# Petroleum Vapor Intrusion Assessment with PVIScreen

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## ABSTRACT

**Vapor intrusion of petroleum differs from that of chlorinated solvents because of the strong 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. 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.**

## BACKGROUND

### Environmental Models and Vapor Intrusion

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.

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, top). 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 source, presence of light non-aqueous phase liquid (LNAPL), and depth to water, among other factors (Figure 1, bottom).

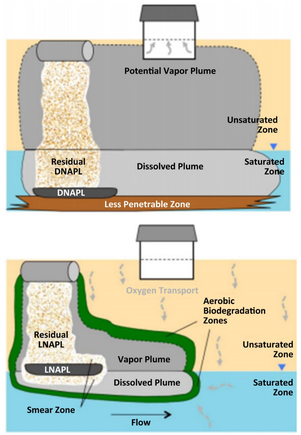



**Figure 1.** Comparison between the processes governing non-biodegrading solvent vapor intrusion (top) and petroleum vapor intrusion (bottom) (U.S. EPA, 2012).

## BioVapor

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 2) 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 are reduced relatively deeply in the vadose zone.

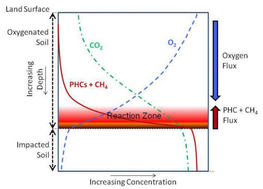



**Figure 2.** Schematic illustration of petroleum hydrocarbon (PHC) flux and distribution and oxygen flux and distribution (US EPA, 2012).

## PVIScreen

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 relative to risk levels, and
- automatically preparing a report of results.

PVIScreen addresses one of the limitations in models described above: uncertainty in parameter choices. In PVIScreen, the building, vadose zone and aquifer are defined in a layout (Figure 3) which relates the bottom of the foundation to a zone of petroleum contamination. Typically, the petroleum contamination will be a region that contains a separate-phase hydrocarbon (non-aqueous phase liquid (NAPL)). Input parameters describe the size and characteristics of each component in the model. Vadose zone contamination might originate from dissolved chemicals in the aquifer. This situation can also be accommodated in PVIScreen (Figure 4).

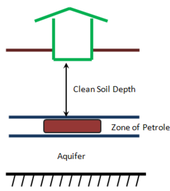



**Figure 3.** Building, vadose zone, petroleum (NAPL) contamination, and aquifer layout used in PVIScreen.

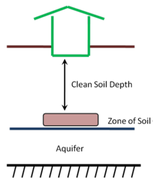



**Figure 4.** Building, vadose zone, ground water contamination layout used in PVIScreen.

### Uncertainty Analysis

Uncertainty analysis, as used here, includes the impact of the inherent sensitivity of the model to changes in parameter values and the magnitude of those changes. 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. These are entered as sets of points defining the curve in a procedure that allows for complete flexibility in specifying the input probabilities. No assumptions of particular distributions (i.e., normal) are needed, although a normal distribution can be approximated empirically.

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 frequency curves for each chemical specified in soil gas (Figure 5). These output frequency curves, along with risk levels, are the main outputs of the model.

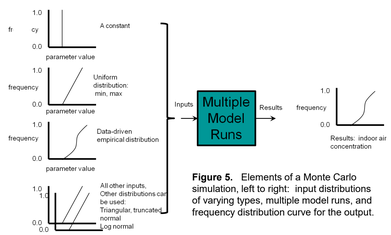



**Figure 5.** Elements of a Monte Carlo simulation, left to right: input distributions of varying types, multiple model runs, and frequency distribution curve for the output.

The main PVIScreen outputs are cumulative 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 6). 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 6) was 31% (horizontal blue arrow on Figure 6).

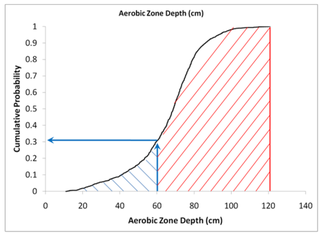
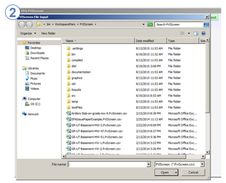


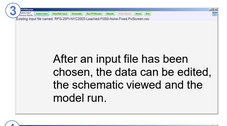

**Figure 6.** Example cumulative probability curve. The probability that the aerobic zone depth is 60 cm is 31%, while the probability that the aerobic zone thickness is greater than 60 cm is 69%.

### The PVIScreen User Interface

1 PVIScreen options run from left to right. Option buttons become available when previously-needed information is available. At the beginning, "Select Input" is the main choice.



2 After choosing "Select Input," available PVIScreen data files show up in the dialog box. An existing file is the starting point for a new application. Several types of files are available with the software.



3 After an input file has been chosen, the data can be edited, the schematic viewed and the model run.

4 Each type of input data is contained on a separate screen. For an individual input a distribution type is chosen (by default either constant – a single value or a uniform distribution defined by a minimum and maximum). Parameters with unknown values should be selected as ranges between the minimum and maximum. For example the length and width of the building should be known, so they can be entered as constants. A crack width, however, is likely to be unknown, so a range should be entered. The combination of constant and variable parameters are used in the Monte Carlo simulation to perform the uncertainty analysis.

5 The building, vadose zone, and aquifer geometries are used to create a schematic view of the problem simulated. Because the relationships may not be clear on the numerical input screens, the schematic should be checked to assure it matches the building simulated.

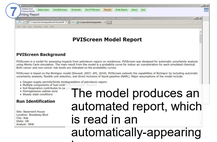
6 After running the Monte Carlo simulation the results are displayed on a series of charts, one for each chemical in the input set.

Both an instantaneous curve (marked with "M") and a cumulative curve are given (marked with "C" and "H"). The cumulative curve is colored red, yellow, and green. The colors give a rough idea if a concentration is likely to be exceeded by other simulation results. For example, the results show that a concentration of 0.01 μg/m³ (log value = -2) is likely to be exceeded because its cumulative frequency is about 0.25, and it falls in the red-colored part of the chart. Higher concentrations that are less likely to be exceeded are colored yellow, or, if unlikely to be exceeded, colored green. The coloration is subjective and can be changed by the PVIScreen user.

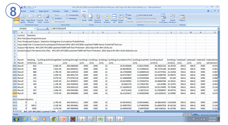
For benzene, the hazard level "H" with quotient of 1.0 corresponds to a concentration of 30.00 μg/L. All simulations were below this level (their frequencies were below 1.0). The 1 x $10^{-5}$ cancer risk level "C" corresponding to 2.9 μg/L was exceeded by only a few simulations (0.65% of them). These both plot in green, indicating that it is unlikely this value would be exceeded.

The single most probable result (marked with an "M") is 0.42 μg/L, which is exceeded by 17.2% of the simulations. The complete frequency response curve from PVIScreen puts the single value in context. (If a single model run was made the context would be lacking.)

7 The model produces an automated report, which is read in an automatically-appearing browser.



8 The results can be read directly from output text files by opening them with Microsoft© Excel.



## AVAILABILITY

Available at :

https://www.epa.gov/land-research/pviscreen

## REFERENCES

American Petroleum Institute, 2010, User's Manual, BioVapor: A 1-D Vapor Intrusion Model with Oxygen-Limited Aerobic Biodegradation, American Petroleum Institute.

DeVaull, G.E., 2007, Indoor Vapor Intrusion with Oxygen-Limited Biodegradation for a Subsurface Gasoline Source, Environmental Science and Technology, 41, 3241-3248.

Johnson P.C., Ettinger, R.A., 1991, Heuristic Model for Prediction the Intrusion Rate of Contaminant Vapors Into Buildings, Environmental Science and Technology, 25, 1445-1452.

Obamascik, M., 2002, EPA home-toxins test "crude and limited"; Widely used computer model often wrong, Denver Post, January 7, 2001, A-1.