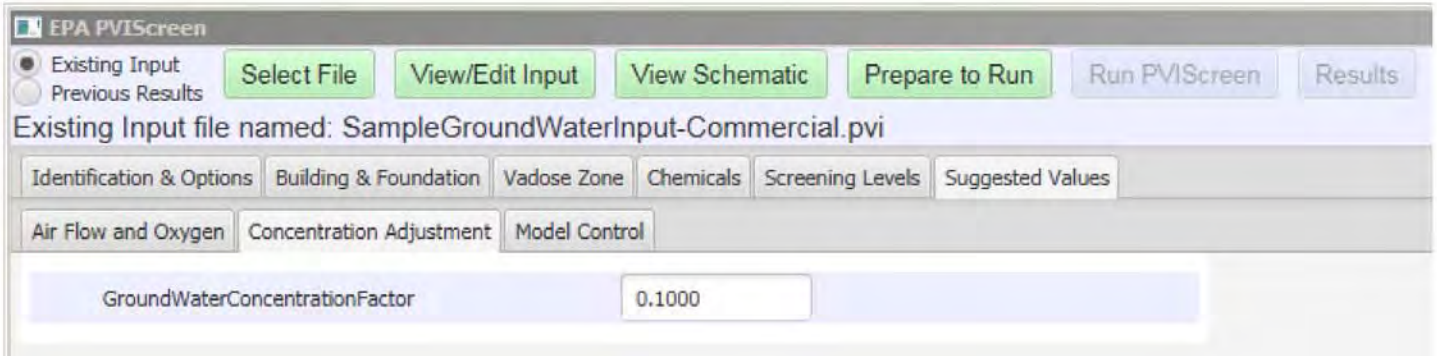


Figure 23. Suggested Value for the ground water concentration factor. This factor is applied to input ground water sample concentrations to generate the source term for PVIScreen. Section "Treatment of Ground Water Samples" discusses the rationale for selecting a value.

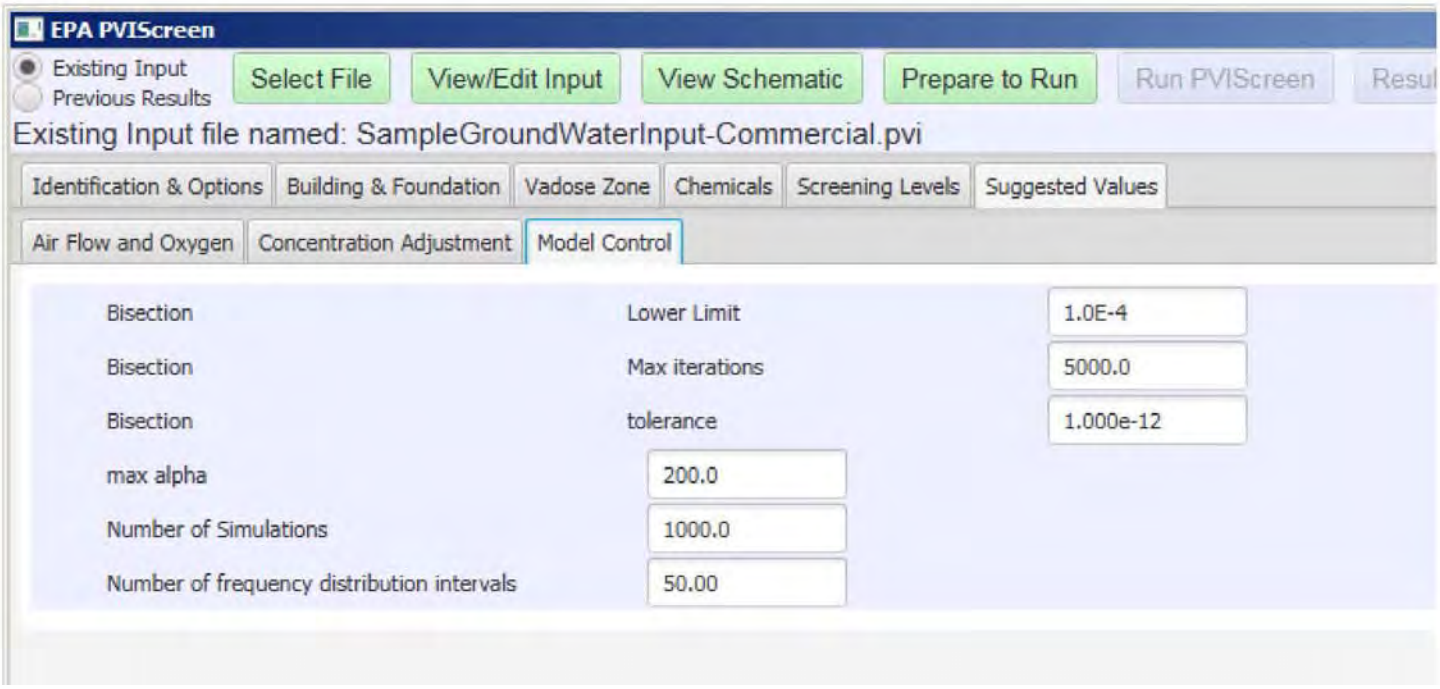


Figure 24. Suggested Values: Model Control input screen.

### *3.1.7 Preparing for Run*

After editing and saving the input file, the schematic should be viewed (Figure 25). The schematic shows the spatial relationships between the foundation, sample and water table. Once the spatial relationships and other data have been checked the "Prepare to Run" button completes preparation for running PVIScreen. If the input data have been changed, a dialog will ask to save changes to the input.

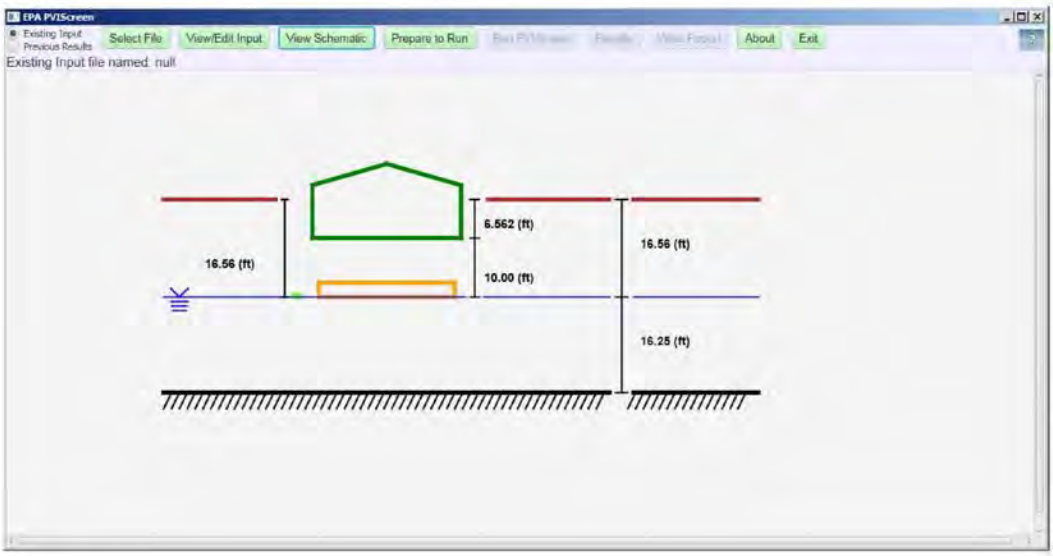


Figure 25. Schematic representation of spatial relationships in a PVIScreen run with a petroleum (NAPL) source.

### *3.1.8 Running PVIScreen*

After editing and checking the input file the "Run PVIScreen" button is used to execute the model (Figure 26). The interface automatically displays the Monte Carlo results when completed. A simulation is shown where none of the benzene simulation results exceeded the screening level (Figure 27).

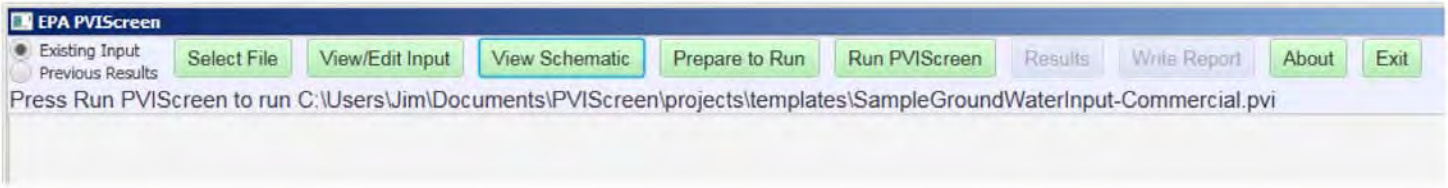


Figure 26. Running PVIScreen after an input file has been selected.

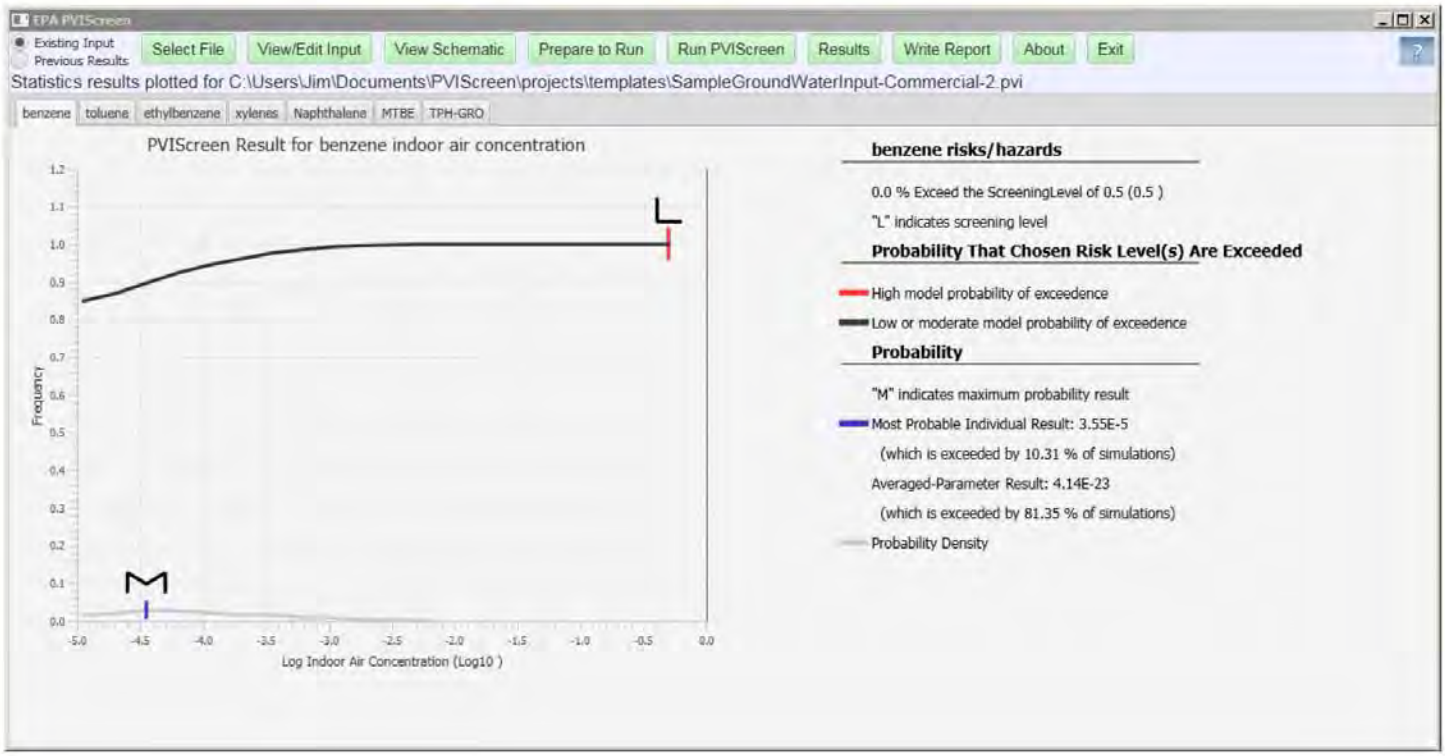


Figure 27. Result for simulation of benzene where petroleum vapor intrusion is unlikely. None of the simulations exceed the screening level of 0.5 as indicated by the "L" on the chart being located at a frequency of 1.0 and the notation in the righthand column that 0.0% of the simulations exceed the screening criteria.

### *3.1.9 Displaying and Understanding Statistics Output*

The model results are presented on separate tabs for each chemical in the simulation. Each tab has a list output (Figure 28) and a chart output (Figure 29), which summarize the same information.

#### 3.1.9.1 List Output

The list form of PVIScreen output gives first the percentage of simulations above the chosen screening level (Figure 28). Here the chemical is benzene, so there are cancer and non-cancer screening levels.

18.58% of the simulations exceeded the $1x10^{-6}$ screening level of 0.29 µg/m$^3$. All of the Monte Carlo simulations fell below the non-cancer hazard level of 30 µg/m$^3$, and no vapor intrusion is indicated by the non-cancer screening. Given the benzene result, the model is indicating a strong possibility of a vapor intrusion problem. Note that this example has a petroleum (NAPL) source fairly close to the bottom of the building (Figure 25).

The list output gives the result of maximum probability ("M") and the averaged-parameter result ("V"). The most probable result is close to the cancer screening level of 0.29 µg/m$^3$, and is another indicator that vapor intrusion could be a problem for this case. The averaged-parameter result is several orders of magnitude lower in concentration (0.00605 µg/m$^3$) and illustrates the necessity for the uncertainty analysis (as it misleadingly indicates no possibility for vapor intrusion).

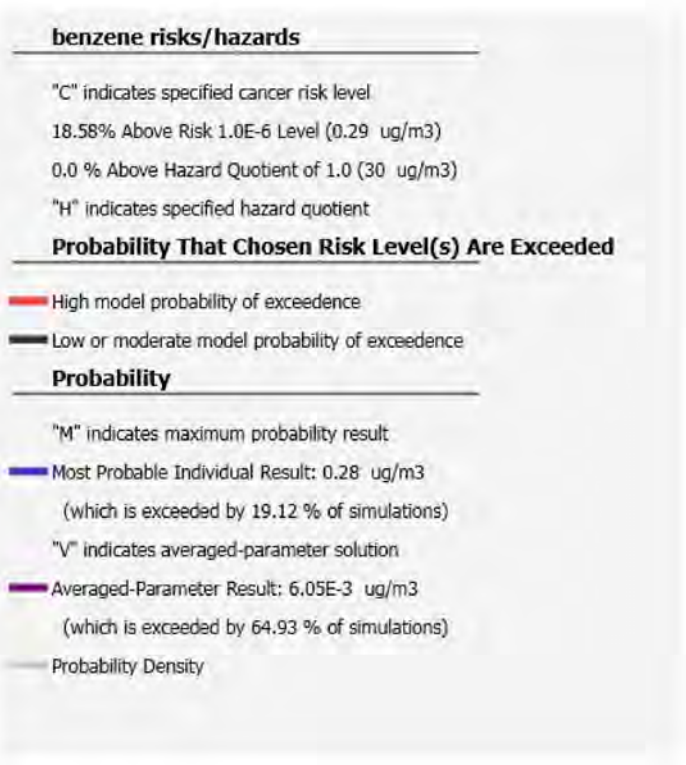


Figure 28. List Form of PVIScreen output.

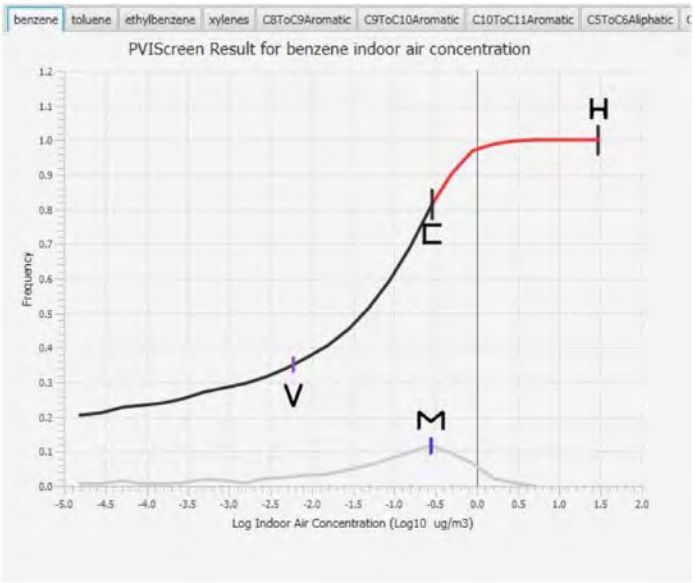


Figure 29. Graphical Form of PVIScreen Output for a case with high potential for vapor intrusion.

#### 3.1.9.2 Graphical Output

The graphical form of output consists of a cumulative probability curve and contains all of the results from the Monte Carlo simulation,[9] ranked from smallest to largest. Concentration is plotted on the horizontal axis and the corresponding cumulative probability (or frequency) is plotted on the vertical axis (Figure 29). Because the calculated indoor air concentrations range over many orders of magnitude in typical problems, the horizontal axis uses a log base 10 scale for concentration. The curve is marked for the cancer and non-cancer screening level concentrations; averaged-parameter and most probable results.

[9]Results with concentrations below $10^{-5}$ µg/m$^3$ are omitted as they are much less than measureable values.

### *3.1.10 Automated Report*

PVIScreen automatically generates a report (Figure 30 and Figure 31). The report is written in HTML and is automatically displayed in a browser window. The report summarizes the model assumptions, specific run information, tabular results and all choices of input parameters. Alternatively, the report can be viewed from a standard browser by double-clicking the html form of the simulation output (Figure 32).


Figure 30. PVIScreen options after simulation completed. Writing the automatically-generated report is now an available option.

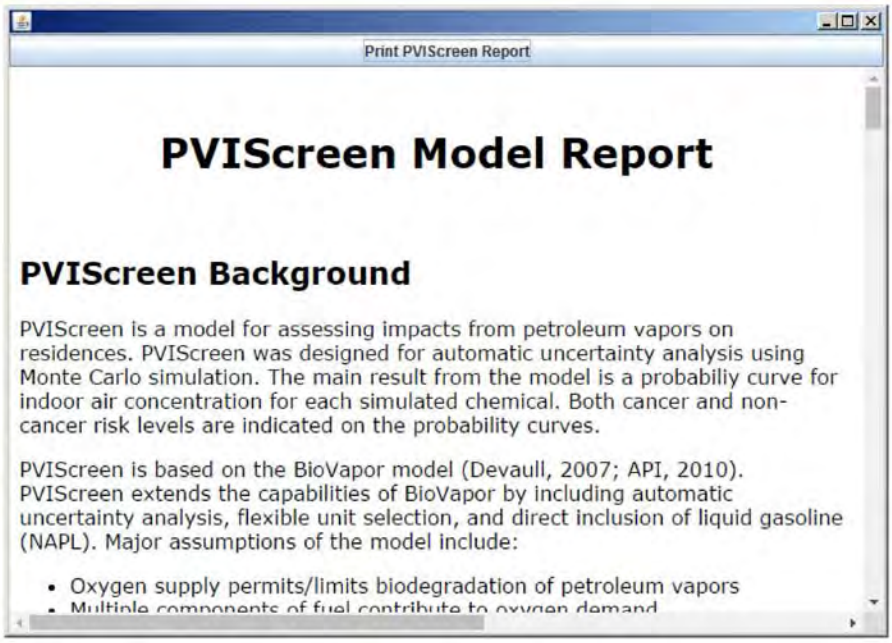


Figure 31. Example PVIScreen-generated report displayed in the User's browser window.

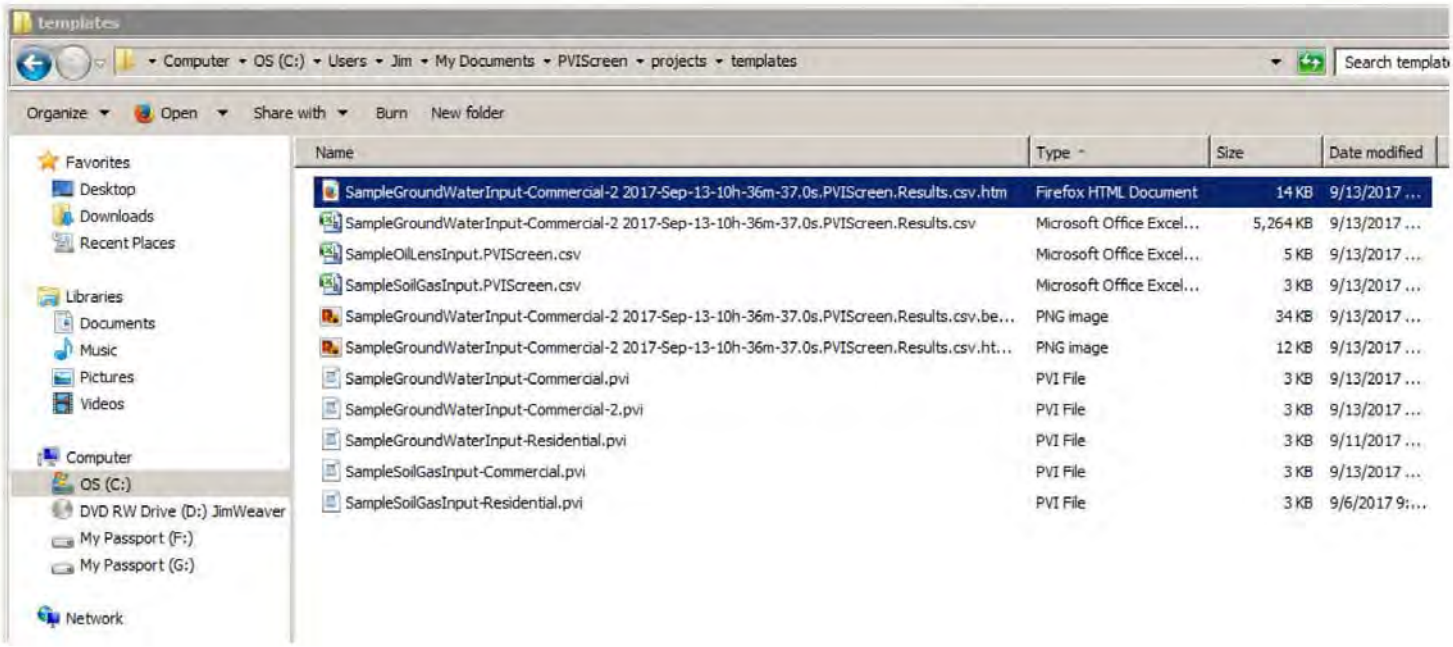


Figure 32. The highlighted HTML file (extension htm) contains an automated report summarizing the output from a run of SampleGroundWaterInput-Commercial.pvi made on 9/13/2017. Double clicking this file displays the report in a default browser.

# 4. Examples

## 4.1 Soil Gas Source Example

### *4.1.1 Site Investigation*

A site with a 2,000 ft$^2$ convenience store and adjacent 4,800 ft$^2$ restaurant (the "off-site restaurant") reported a release in August 2010 (Figure 33). The gas station was active with two 10,000 gallon and one 8,000 gallon tanks. The release was assumed to be from spills and overfills. Four field investigations were made between 2010 and 2015 with 22 monitoring wells and 7 borings made. The groundwater ranged from 5.5 ft to 7.5 ft deep (Figure 34). A 3 ft deep boring was made at the edge of the restaurant. Soil gas data from this boring was used as the source of contamination for the simulation (Table 2). Because the observed concentrations are low (1$^{st}$ row of Table 2), the model result is expected to show that there is a low possibility of vapor intrusion at this location. The complete input file can be found at ***projects/examples/LUSTLineRestaurantExample.pvi.***

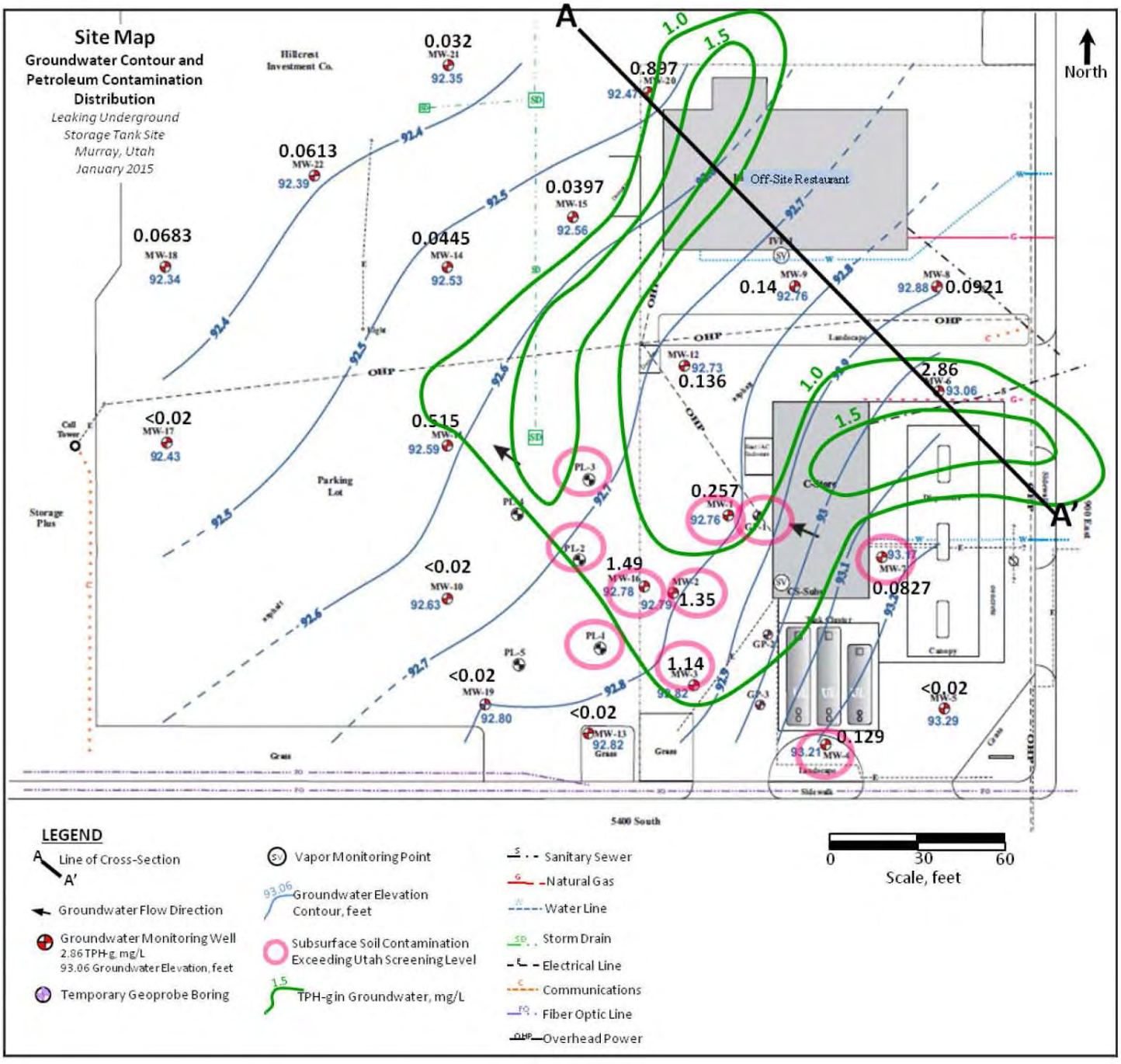


Figure 33. Site plan for the convenience store and off-site restaurant simulations.

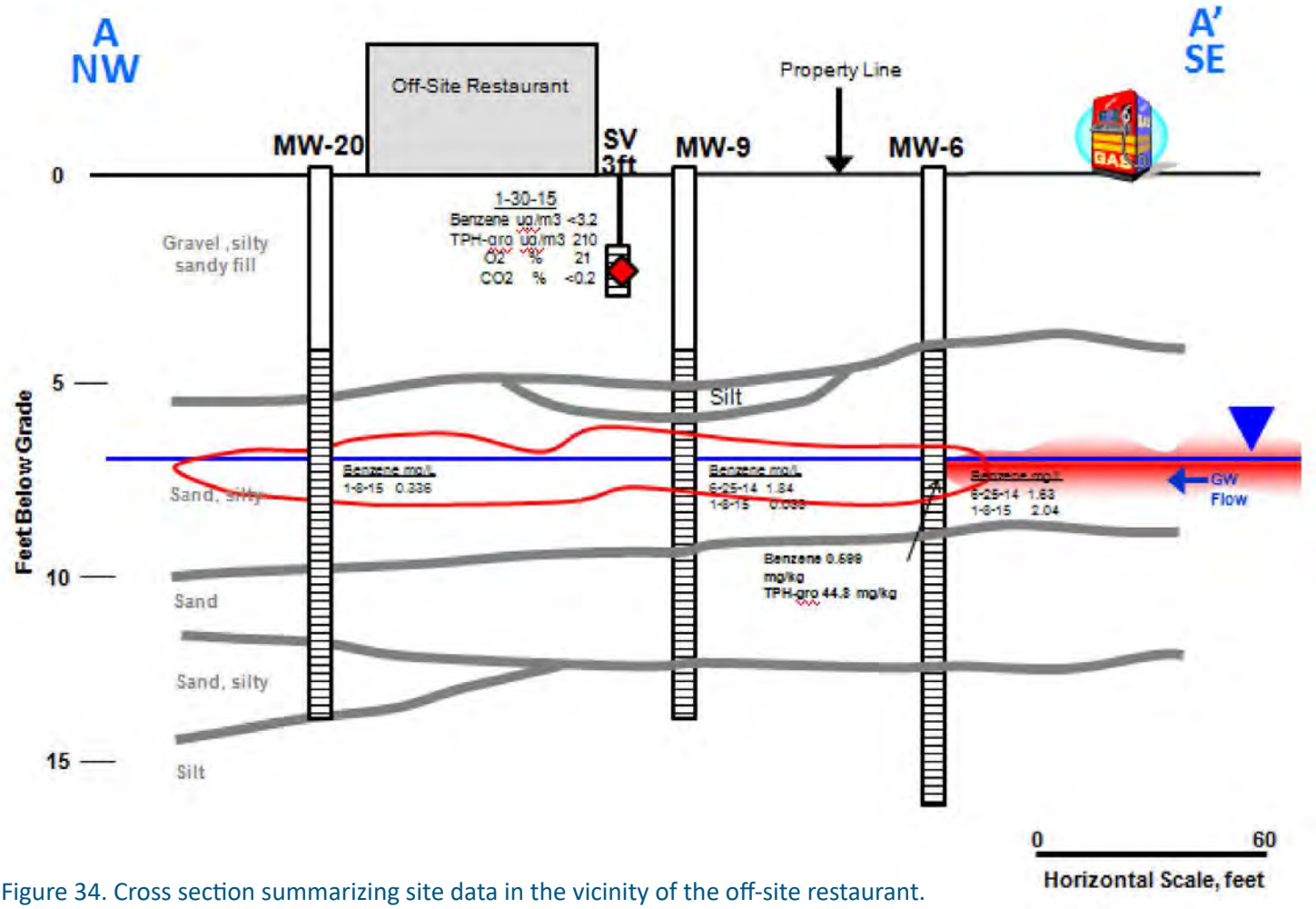


Figure 34. Cross section summarizing site data in the vicinity of the off-site restaurant.

Table 2. Field results, PVIScreen input concentrations and Utah DEQ screening levels for the Off-Site Restaurant simulation.

| ID | Sample Depth (ft) | Benzene (µg/m³) | Toluene (µg/m³) | Ethylbenzene (µg/m³) | Total Xylenes (µg/m³) | Naphthalene (µg/m³) | TPH-GRO (µg/m³) | MTBE (µg/m³) |
|---|---|---|---|---|---|---|---|---|
| SVP-1 | 3 | < 3.2 | 10 | < 4.4 | 41 | < 5.3 | 210 | < 3.6 |
| PVIScreen Input | 3 | 1.6 | 10 | 2.2 | 41 | 2.85 | 210 | 1.8 |
| Utah DEQ Screening Levels, indoor air, commercial | n/a | 0.5 | 7310 | 1480 | 148 | 4.39 | 307 | 4380 |

### 4.1.2 PVIScreen Model Parameters

The input parameters for simulation are shown in Figures 35 to 39. The width and length of the building was entered as measured (60 ft x 80 ft), the ceiling height was assumed to be 9 ft, and thickness of foundation 10 cm. The crack width was considered as a variable parameter, using a US EPA range of values (0.5 mm to 5.0 mm). The air exchange rate was set to a range of 3 $hr^{-1}$ to 10 $hr^{-1}$ to represent commercial buildings (Figure 36).

Site-specific values were entered for the depth to sample (3 ft), and depth to water (7.5 ft). The other vadose zone parameters were given wide ranges as site-specific values were not available (Figure 37).

The source of contamination was taken to be the soil gas data from the 3 ft deep boring at the edge of the building (SVP-1 on Figure 33). Concentration values reported at less than the reporting limit were set to half the reporting limit (Table 2 and Figure 38). Site-specific screening levels were calculated from Guidelines for Utah's Corrective Action Process for Leaking Underground Storage Tank Sites (Utah, 2010) and used as input (Figure 39).

### 4.1.3 PVIScreen Model Results

The PVIScreen simulation showed that all runs of the model were below the screening level of 0.5 µg/$m^3$ for benzene (Figure 40). Although not shown, the same result was found for each of the other chemical constituents. Therefore, the model results suggest that there is a very low chance of vapor intrusion at the restaurant.

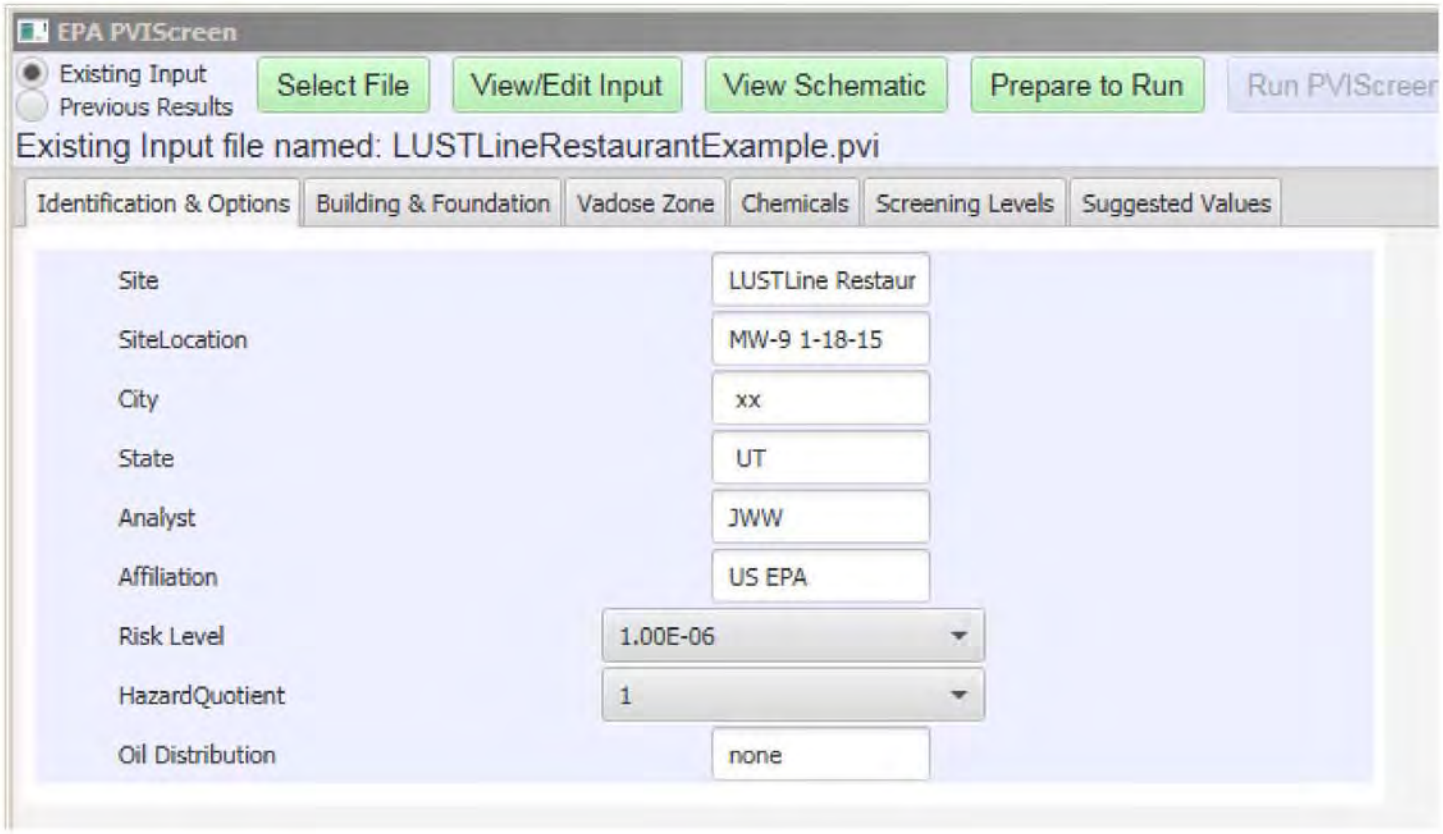


Figure 35. Identifications and Options input screen for the off-site restaurant simulation.

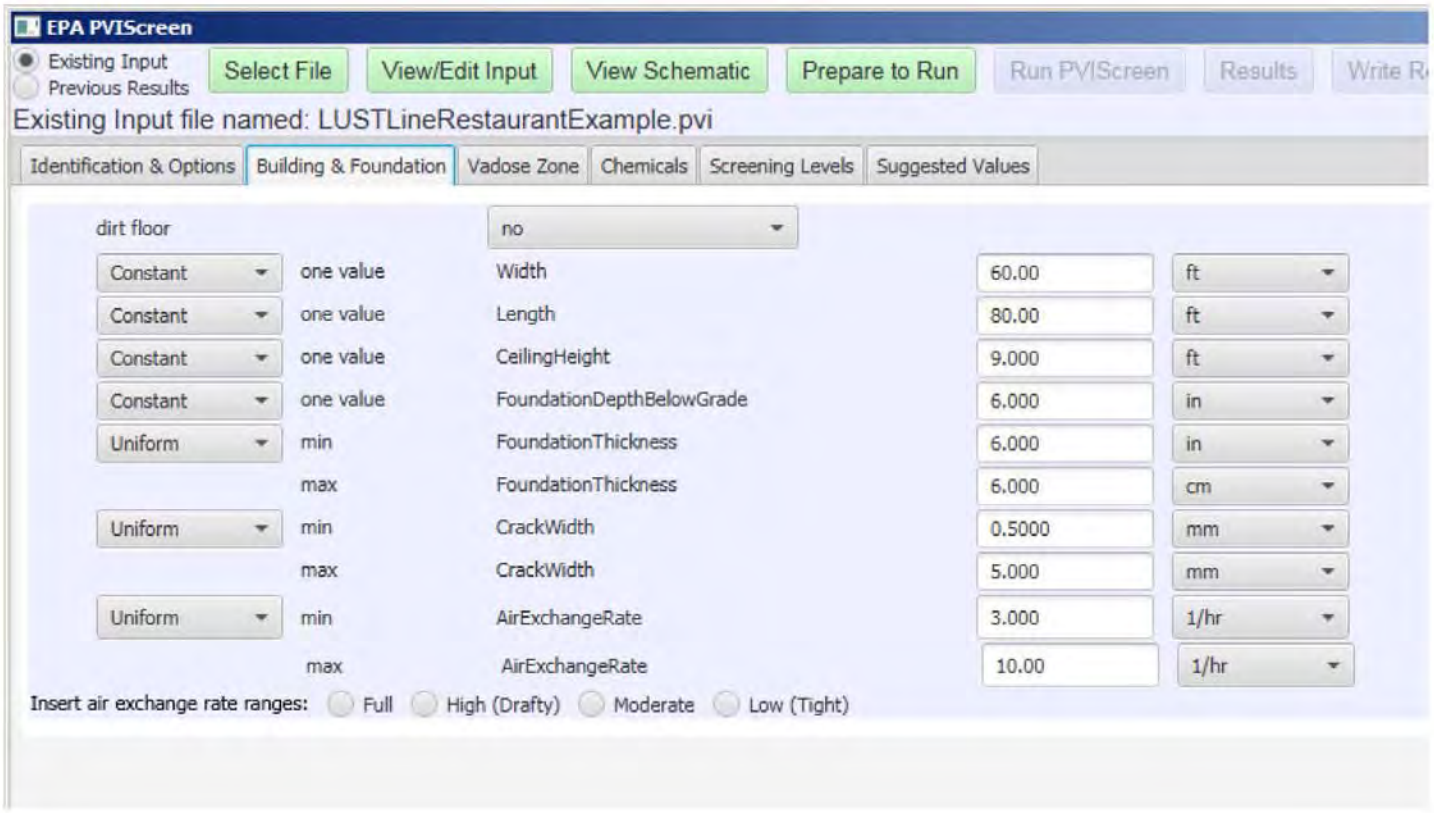


Figure 36. Building and Foundation input screen for the off-site restaurant simulation.

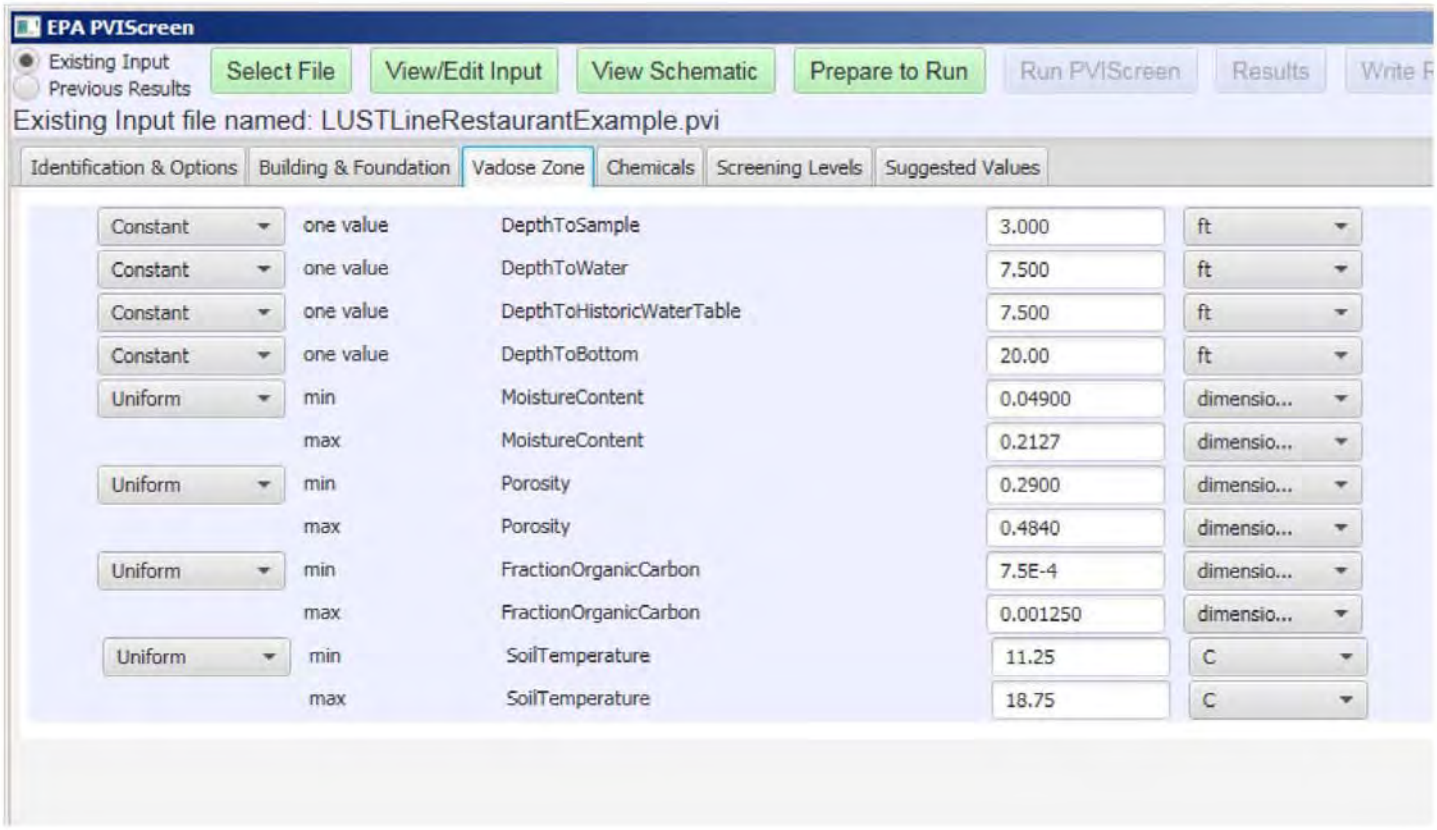


Figure 37. Vadose Zone input screen for the off-site restaurant simulation.

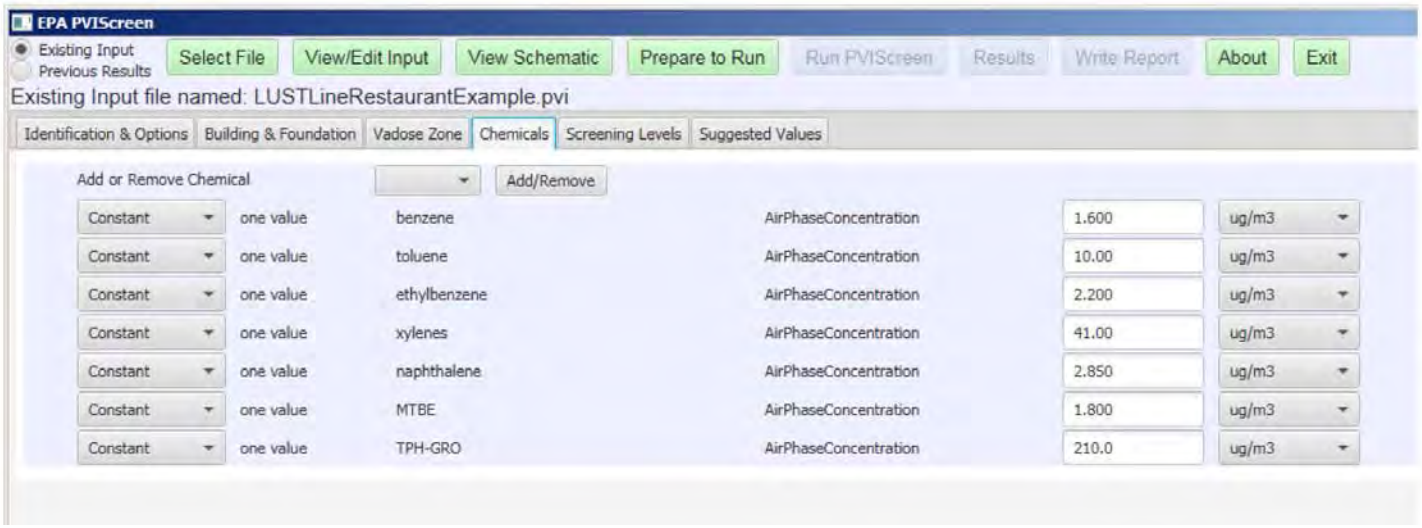


Figure 38. Chemicals input screen for the off-site restaurant simulation.

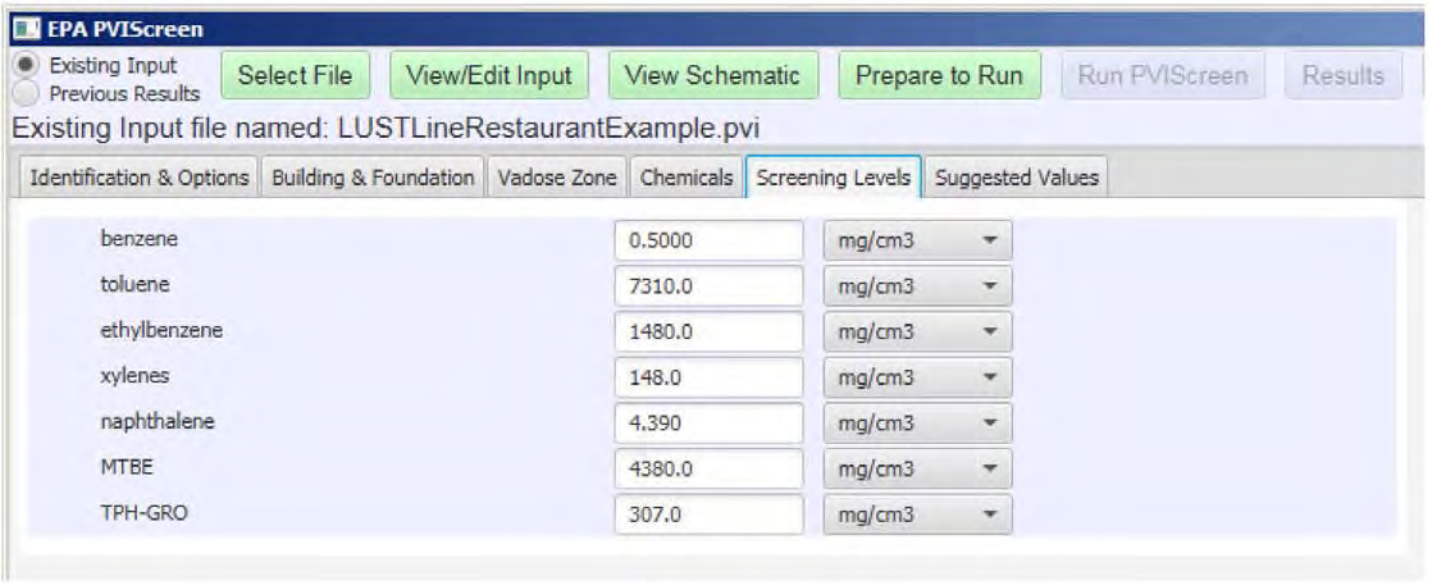


Figure 39. Screening Levels input screen for the off-site restaurant simulation.

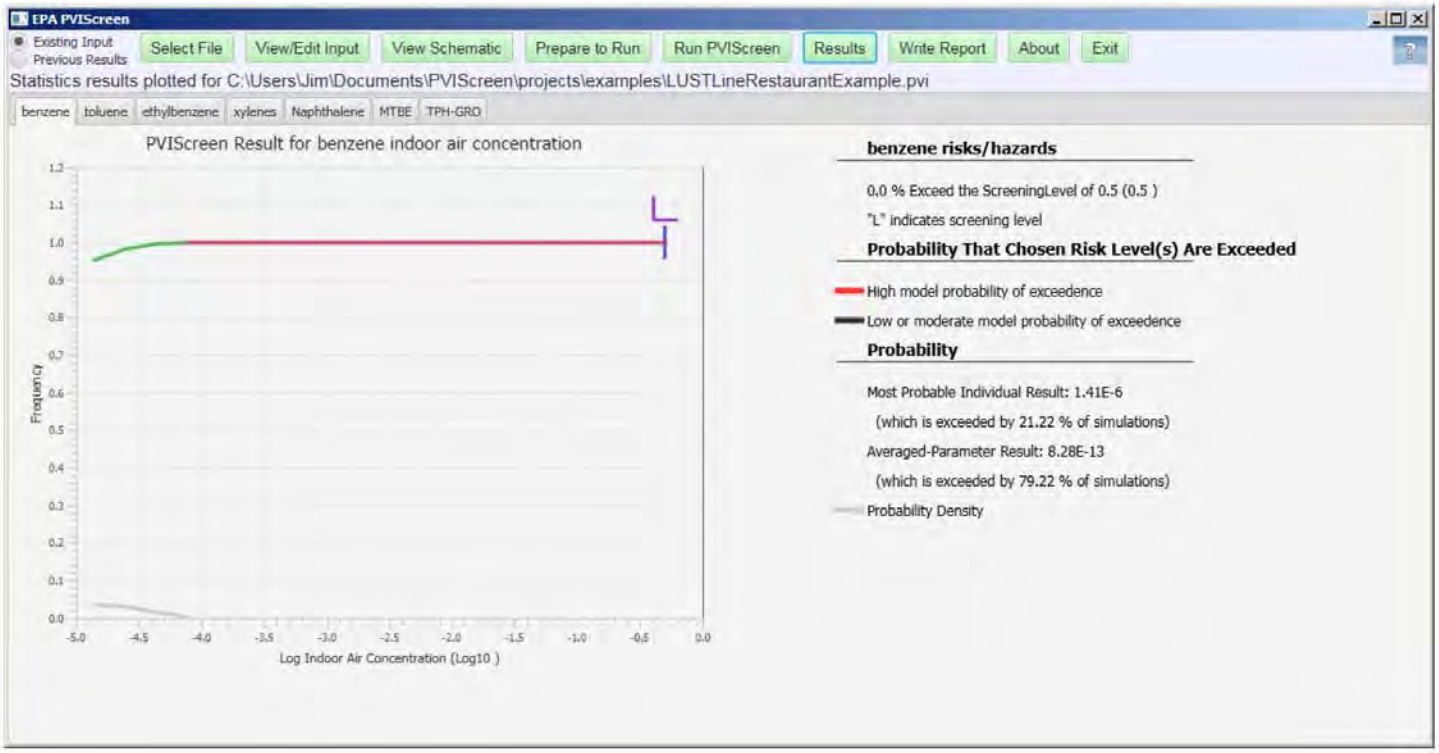


Figure 40. Off-site restaurant simulation of benzene showing no simulation results above the screening level of 0.5 µg/m$^3$. The most probable and averaged-parameter results are below the minimum plotting concentration of $10^{-5}$ µg/m$^3$.

## 4.2 Ground Water Data Example

The restaurant simulation can also be run using ground water data. The chemical concentrations, their type (i.e., water phase concentration), and depths differ from the previous simulations; all the other parameters were unchanged. The location of the monitoring wells relative to the building guides the selection of the data to drive the model simulation. MW-9 is the closest monitoring well that is upgradient to the building. This well is close to the building, but between the contamination and the building and is the best choice of these for use in the model. MW-20 is downgradient and might be less representative of the potential exposure in the building. MW-6 is located just on the edge of the source, with benzene concentration characteristic approaching that of NAPL[10]. For comparison purposes the results of simulation with all three wells is presented below. The schematic and result for MW-9 with 10 x ground water adjustment factor are shown in Figure 41 and Figure 42.

For comparison purposes data from each of the monitoring wells was used in simulation (highlighted in Table 3). The results from MW-9 (Table 4) show that none of the simulations indicated the possibility of vapor intrusion above the screening level. This was the result for both ground water reduction factors. (Note that if the results show no impact for a reduction factor of 10, the result when using the reduction factor of 100 must also show no impact as the condition is less stringent). Similar results were obtained in this case for MW-20.

For MW-6, which lies on the edge of the NAPL zone (Figure 34), at the reduction factor of 10, a very small number of simulations (0.12%) exceed the screening level for benzene. At the reduction factor of 100, none exceed the screening level. Accepting the conceptualization of the model, in this case the occurrence of an impact depends on the nature of transport across the capillary fringe. Since the true nature of that transport is unknown from the available data, a policy decision is needed for dealing with borderline cases as this. The case is borderline because only a very few simulations exceed the screening level (0.12%), and because the ground water concentration reduction factor of 100 results in 0.0% exceedance.

[10]In the EPA PVI benzene concentrations >5 mg/L are presumed to indicate NAPL. Peargin & Kolhatkar presume the presence of NAPL for benzene concentration of 1 mg/L or higher.

| Table 3. Ground water data for MW-6, MW-9, and MW-20 of Figure 34. | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Well/ Elev. | Date | DTW (feet) | MTBE (mg/L) | Benzene (mg/L) | Toluene (mg/L) | Ethylbenzene (mg/L) | Xylenes (mg/L) | Naphthalene (mg/L) | TPH-GRO (mg/L) |
| **MW-6** | | | | | | | | | |
| 99.57 | 2/18/11 | 5.35 | < 0.00200 | 2.73 | 0.181 | 0.183 | 0.433 | 0.138 | 4.58 |
| | 7/11/11 | 5.29 | < 0.00200 | 1.58 | 0.0635 | 0.136 | 0.231 | 0.129 | 3.10 |
| | 12/4/12 | 6.15 | < 0.00200 | 1.93 | 0.00455 | 0.0141 | 0.0276 | 0.130 | 2.67 |
| | 12/19/13 | 6.61 | < 0.00200 | 0.590 | < 0.00200 | 0.00803 | 0.0129 | 0.0786 | 1.02 |
| | 6/25/14 | 6.08 | < 0.00200 | 1.63 | 0.0254 | 0.0979 | 0.171 | 0.0974 | 2.76 |
| | **1/8/15** | **6.51** | **< 0.00200** | **2.04** | **0.00404** | **0.0179** | **0.0296** | **0.180** | **2.86** |
| **MW-9** | | | | | | | | | |
| 99.66 | 12/20/13 | 7.18 | < 0.00200 | 0.813 | < 0.00200 | < 0.00200 | 0.0298 | 0.0136 | 1.29 |
| | 6/25/14 | 6.47 | < 0.00200 | 1.84 | 0.00260 | 0.00268 | 0.00515 | 0.0160 | 2.40 |
| | **1/8/15** | **6.90** | **< 0.00200** | **0.0330** | **< 0.00200** | **< 0.00200** | **< 0.00200** | **< 0.00200** | **0.140** |
| **MW-20** | | | | | | | | | |
| 98.90 | **1/9/15** | **6.43** | **< 0.00200** | **0.336** | **< 0.00200** | **< 0.00200** | **0.0126** | **0.0349** | **0.897** |

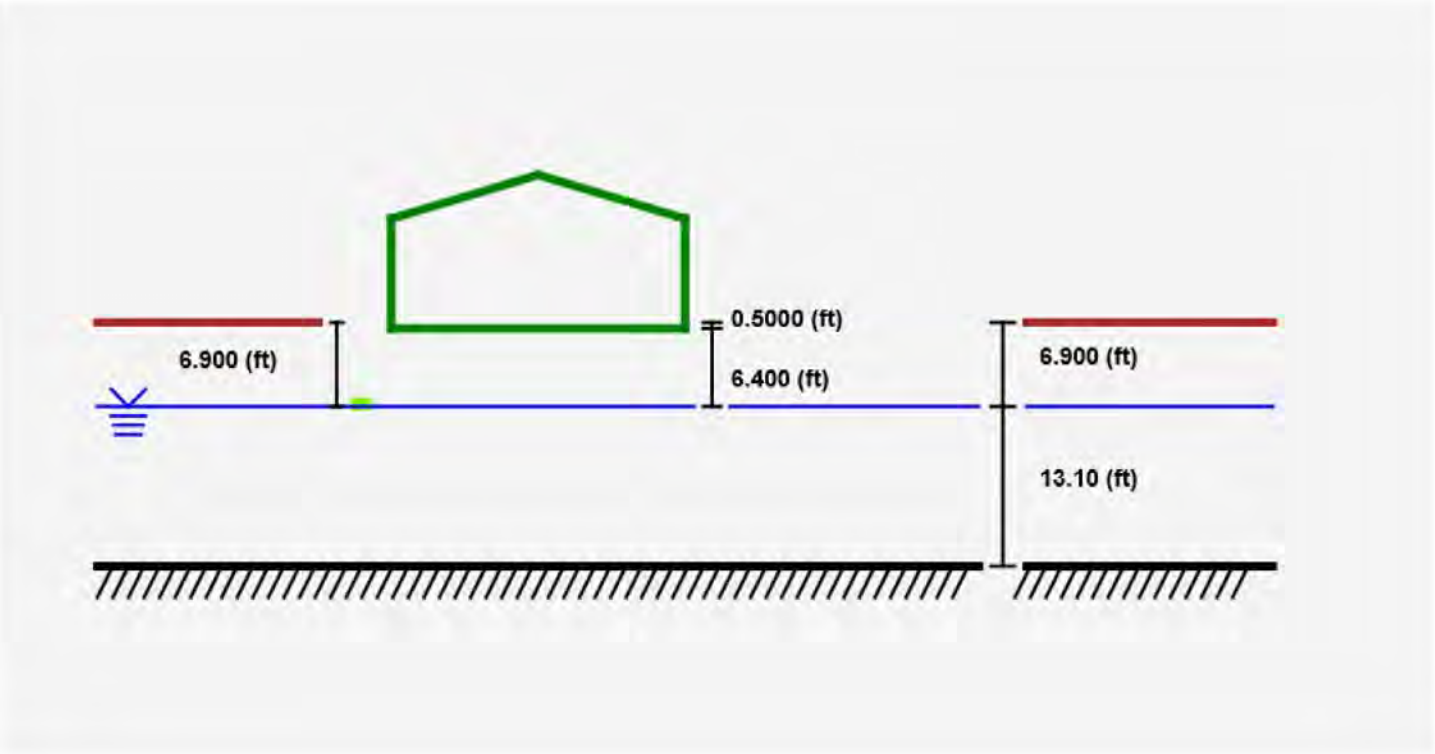


Figure 41. Schematic for the MW-9 simulation with sample depth of 6.9 ft.

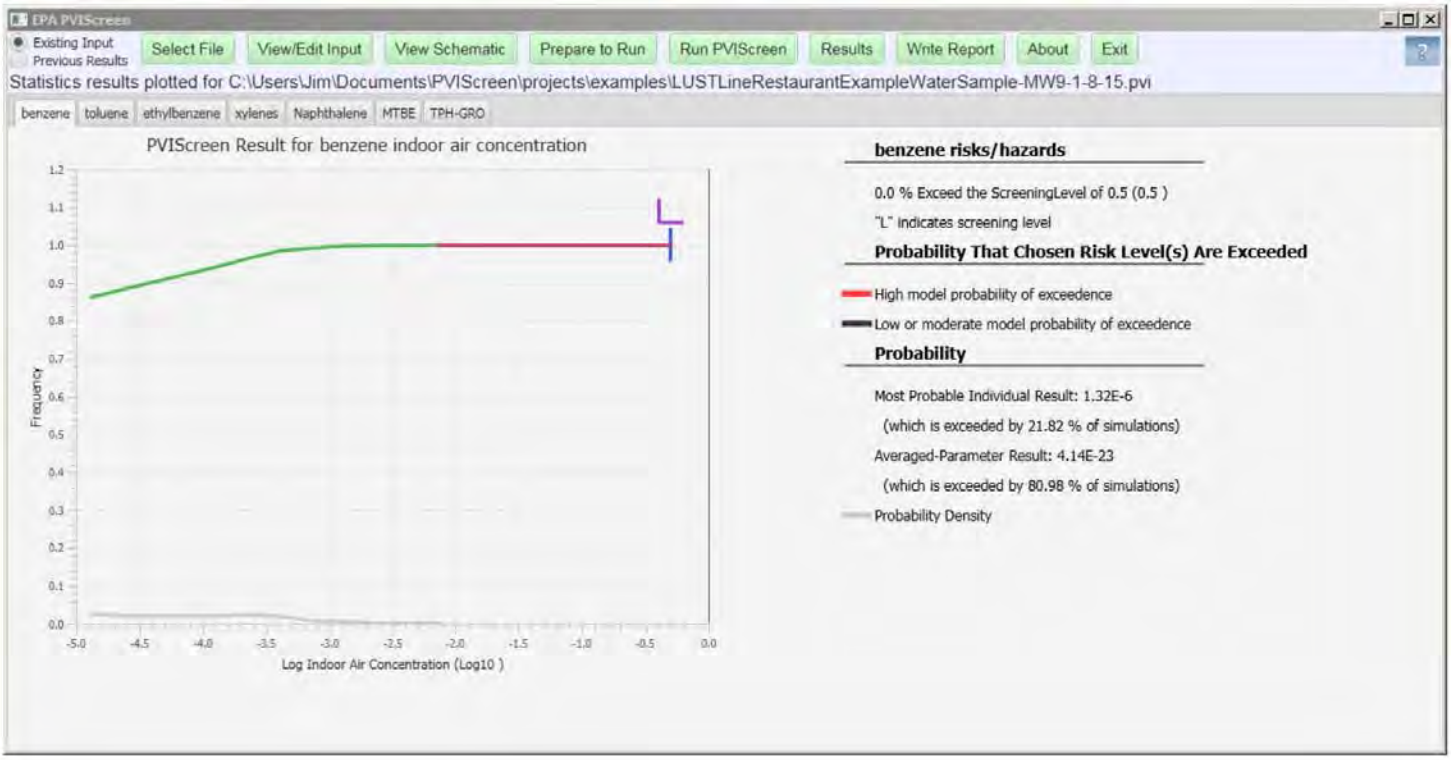


Figure 42. Simulation results for MW-9 using ground water data.

Table 4. Benzene simulation results for the restaurant with ground water concentration data as the source of contamination.

| Ground Water Data | Simulations Exceeding Screening Level |
|---|---|
| MW-6 | 0.12% |
| MW-9 | 0.0% |
| MW-20 | 0.0% |

## 4.3 Ground Water Example Indicating Possibility of Vapor Intrusion

The Utah Department of Environmental Quality (UDEQ) investigated potential petroleum vapor intrusion at a convenience store, where leaking underground storage tanks (USTs) released gasoline into soil and groundwater (Figure 43). The potential for PVI was determined highly likely due to presence of free product less than 15 feet below ground surface (bgs) under the site convenience store, and extremely high subslab vapor concentrations of total petroleum hydrocarbons (TPH) and benzene. PVI was ultimately confirmed through collection of indoor air samples from the convenience store in April 2015, which indicated the presence of TPH, benzene, and other gasoline component vapors at concentrations that exceeded risk-based screening levels (see Table 6, Figure 44, and Davis (2015) for site details and a summary of the site investigation).

Analyte concentrations from MW-4 taken on 10/2/2013 were used to drive the simulation. Since these concentrations were high the possibility exists for an impact to indoor air. The input parameter values are found on Figure 45 to Figure 47, and the site schematic is shown on Figure 48. The model results are suggestive of petroleum vapor intrusion with 69% of the benzene (Figure 49), 69% of the TPH-GRO (Figure 50), and 21% of the TPH-DRO (Figure 51) simulations indicating the potential for petroleum vapor intrusion. These results are consistent with the state's findings (Table 6).

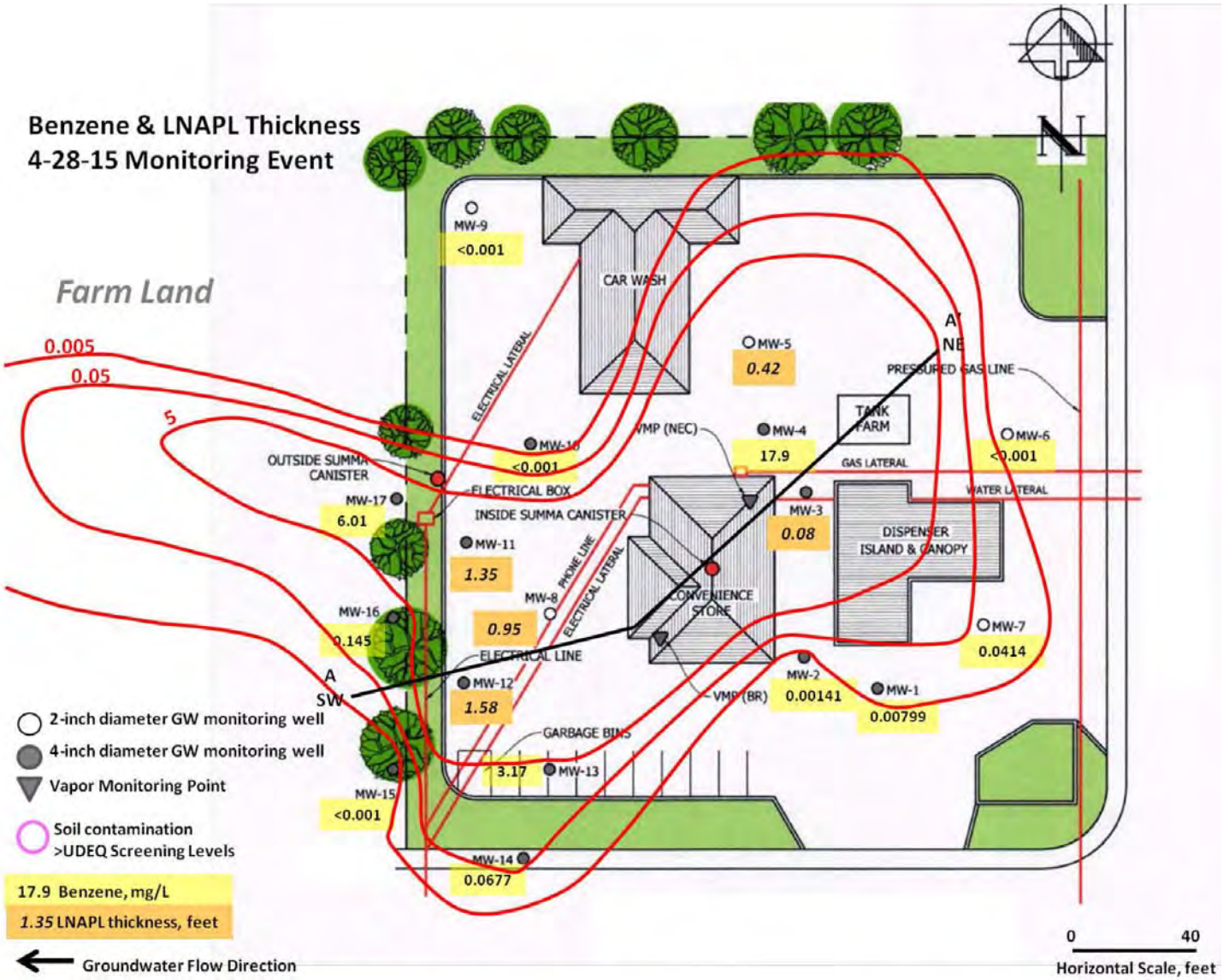


Figure 43. Site plan indicating benzene concentration and free product thicknesses for April 28, 2015.

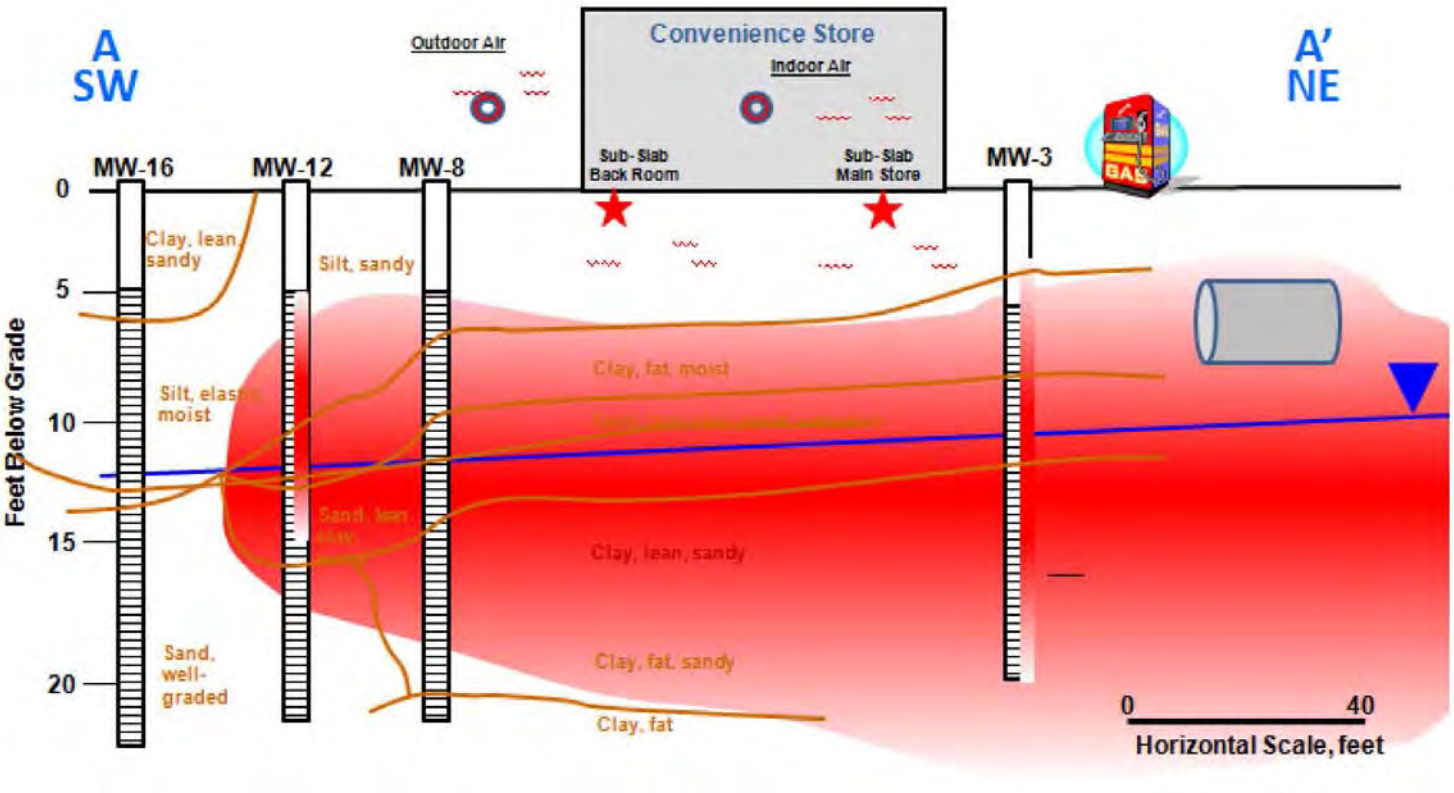


Figure 44. Cross section summarizing site data in the vicinity of the convenience store.

Table 5. Ground water sampling data from MW-3 and MW-4 when no free product was present.

| Date | Benzene (mg/L) | Toluene (mg/L) | Ethylbenzene (mg/L) | Xylenes (mg/L) | Naphthalene (mg/L) | MTBE (mg/L) | TPH-GRO (mg/L) | TPH-DRO (mg/L) | Depth to Water (ft) |
|---|---|---|---|---|---|---|---|---|---|
| **MW-3** | | | | | | | | | |
| 10/2/13 | 39.4 | 49.0 | 3.26 | 17.2 | 0.688 | < 0.2 | 118 | 0.396 | 9.78 |
| 5/3/13 | 13.4 | 12.6 | 0.929 | 5.76 | 0.239 | < 0.2 | 34.2 | < 0.2 | 10.09 |
| **MW-4** | | | | | | | | | |
| 4/28/15 | 17.9 | 0.774 | 2.51 | 10.5 | 0.246 | < 0.02 | 33.1 | < 2.0 | 11.16 |
| 10/2/13 | 26.1 | 53.1 | 3.76 | 17.4 | 0.426 | < 0.04 | 128 | < 0.4 | 9.88 |
| 5/3/13 | 28.6 | 42.9 | 1.92 | 11.1 | < 1.0 | < 1.0 | 84.4 | < 10.0 | 10.2 |

| Table 6. Sub-slab, indoor air, and screening concentrations for the Utah convenience store. | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | Benzene (µg/m³) | Toluene (µg/m³) | Ethylbenzene (µg/m³) | Xylenes (µg/m³) | Naphthalene (µg/m³) | MTBE (µg/m³) | TPH-GRO (µg/m³) | TPH-DRO (µg/m³) |
| **Results** | | | | | | | | |
| 8-hour indoor air | 55 | 13 | 2 | 12 | < 0.53 | < 0.73 | 2,200 | |
| 24-hour indoor air | 210 | 14 | 4 | 25 | < 2.7 | < 3.6 | 6,400 | |
| Sub-slab main store | 333,000 | < 20,000 | < 10,000 | < 10,000 | < 2,000 | < 10,000 | 8,700,000 | |
| Sub-slab back room | 690 | < 4,000 | < 2,000 | < 2,000 | < 400 | < 2,000 | 420,000 | |
| **Screening Levels** | | | | | | | | |
| Commercial Indoor Air | 0.5 | 7,154 | 1,482 | 148 | 4 | 4,395 | 307 | 307 |
| Commercial Sub-slab | 16.4 | 243,667 | 49,333 | 4,933 | 146 | 146,000 | 10,233 | 10,233 |

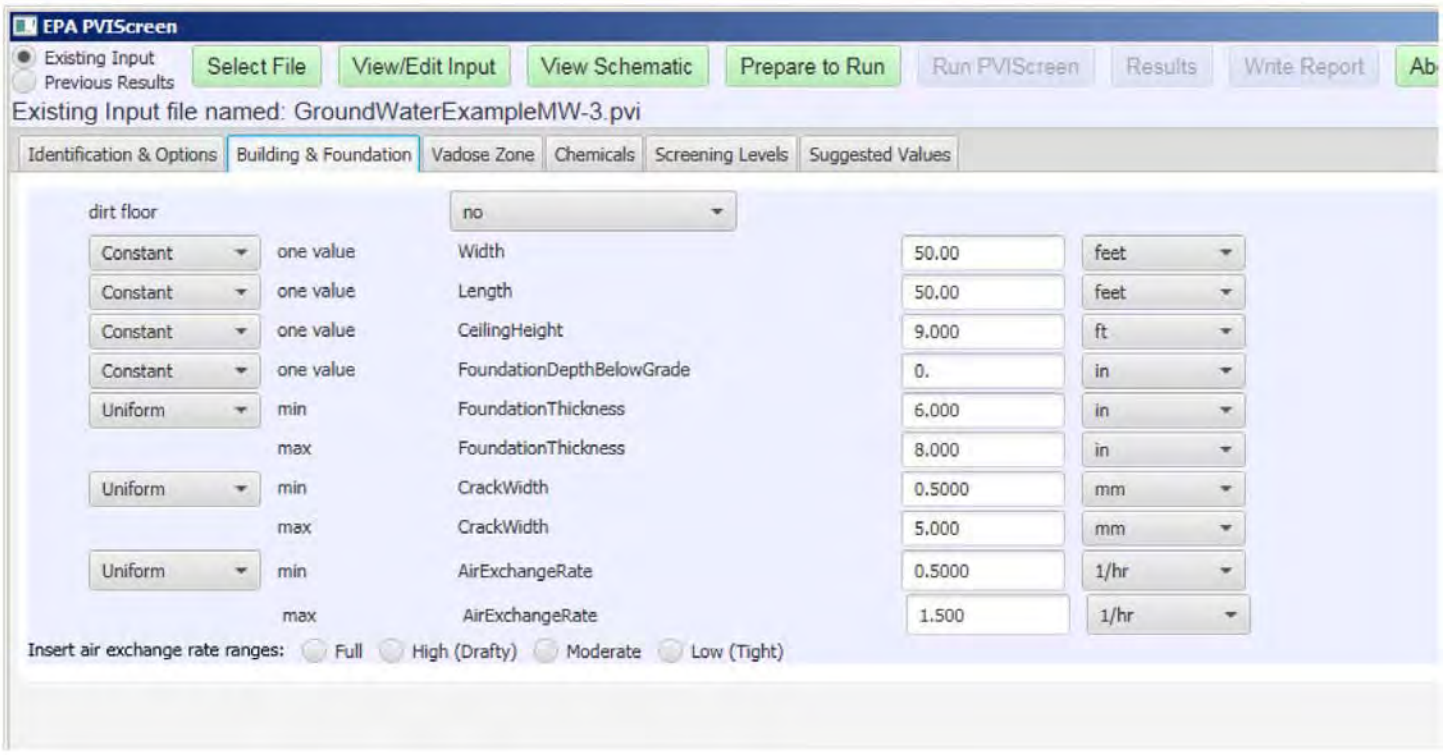


Figure 45. Building and foundation input parameters for convenience store simulation.

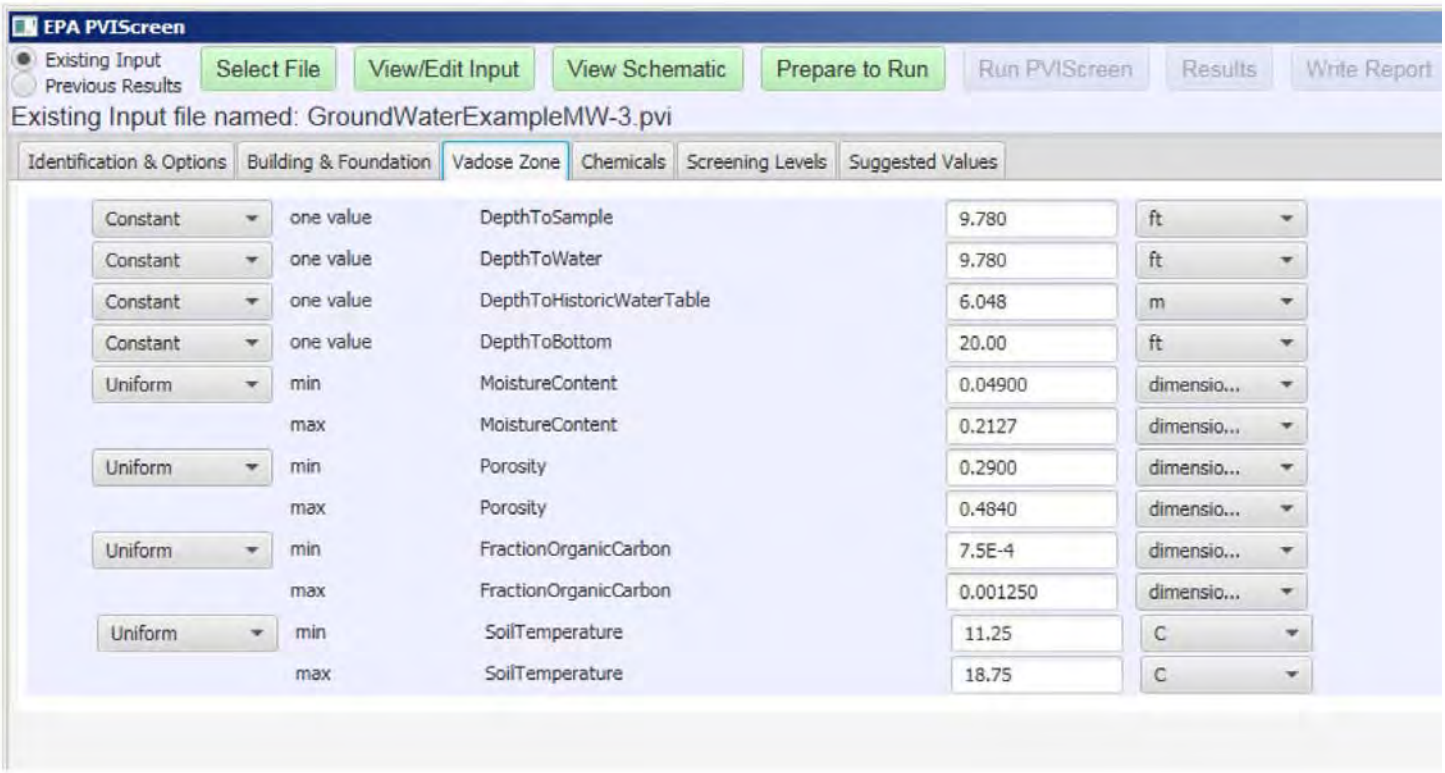


Figure 46. Vadose zone inputs for convenience store simulation.

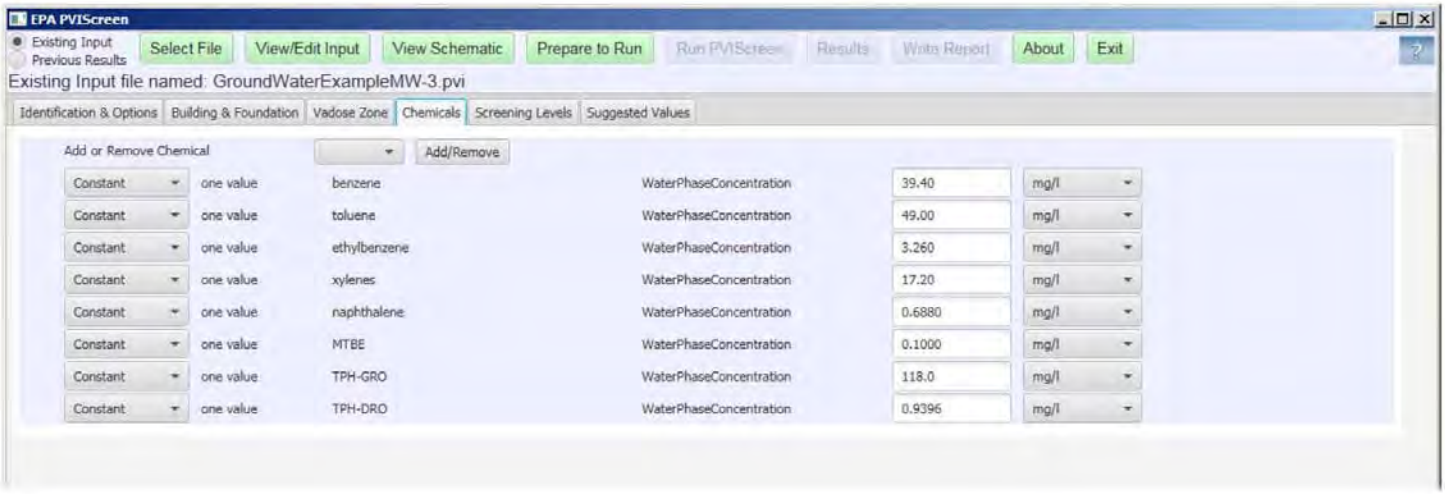


Figure 47. Chemical inputs for convenience store simulation.

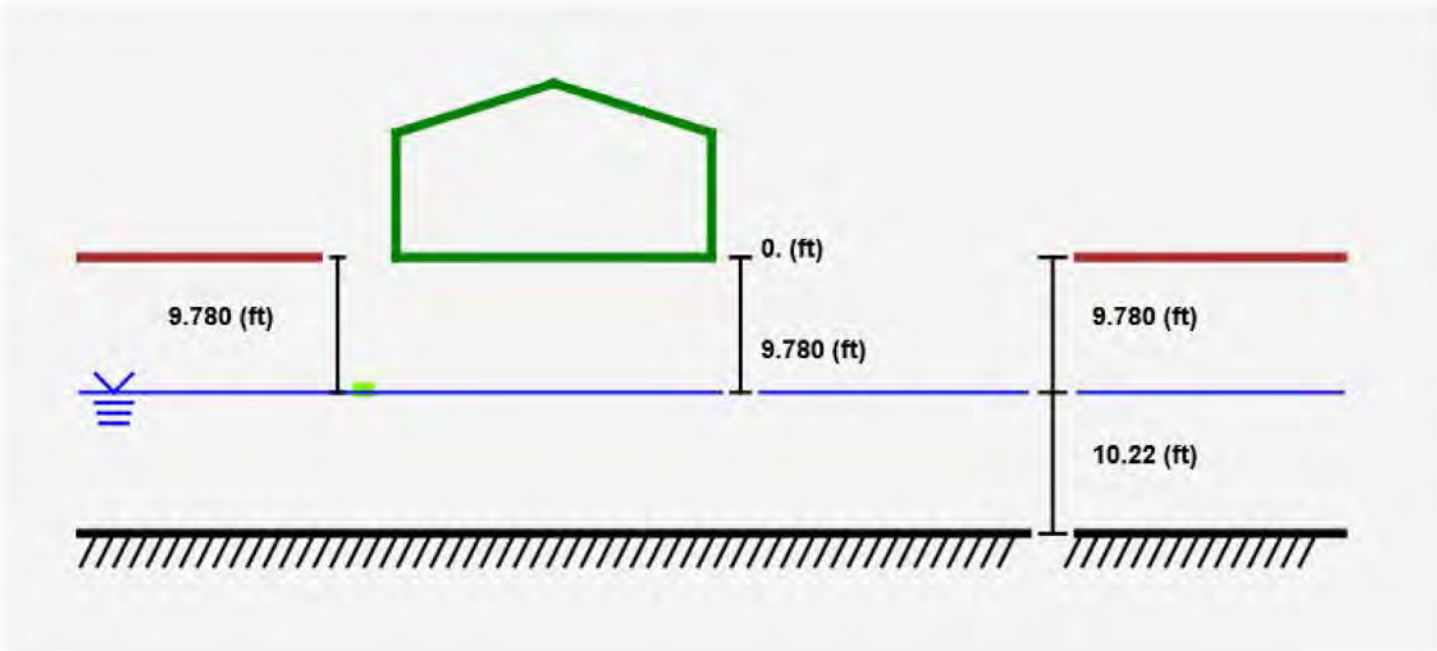


Figure 48. Schematic for simulation of convenience store.

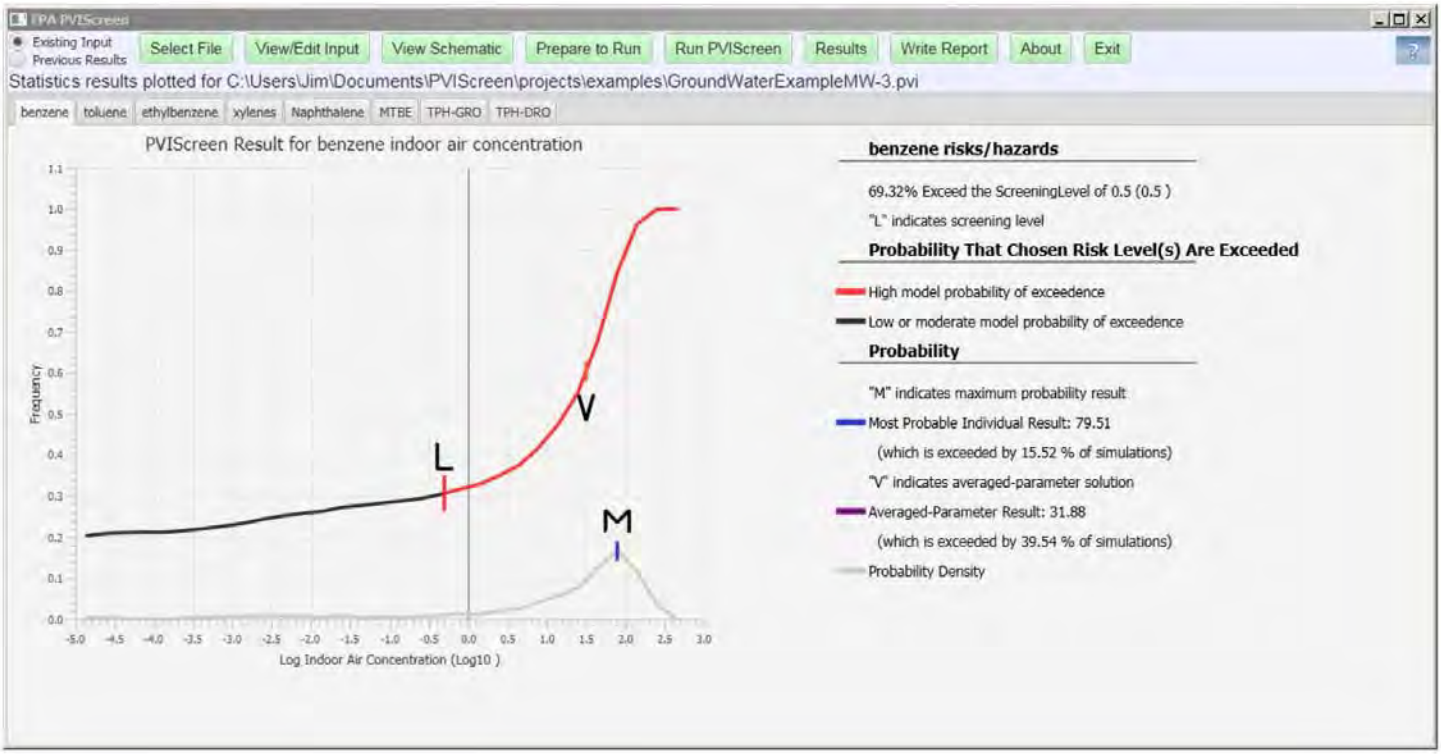


Figure 49. Benzene results indicating high probability for petroleum vapor intrusion. As indicated on the graph (left) and the table (right), 69% of the simulations exceeded the site-specific screening level of 0.5 µg/m$^3$.

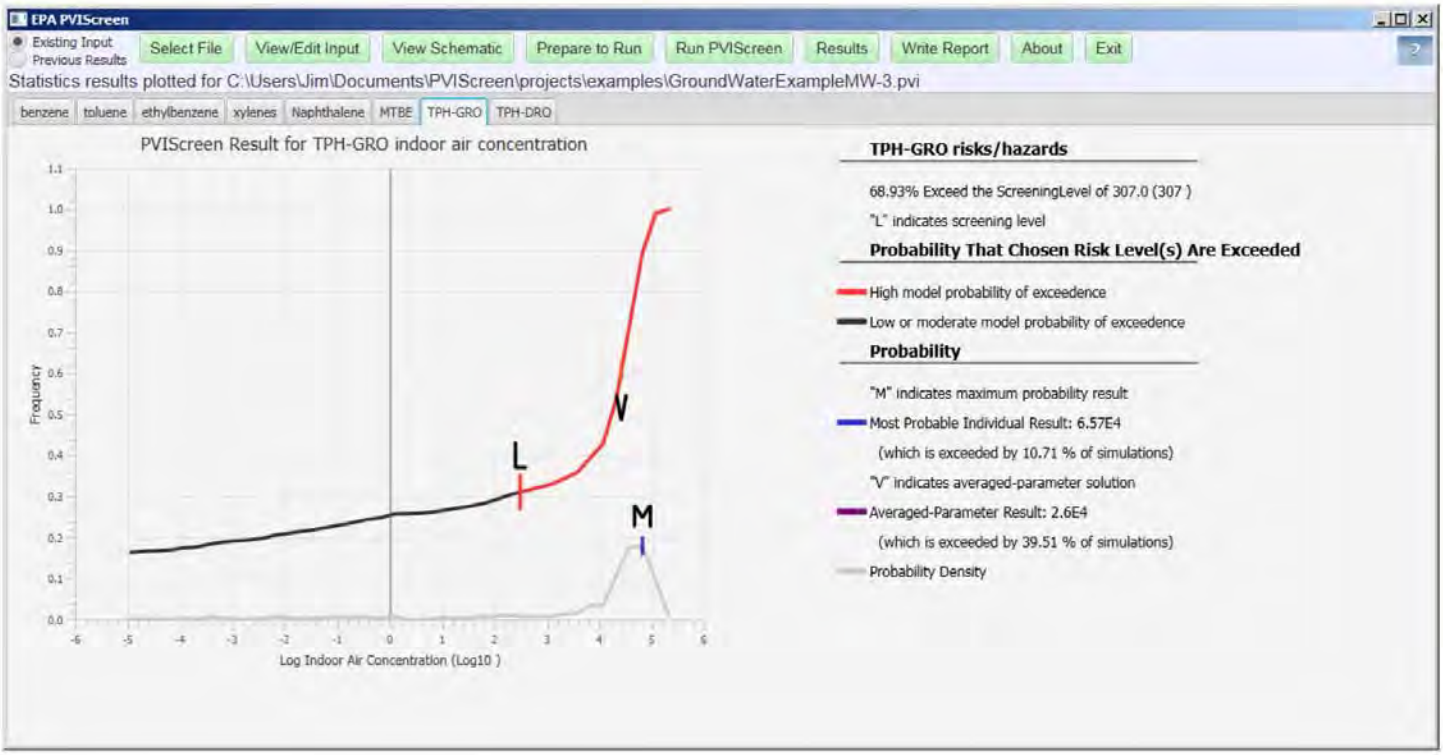


Figure 50. Gasoline range organics (TPH-GRO) results indicating high probability for petroleum vapor intrusion. As indicated on the graph (left) and the table (right), almost 69% of the simulations exceeded the site-specific screening level of 307 µg/m$^3$.

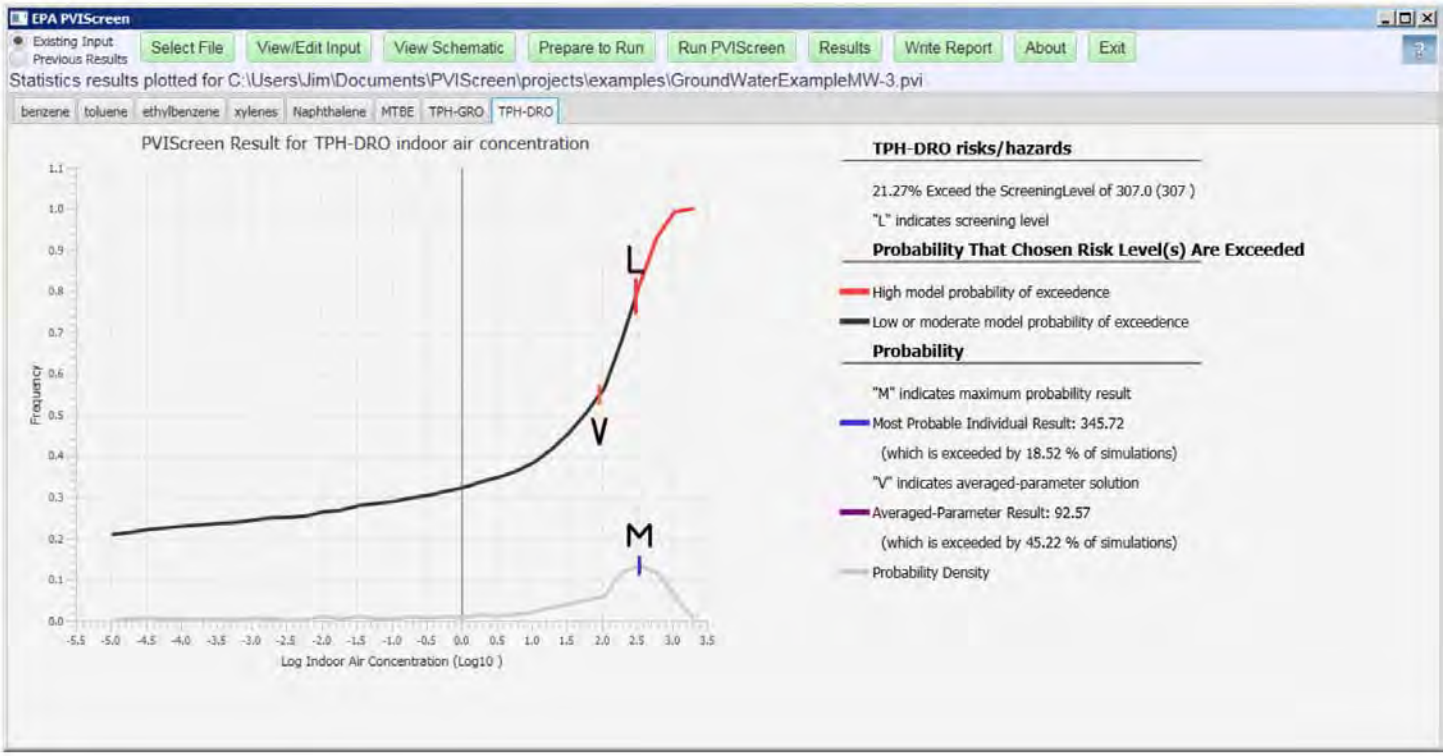


Figure 51. Diesel range organics (TPH-DRO) results indicating a strong possibility of vapor intrusion. As indicated on the graph (left) and the table (right), 21% of the simulations exceeded the site-specific screening level of 307 µg/m$^3$.

# 5. Theoretical Background

Over ten years ago vapor intrusion and its evaluation through modeling approaches were identified as a potential problem at subsurface contamination sites (Obamascik, 2002). Application of simplified models using mostly generic default parameters has contributed to confusion over appropriate assessment strategies for these sites. One of the primary models in use, the Johnson-Ettinger model was presented as a heuristic screening model (Johnson and Ettinger, 1991). Essentially the model consists of two completely-mixed compartments, one representing the interior of a building and the other the soil below. This conceptualization reflects the potential for both features of the building and the subsurface to contribute to indoor air contamination. Although models may represent important processes, the ability to determine definitively that there are no vapor impacts to buildings ("screen for PVI") also depends on application-related factors. These factors include the degree to which the site conceptual model matches the structure of the screening model, the inherent limitations imposed by the model assumptions, the values chosen for input parameters, and the ability to calibrate the model to site conditions.

Analysis of the Johnson-Ettinger model (JEM) using a one-at-a-time sensitivity analysis showed a moderate level of uncertainty resulting from parameter uncertainty (Johnson 2005). With a bounding value analysis Tillman and Weaver (2006) showed that synergistic effects dominate uncertainty because parameters of the model do not act independently but interact. For JEM, the interactions are clear as the model can be formulated in dimensionless form using three dimensionless parameter groups. Tillman and Weaver (2006) showed that the uncertainties were one to two orders of magnitude higher when parameter interactions were considered, and constructed a generic ordering of parameter importance (Tillman and Weaver, 2007).

The Johnson and Ettinger model does not account for biodegradation and so inherently over-predicts indoor air concentrations for situations where biodegradation occurs. A primary and geographically-extensive example occurs at petroleum hydrocarbon release sites, where many studies have shown extensive aerobic biodegradation. In response to these problems, the BioVapor model (Devaull, 2007) was developed to include the effects of oxygen-limited biodegradation, native soil respiration, and multiple hydrocarbon species on vapor intrusion, all within a simplified modeling context. The model is based on the assumption of steady-state diffusive transport in a homogeneous vadose zone. Consequently, an analytical solution was obtained.

## 5.1 Oil Phase Weathering

If the oil is uniformly leached due to flowing water and volatilization to the vadose zone, then the mass conservation equation for each constituent $i$ becomes

$$\frac{dM_i}{dt} = -\iint i\,K_w(S_w)\,C_{iw}\,dy\,dz - A\,D_{eff}J_{s,i}$$

where $i$ is the absolute value of the hydraulic gradient, $K_w(S_w)$ is the effective conductivity at water saturation, $S_w$, $D_{eff}$ is the effective diffusion coefficient for the vadose zone, and $J_{s,i}$ is the flux of chemical leaving the source through the gaseous phase. If the source is a rectangular block of width, Y, then the mass balance that accounts for the variation of flow with water saturation is

$$\frac{dM_i}{dt} = -Y\int i\,K_w(S_w)\,C_{iw}\,dz - A\,D_{eff}J_{s,i}$$

Solution of this equation provides a boundary condition based on emplacement of a fuel phase and consistent changes in composition due to weathering. When coupled with transport in the soil gas as calculated by BioVapor, the changes are assumed to occur slowly enough so that the transients in the vadose zone are negligible. In the simplest application of the model, leaching is assumed to occur up to a specified time, and the composition of the oil phase is then used as input to PVIScreen.

## 5.2 BioVapor Equations

Using the Johnson-Ettinger equations as the basis for representing transport from the subsurface into a building, the BioVapor equations extend the modeling approach to include an analytical solution of steady-state diffusion-driven transport in the vadose zone (DeVaull, 2007 and API, 2010). Multiple constituents of gasoline diffuse from a soil gas or ground water source. Oxygen is supplied at the foundation bottom either limited by atmospheric concentration or the foundation flux. It is then transported downward by diffusion and it is available to react with the upward-diffusing petroleum hydrocarbons. The sum of the oxygen demands determines the extent of oxygen penetration into the vadose zone, and the concentration of intruding chemicals for the oxygen concentration limited solution, according to:

$$c_{f,O} - c_{t,O} = \sum \frac{1}{\phi_i} \frac{D_{eff,i}}{D_{eff,O}} (c_{f,i} - c_{t,i}) - \frac{\rho_b \Lambda_{base,O}}{D_{eff,O}} \frac{L_a^2}{2} + \frac{L_a}{D_{eff,O}} \sum \frac{1}{\phi_i} J_{t,i}$$

where $c_{f,O} - c_{t,O}$ is the difference in oxygen concentration between the foundation and the transition point between the aerobic and anaerobic zones, $\phi_i$ is the stoichiometric utilization factor for complete mineralization, $D_{eff,i}$ and $D_{eff,o}$, are the effective diffusion coefficients for the chemical, and oxygen, $c_{f,i} - c_{t,i}$ is the difference in chemical concentration between the foundation and the transition point, $\rho_b$, is the bulk density, $\Lambda_{base,O}$ the baseline soil respiration rate, $L_a$, the aerobic zone depth, and $J_{t,i}$ the chemical flux at the transition point. The oxygen flux equation is

$$J_{f,O} - J_{t,O} = \sum \frac{1}{\phi_i} (J_{f,i} - J_{t,i}) + \rho_b L_a \Lambda_{base,O}$$

where the change in oxygen flux between the foundation and the transition between aerobic and anaerobic is denoted $J_{f,O} - J_{t,O}$, and is determined from the utilization factor, $\phi_i$ the change flux of each chemical constituent, $i(J_{f,i} - J_{t,i})$ and the baseline soil respiration. The latter is calculated from the bulk density, $\rho_b$, the aerobic zone depth, and the soil baseline oxygen utilization rate, $\Lambda_{base,O}$. The model is solved for the aerobic zone depth by bisection iteration, using either an oxygen concentration or an oxygen-flux limitation. See API 2010 for the complete model details.

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# Appendix A
## Running PVIScreen in Command Line and Batch Mode

### A.1 Batch Mode

In command line mode, PVIScreen can be used to run multiple sets of input files. The names for these files are listed in a control file named:

**00InputSetsToRun.csv**

Each complete PVIScreen input file is listed on a separate line of this file. Double clicking on the PVIScreen executable jar file – PVIScreenBatchLibrary.jar (Figure A1) causes each input file to be run in turn.

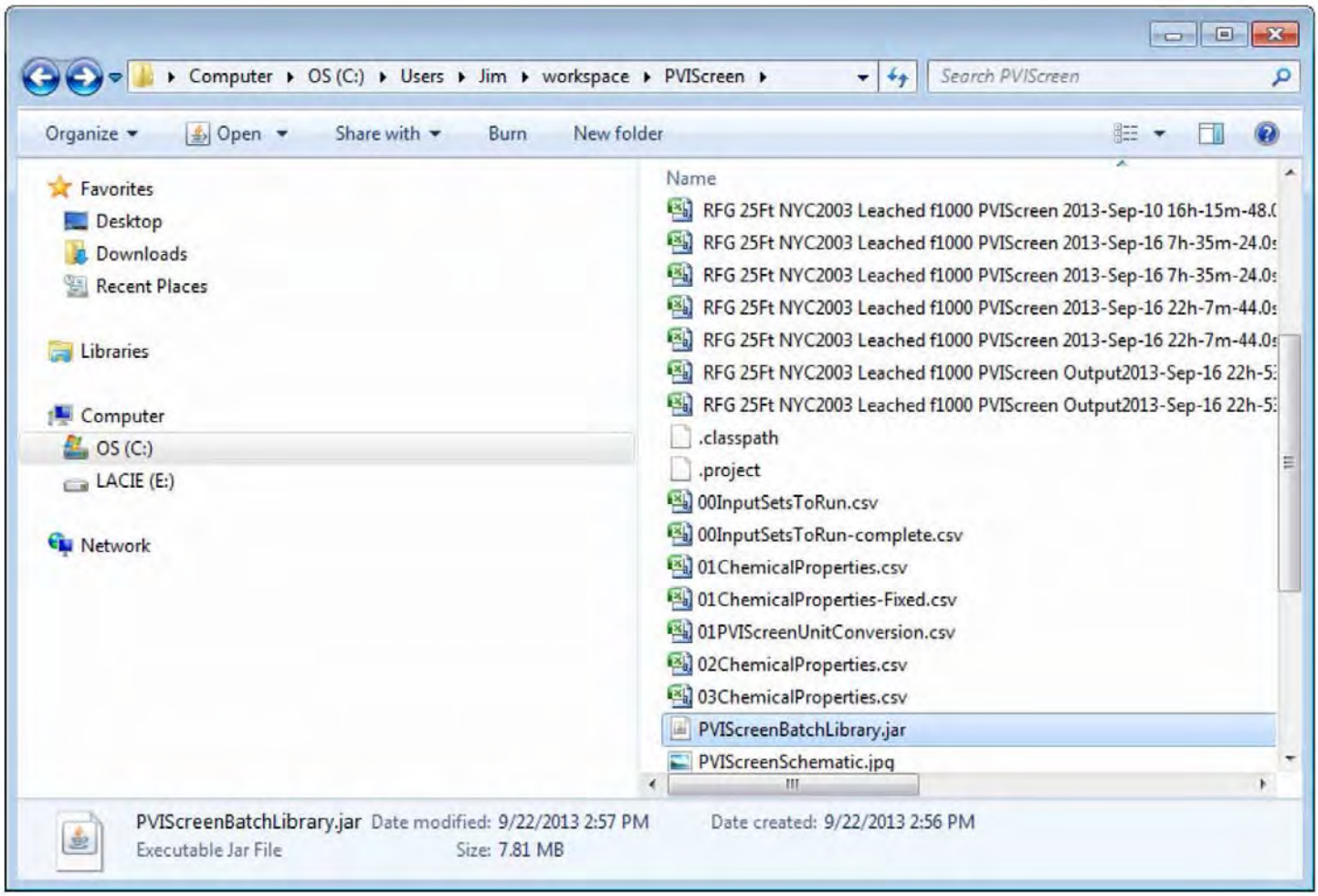



Figure A1. Executable jar file (PVIScreenBatchRun.jar) used to execute the batch version of PVIScreen.

# Appendix B
## Microsoft Excel Comma Separated Value (.csv) Format

File types are selected from the MicroSoft Excel “Save As” menu (Figure B1). Then the Comma Separated Value (.CSV) format is chosen from the selections (Figure B2).

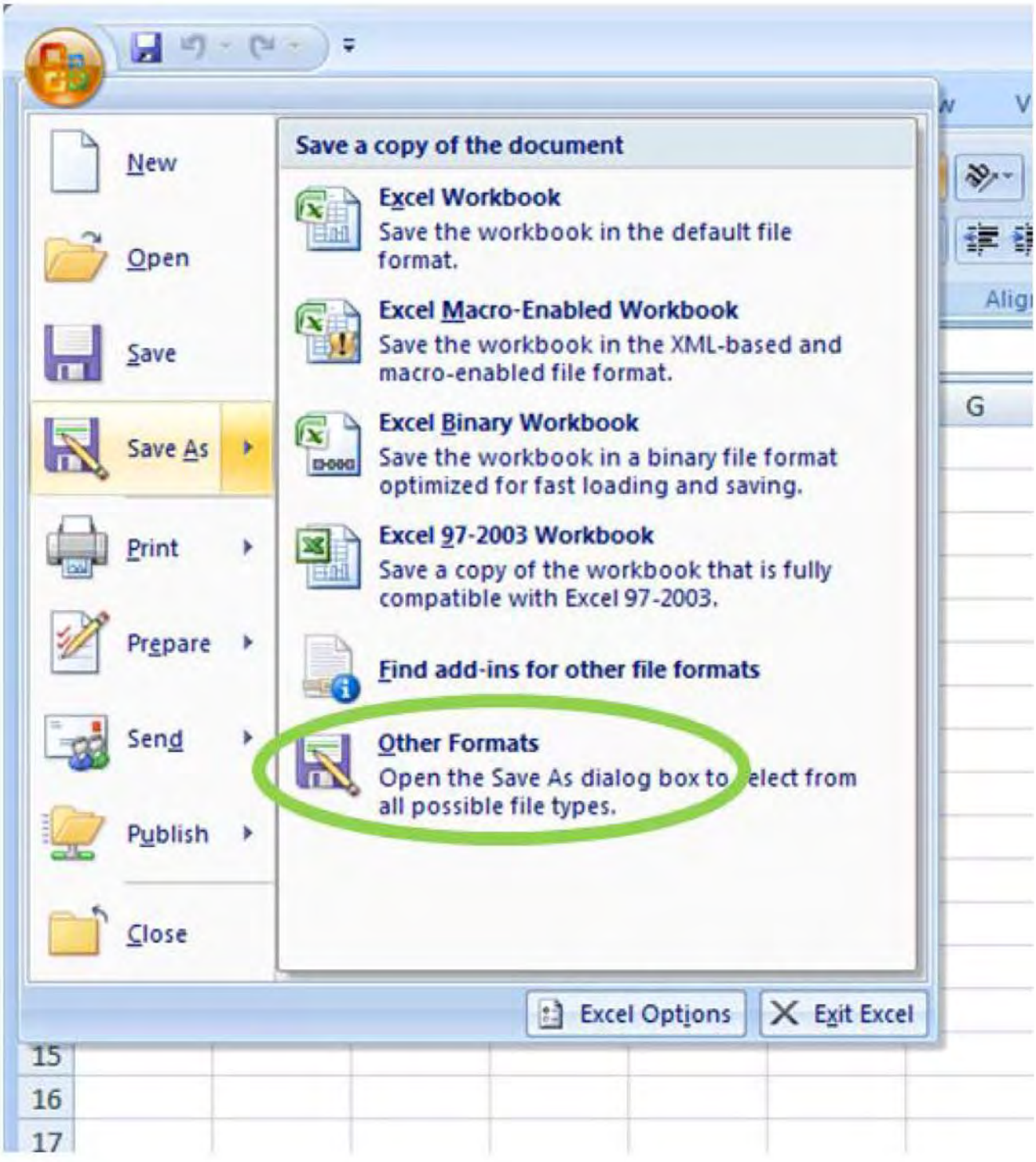



Figure B1. Microsoft Excel output (“Save As”) dialog box showing choice of **Other Formats** to write a comma separated value (*.csv) file.

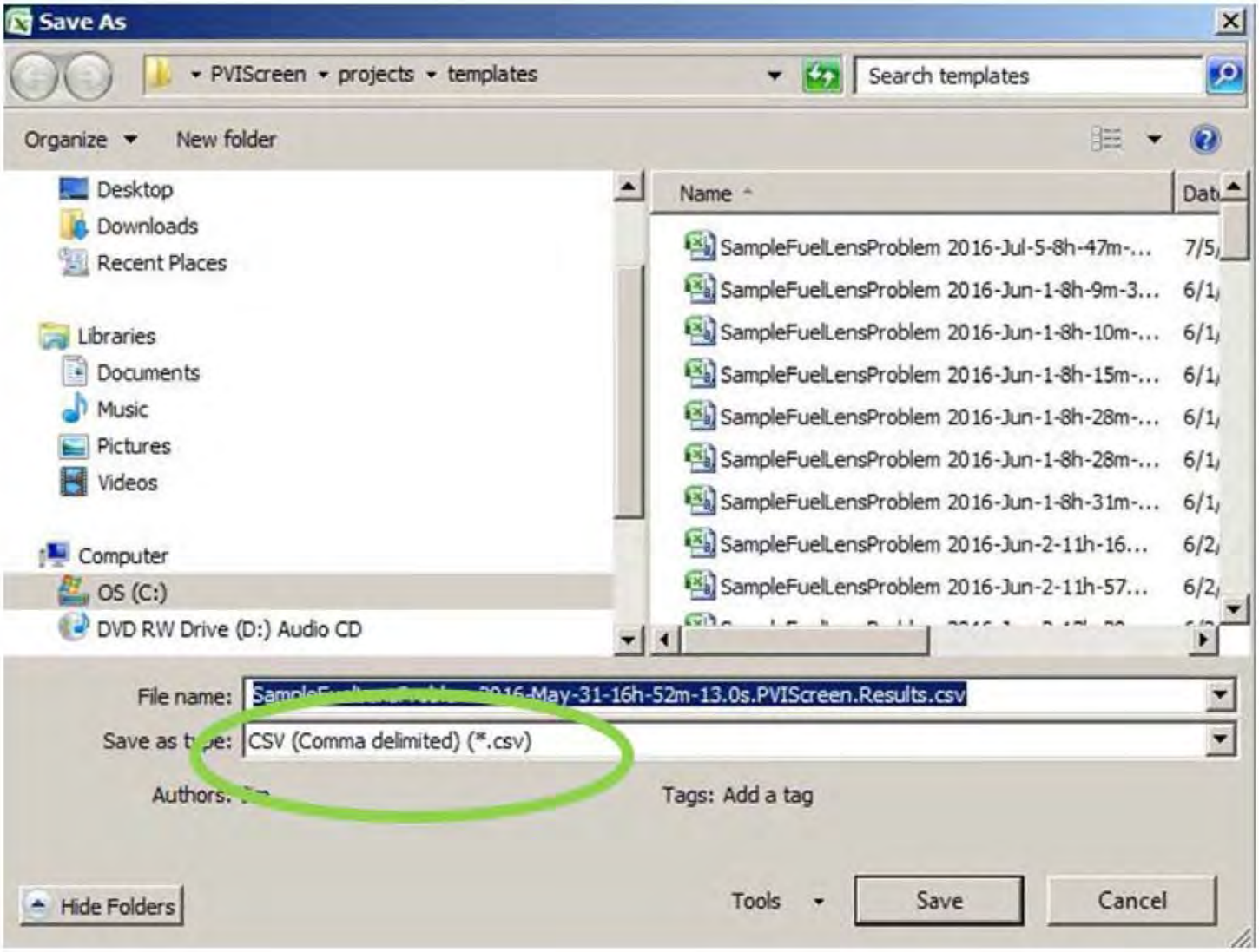



Figure B2. Microsoft Excel output dialog showing “CSV” file type selected for PVIScreen input file.

# Appendix C
## Unit Conversions in PVIScreen

A special subset of the Control group is the unit conversion factors. The allowable unit conversions are summarized in the file 01PVIScreenUnitConversion.csv. Most PVIScreen users will never have to view or change this file. Editing the unit conversion file is needed only to add a new set of units.

The unit conversion system is based on the idea that there is an internal set of units that are used in the model. For the PVIScreen the unit set is:

| quantity | unit |
|---|---|
| time | second |
| length | cm |
| mass | kilogram |
| concentration | mg/L |

Any of the optional units (Table C1) can be used for an input data set, the specified unit conversions to the model's internal unit set are made when the input data are read. Unit choices can be made for outputs.

Although not necessary for running the model, the following describes the operation of the unit conversion system:

When a parameter is read by the model, the name of the unit is included in the input group. The unit appears in input immediately after the numeric value. The unit name and type is used to identify the appropriate unit conversion factors. As many as five variants on the name are allowed. For example, the area in square meters can be designated by sm, squaremeter, square meters, squaremeters, or m2. The case is unimportant so SM, Square Meter, etc. are also accepted.

When the unit is identified as belonging to a type (say area), the unit conversion to the model unit is performed. The file indicates which units are the model units mostly for convenience as all input values undergo unit conversions. A model unit always has the unit conversion factor of 1.0. The unit conversion factors for an optional unit give conversion to the model unit. For example, to convert square feet to square meters a unit conversion of 0.3048 m per ft is applied twice. In the unit conversion file, the unit conversion factors are supplied as up to four values. This is done for clarity. To get square meters from square feet multiply the value in square feet by 0.3048 twice.

If the specified unit does not appear in the list of units from 01PVIScreenUnitConversion.csv, additional unit conversions can be added to the 01PVIScreenUnitConversion.csv file as needed.

Table C1. Excerpt of file showing default set of unit conversion factors in file 01PVIScreenUnitConversion.csv.

| Control | heading | type | status | ucf0 | ucf1 | ucf2 | ucf3 | name0 | name1 | name2 |
|---|---|---|---|---|---|---|---|---|---|---|
| Control | unit | length | model | 1 | 1 | 1 | 1 | cm | centimeter | centimeters |
| Control | unit | length | optional | 100 | 1 | 1 | 1 | m | meter | meters |
| Control | unit | length | optional | 12 | 2.54 | 1 | 1 | ft | foot | feet |
| Control | unit | length | optional | 2.54 | 1 | 1 | 1 | in | inch | inches |

# Appendix D
## Post-Processed Output File

After completing stochastic (Monte Carlo) simulation runs, the main result file is read back into the model and the results post-processed. The purpose of the post-processing is to generate statistical characterization of the results, including simple statistics and histograms.

### D.1 File Identification

The post-processed output file begins by listing the input and output files upon which it is based. Example output files are provided with the executable PVIScreen file.

### D.2 Reprinting Output Results

All of the results from the main output file are read and reprinted (not shown here).

### D.3 Simple Statistical Results

A set of simple statistical calculations is performed on the output. These include:

- Minimum
- Average
- Maximum
- Range
- Variance
- Standard Deviation
- $5^{th}$, $95^{th}$ Percentiles
- First, third Quartiles
- Median
- Inter-quartile range
- Median + ½ inter-quartile range

As for the main output file results, two tables show major parts of the statistical results.

### D.4 Histograms

Histograms are used to determine the distribution of the results. In the histogram, the results, say for peak concentration, are placed in binned intervals of the total output range. From these the most likely – and other – bins can be determined. For each bin, the histogram gives the:

- Interval mid-point
- Count (number of results within the bin)
- Frequency (fraction of results in this bin relative to the total)
- Cumulative frequency

The histogram ends with a sum of points, which should equal the number of Monte Carlo runs, and the sum of the frequencies, which should equal 1.0.

# Appendix E
## Entry of Deterministic and Stochastic (Monte Carlo) Data

PVIScreen has the capability of running either a deterministic or a stochastic (Monte Carlo) model. Many of the input parameters may be specified as being variable ("stochastic"), but to do so the input probability distribution must be specified. To simplify the input of data, the input for constant ("deterministic") and variable parameters follow the same pattern.

For other than constant and uniformly distributed parameters, the inputs must be specified using the command line version of PVIScreen, because the Graphical User Interface only allows for constant and uniformly distributed parameters.

### E.1 For Deterministic Models

Each input parameter has only one value. A parameter is entered with a key word to indicate the parameter group (here "building"), followed by the specific parameter ("width"). Next a key word indicates that the parameter has only one value. The key word is "constant". The value and unit are entered followed by the second key word which indicates the cumulative frequency is 1.0. The frequency value is not used in deterministic models, but is included for compatibility with stochastic models. An example of this input is:

Building, Width, *Constant*, *value, unit symbol, 1.0, comment*

### E.2 For Stochastic (Monte Carlo) Models

Each stochastic model parameter is described by a cumulative probability distribution. These are entered by a series of values. These are essentially empirical distributions. If the use of a parametric distribution is needed, these can be entered as described below. The following describes how constant and varying values are entered in stochastic models.

#### *E.2.1 Constant Parameter Values in Stochastic Models*

Although every parameter in PVIScreen can be treated as variable, typically stochastic models will have some fixed parameters. In that case, the parameter is designated as "constant." The entry of these values is given in the previous section.

A constant or deterministic parameter has a single value. The probability of this value is 1.0, so a single entry is made for the value with the frequency set at 1.0 (Figure E1). To use a constant value for hydraulic conductivity of 15 ft/d, the line of input for this parameter would be:

GroundWater, Hydraulic Conductivity, constant, 15, ft/d, 1.0

Alternatively, the deterministic parameter can be entered as if it is stochastic. Why would you want to do this? If you are testing the effect of parameter variability, you might want to begin with a parameter following a uniform distribution but later assign a constant value. To avoid inserting and deleting lines from the input file, two input lines are specified:

GroundWater, Hydraulic Conductivity, stochastic, 15, ft/d, 0.0

GroundWater, Hydraulic Conductivity, stochastic, 15, ft/d, 1.0

These lines are interpreted as specifying an input probability distribution with a uniform distribution with no values less than 15 (first line) and no values higher than 15 (second line). Effectively, the parameter is set at 15 ft/d (Figure E2) for all simulations. The impact on efficiency of running the model is negligible.

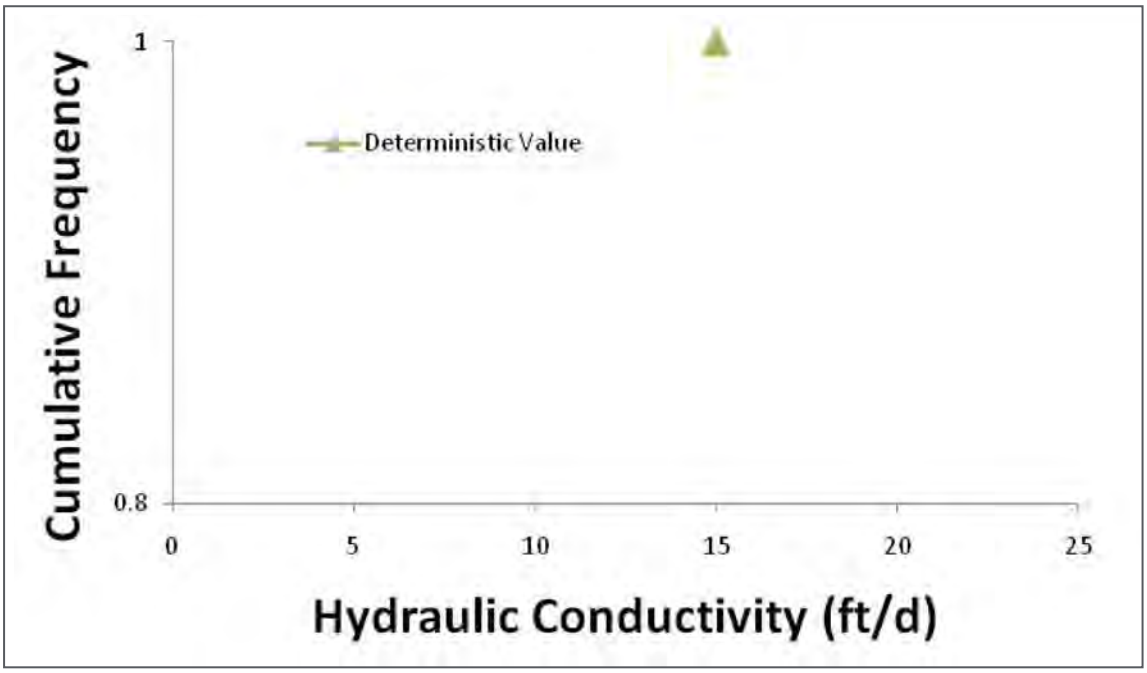



Figure E1. Cumulative frequency for a constant or deterministic parameter. Here the value is 15 ft/d which is used for every simulation.

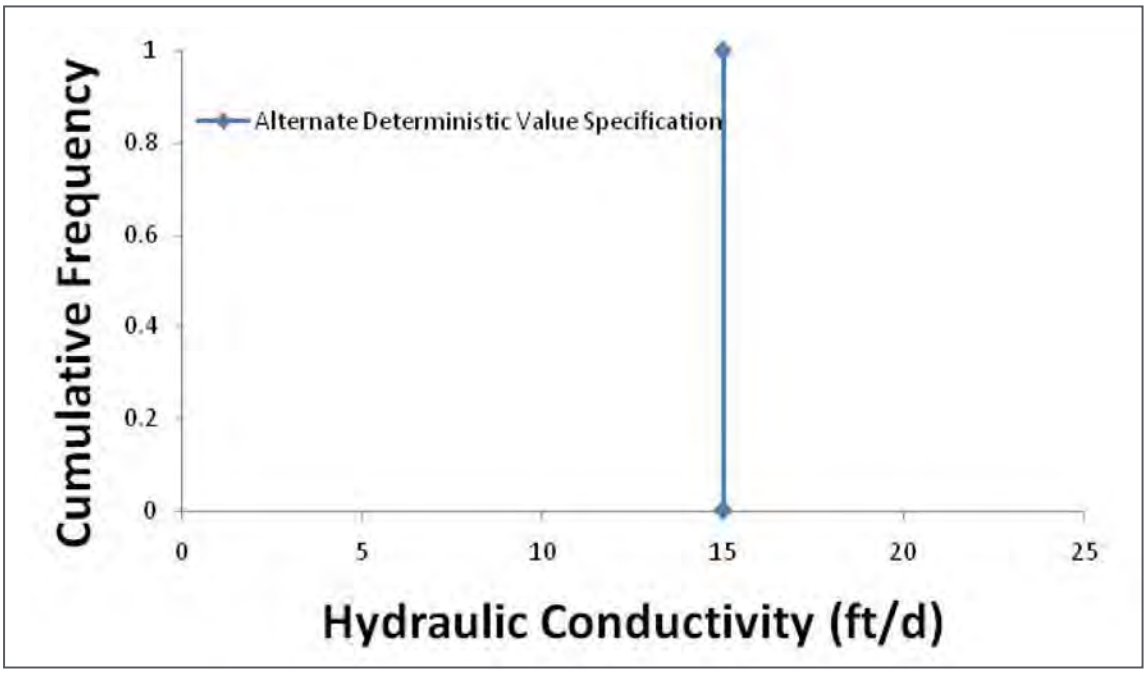



Figure E2. Alternate specification of constant parameter by specifying a uniform probability distribution with no values less than 15 ft/d and no values higher than 15 ft/d. Effectively the value is set at a constant 15 ft/d.

### *E.2.2 Variable Parameters in Stochastic Models*

For parameters considered to be stochastic, cumulative probability distributions are entered as input. These are values paired with a cumulative frequency. The cumulative probability distribution begins with the probability that ***no*** value is less than and ends with the value that ***all*** values are less than.

In the example (Table E1), no value of the parameter is less than 10.0 hence its cumulative probability is 0.0. Similarly, no value is greater than 20.0 and its cumulative probability is 1.0. The intermediate values represent cumulative probabilities between the extremes.

Table E1. Cumulative probability curve example.

| Parameter Values | Cumulative Probability |
|---|---|
| 10.0 | 0.0 |
| 10.5 | 0.00135 |
| 12.0 | 0.0228 |
| 13.5 | 0.1587 |
| 15.0 | 0.5 |
| 16.5 | 0.8413 |
| 18.0 | 0.9772 |
| 19.5 | 0.99865 |
| 20.0 | 1.0 |

## E.3 Uniformly Distributed Parameter Values

If a parameter distribution is uniform (i.e., all values are equally probable between a minimum and maximum value), two entry values are entered for a uniform distribution. The minimum value is assigned a frequency of "0.0" and the maximum value is assigned a value of "1.0."

To specify a uniform distribution with, say, a minimum value of 10 ft/d and maximum value of 20 ft/d (Figure E3) two input lines are used:

GroundWater, Hydraulic Conductivity, stochastic, 10, ft/d, 0.0

GroundWater, Hydraulic Conductivity, stochastic, 20, ft/d, 1.0

The first line gives the minimum parameter value (10 ft/d) and cumulative probability of 0.0. This value indicates that there are no hydraulic conductivity values less than 10 ft/d. The second line gives the maximum parameter value of 20 ft/d and cumulative probability of 1.0, indicating that there are no hydraulic conductivity values greater than 20 ft/d.

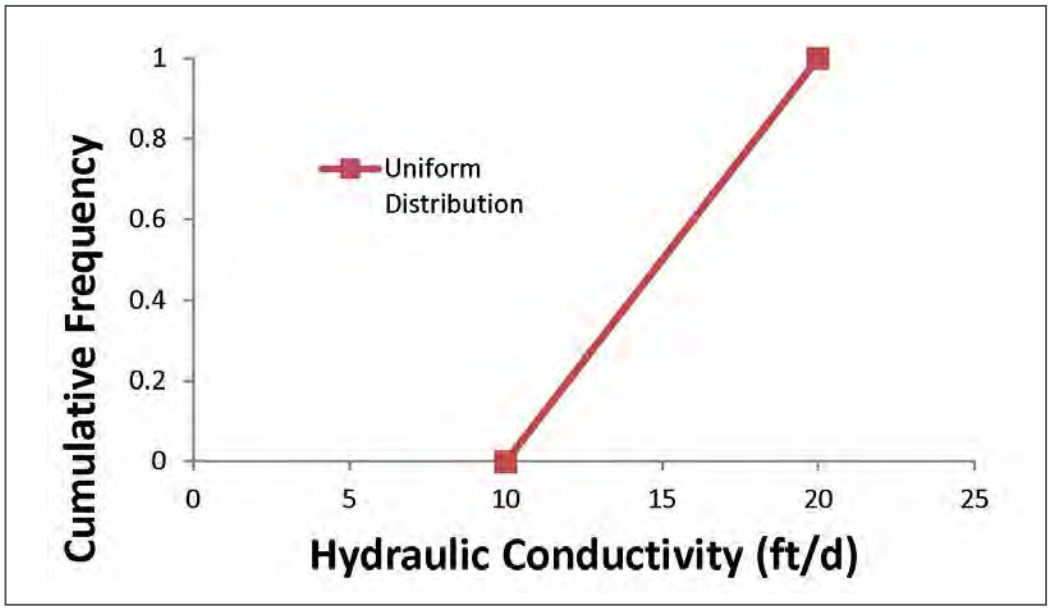



Figure E3. Uniform cumulative probability distribution with a range from 10 ft/d to 20 ft/d.

Options for entering triangular distributions where the minimum, maximum and most likely value are specified, and truncated normal distributions are given in the appendix.

## E.4 Triangular Distribution

A triangular distribution is specified from a minimum, maximum, and most likely value of a parameter. The triangular cumulative probability distribution is determined from:

$$f(x) = \begin{cases} 0; & x < a \\ \dfrac{(x-a)^2}{(b-a)(c-a)}; & a < x < c \\ 1 - \dfrac{(b-x)^2}{(b-a)(b-c)}; & c < x < b \\ 1; & x > b \end{cases}$$

where $f(x)$ is the cumulative probability, $a$ is the minimum, $b$ is the maximum and $c$ is the most likely value. For a parameter with minimum of 10, maximum of 20 and most likely value of 13, the cumulative probability curve is approximated by 11 points (Figure E4 and Table E2). The figure illustrates the cumulative probability curve determined from 41 points (using an increment of 0.25 ft/d) and its approximation by 11 points (squares). A spreadsheet illustrating these calculations is available from the author (weaver.jim@epa.gov).

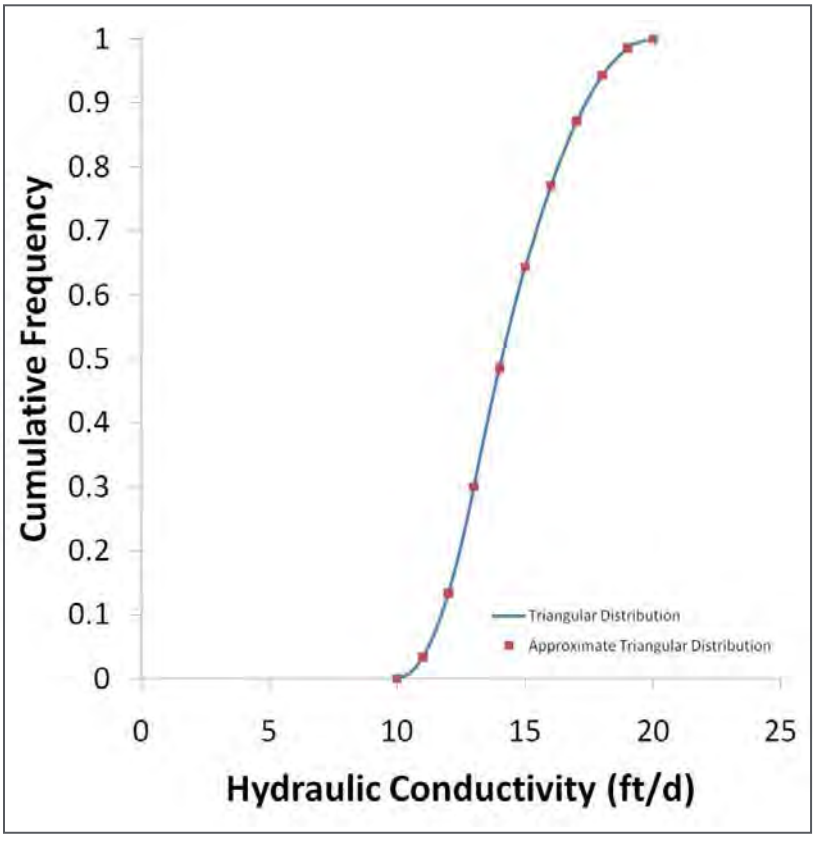



Figure E4. Triangular distribution (line) and its approximation by 11 points (squares).

Table E2. Approximate triangular distribution with minimum of 10, maximum of 20 and most likely value of 13.

| Hydraulic Conductivity (ft/d) | Cumulative Probability |
|---|---|
| 10 | 0 |
| 11 | 0.033333 |
| 12 | 0.133333 |
| 13 | 0.3 |
| 14 | 0.485714 |
| 15 | 0.642857 |
| 16 | 0.771429 |
| 17 | 0.871429 |
| 18 | 0.942857 |
| 19 | 0.985714 |
| 20 | 1 |

## E.5 Truncated Normally Distributed Parameter Values

Parameters with a truncated normal distribution can also be entered by specifying the cumulative distribution (Figure E5). A specific set of nine cumulative frequencies are needed to specify the distribution (Table E3). The distribution is truncated because the normal distribution ranges from negative to positive infinity. For practical calculation purposes, range is truncated at a minimum and maximum value. For this example the input lines are

GroundWater, Hydraulic Conductivity, stochastic, 10.0, ft/d, 0.0
GroundWater, Hydraulic Conductivity, stochastic, 10.5, ft/d, 0.00135
GroundWater, Hydraulic Conductivity, stochastic, 12.0, ft/d, 0.0228
GroundWater, Hydraulic Conductivity, stochastic, 13.5, ft/d, 0.1587
GroundWater, Hydraulic Conductivity, stochastic, 15.0, ft/d, 0.5
GroundWater, Hydraulic Conductivity, stochastic, 16.5, ft/d, 0.8413
GroundWater, Hydraulic Conductivity, stochastic, 18.0, ft/d, 0.9772
GroundWater, Hydraulic Conductivity, stochastic, 19.5, ft/d, 0.99865
GroundWater, Hydraulic Conductivity, stochastic, 20.0, ft/d, 1.0

The truncated normal distribution is contained between 10.0 ft/d and 20.0 ft/d. Note that for the distribution to approximate the normal distribution, the mean value less three standard deviations (10.5) must be above the minimum (10.0), and the mean value plus three standard deviations (19.5) must be below the maximum value (20.0).

Table E3. Cumulative normal distribution frequencies, symbolic values and example.

| Normal distribution cumulative frequency | Symbolic values mean (μ) and standard deviation (σ) | Example with mean of 15, standard deviation of 1.5 |
|---|---|---|
| 0.0 | minimum | 10.0 |
| 0.00135 | μ - 3σ | 10.5 |
| 0.0228 | μ - 2σ | 12.0 |
| 0.1587 | μ - σ | 13.5 |
| 0.5 | μ | 15.0 |
| 0.8413 | μ + σ | 16.5 |
| 0.9772 | μ + 2σ | 18.0 |
| 0.99865 | μ + 3σ | 19.5 |
| 1.0 | maximum | 20.0 |

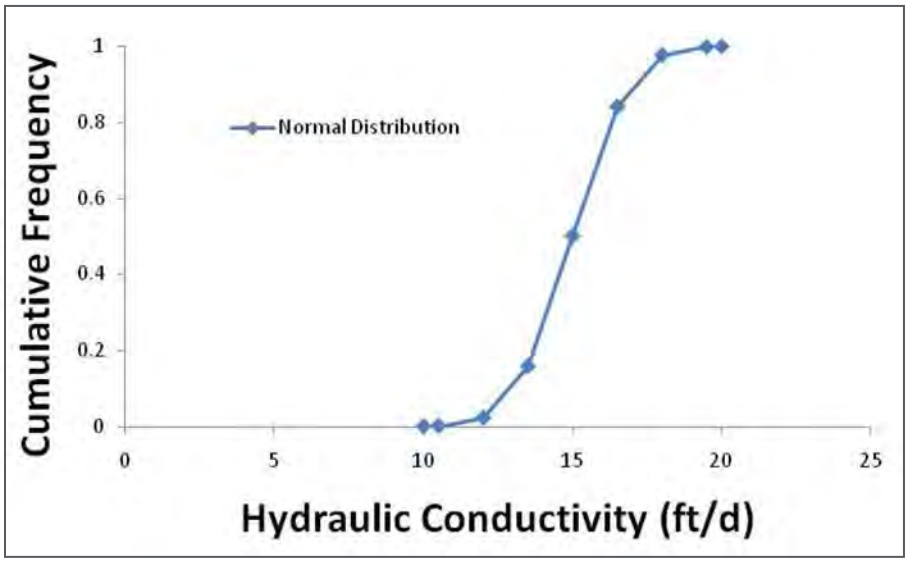
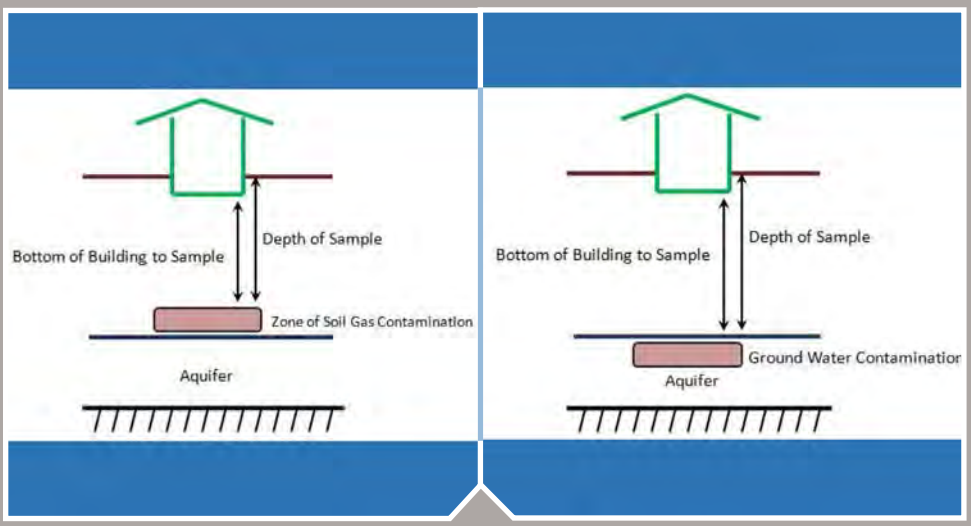



Figure E5. Truncated cumulative normal distribution with mean of 15 ft/d and standard deviation of 1.5 ft/d. The distribution is defined by seven points (Table E3).

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