



## Inverse Groundwater-Plume Modeling Applied to Dose Reconstruction

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### Introduction

In toxic tort claims, questions often arise regarding exposure of individuals (receptors) to chemicals of potential concern (COPCs). In these cases, the concentration of the COPCs in an environmental medium that a receptor has been in contact with (termed the “dose”) is a key component in assessing the amount of the chemical that may have entered the body via dermal absorption, ingestion, or inhalation. However, if the exposure occurred in the past, and records of direct measurements of COPC concentrations are not available, it is necessary to estimate historical concentrations, which requires a dose reconstruction approach.

This Environmental Forensics Note presents the application of inverse groundwater-plume modeling to estimate past concentrations of volatile COPCs in groundwater and soil vapor, which could have historically exposed a receptor to those COPCs via two pathways—drinking water and soil vapor intrusion. A hypothetical setting of a rural neighborhood downgradient from a release is used to illustrate this dose reconstruction approach.

### Properties of COPCs

The critical properties that determine the migration of a COPC in groundwater include its solubility and the degree to which a dissolved COPC would tend to evaporate (vapor pressure). The relationship between the solubility and the vapor pressure is unique to any given COPC (and is quantified as the Henry’s constant, or H), and it dictates the degree to which it may volatilize from the groundwater into the soil vapor in the vadose zone, which is the zone of unsaturated soil between the ground surface and the top of the groundwater table. The pore spaces between soil particles in the vadose zone are filled with air, which can be affected by volatile COPCs (such as benzene or trichloroethylene), depending on the value of Henry’s constant (the greater the value of H, the more likely a COPC will tend to partition into soil vapor from groundwater).

In addition to volatilization, some COPCs sorb to the aquifer soil, which retards the migration of the COPC. The amount of organic carbon in the soil that makes up the aquifer has the strongest effect on the degree of retardation, particularly for many organic compounds. COPCs can adsorb to clays and iron oxides, which also influence retardation. Other types

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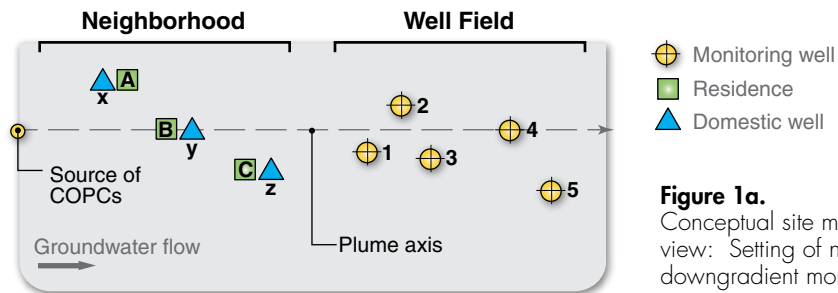
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of COPCs (e.g., perchlorate, 1,4-dioxane, etc.) do not react with or adsorb to soils to any significant degree, regardless of the organic carbon content, and these non-reactive constituents migrate at approximately the same velocity as the groundwater. Also, some COPCs (e.g., certain chlorinated solvents and certain petroleum hydrocarbons) degrade by biotic and abiotic processes to other compounds. These other compounds may be more toxic than the original compound (e.g., vinyl chloride is a degradation product of trichloroethylene), or may be relatively innocuous compounds (e.g., benzene degrades to carbon dioxide or methane).

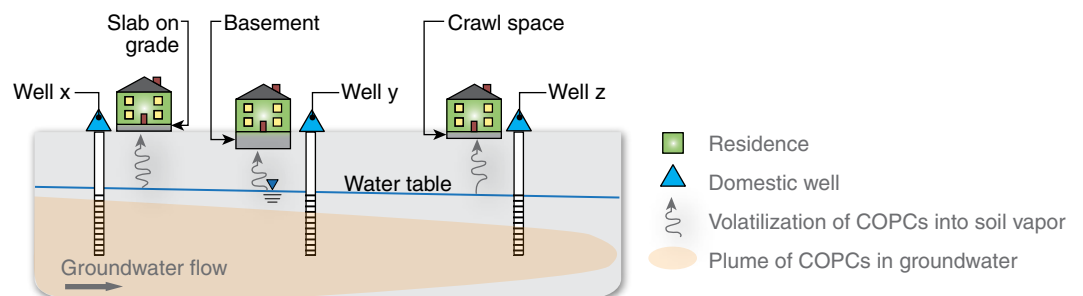
## Conceptual Site Models

A conceptual site model (CSM) describes known and suspected sources of contamination, types of contaminants and affected media, routes of migration, and human and environmental receptors. A CSM depicting a hypothetical plume of volatile COPCs to residents of a neighborhood is presented in Figures 1a and 1b. In this scenario, the residences are supplied with their own well water, and the groundwater is relatively shallow. Potential exposure pathways to COPCs for the residents are from (i) well water, including ingestion by drinking, inhalation from volatilization of the COPCs (e.g., during showering), and dermal exposure during bathing, washing, or gardening; and (ii) inhalation of COPCs in indoor air that has been affected by soil vapor intrusion (SVI).

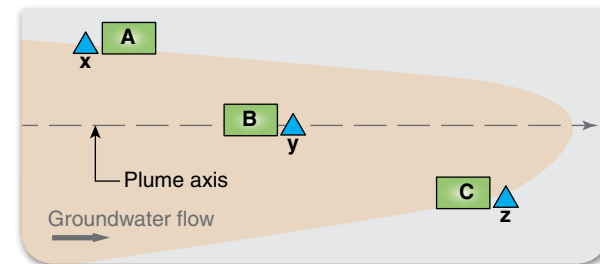


**Figure 1a.**  
Conceptual site model—Plan view: Setting of neighborhood and downgradient monitoring well field

### Cross section



### Plan view



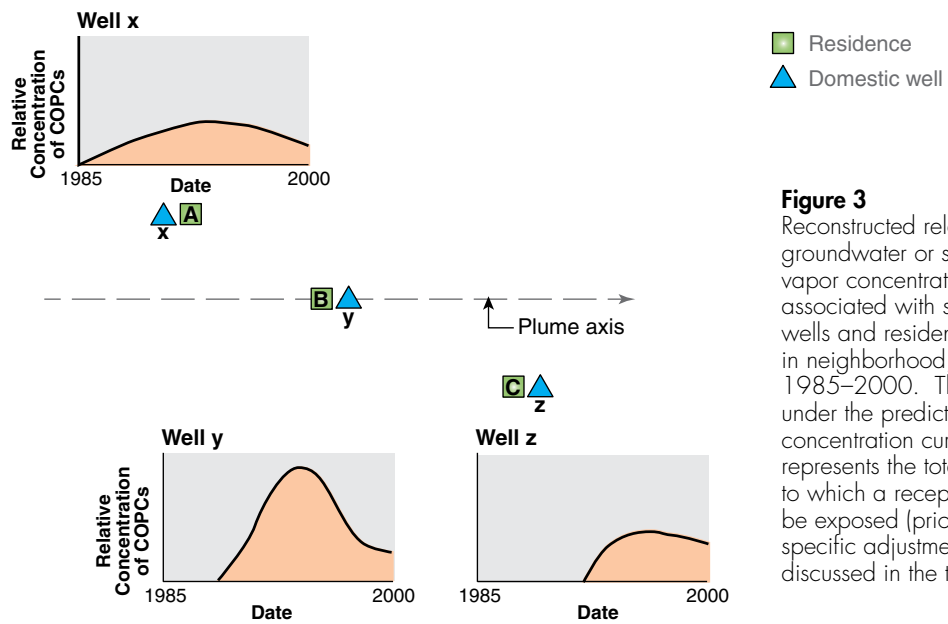
**Figure 1b.**  
Conceptual site model of neighborhood: Profile and plan view



modeling. For example, if a groundwater-well network was sampled from 2005 to 2010 (Figures 2a and 2b), and the plume variables were estimated on the basis of that sampling, the concentrations of COPCs in groundwater could be determined back to the point in time when the COPC plume in shallow groundwater would have first reached the neighborhood, say in 1985. In particular, the groundwater concentrations at the locations of domestic wells can be estimated for any point in time. This is an essential and critical step in determining the dose of COPCs to which the residents may have been exposed over time.

## Modeled Exposure Concentrations

Figure 3 depicts relative time-concentration plots of past COPC concentrations in groundwater that was pumped from wells x, y, and z for use by residences A, B, and C, respectively, between 1985 and 2000. The area under the curve in each graph represents the total amount of COPC (or maximum dose) to which an occupant of each residence could potentially be exposed during the use of well water (e.g., via ingestion, inhalation, or dermal contact) for the six-year period, based on the results of the inverse plume model results.



**Figure 3**  
Reconstructed related groundwater or soil vapor concentrations associated with specific wells and residences in neighborhood; circa 1985–2000. The area under the predicted time-concentration curves represents the total dose to which a receptor may be exposed (prior to site-specific adjustments, as discussed in the text).

The soil gas concentration in the vadose zone that would have resulted in the past exposures associated with the contaminants immediately above the groundwater table can also be calculated based on the Henry's law relationship. In the examples presented in Figure 3, the residences are located very near the associated wells, so the time-concentration plots of past soil vapor concentrations beneath residences A, B, and C would closely parallel the patterns for groundwater (except that the concentrations would be measured as mass per volume of air [ $\mu\text{g}/\text{Lair}$ ], as opposed to mass per volume of groundwater [ $\mu\text{g}/\text{L groundwater}$ ]). Therefore, the graphs presented in Figure 3 also represent the relative exposure concentrations in soil vapor at any point in time at any of the residences A, B, and C. Further, the total amount of a COPC in soil gas to which receptors in each residence could potentially be exposed due to soil vapor intrusion (e.g., via inhalation) for the six-year period can also be determined based on the results of the inverse plume model results.

## Estimation of Dose

Risk assessment professionals use the historical exposure concentration estimated by the inverse plume model to estimate an average daily and/or cumulative dose of the COPCs. A detailed discussion of the dose assessment is beyond the scope of this EF note, but it would consider the

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activities and behavior of the residents, such as their individual bathing, gardening, recreational (e.g., whether the residence has a swimming pool), and cooking habits, and the frequency and duration of time they are home (e.g., work and travel habits).

The historical exposure concentration in soil vapor can also be used to estimate the total amount of COPCs that reached the indoor breathing space in the residence. One of the more important variables that affect the relative amount of a COPC that may ultimately reach the indoor breathing space is the type of foundation upon which the residence is situated. In addition, and similar to the analysis for groundwater exposure, the activities and habits of the residents would be evaluated in any final site-specific exposure assessment.

## Summary and Conclusions

In toxic tort cases where past exposures to COPCs are an issue, but for which contemporaneous data are not available, inverse plume modeling is a useful and potentially essential tool. Inverse plume modeling is used to predict the exposure concentration in groundwater and soil vapor at any point in time, and a total amount of COPC to which a well or structure may be subjected, respectively. This is particularly important when there are multiple potential claims of exposure in a specific area. Receptors will have been exposed to varying levels of COPCs, even over relatively small distances. Typically, the results from an inverse plume model are used by risk assessors, incorporating other information to develop a complete exposure assessment that estimates the dose of COPCs that a receptor has received.

## References

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## Biographical Sketch

Mr. Peter Mesard is a Principal Engineer in Exponent's Environmental Science practice in Oakland, California. Mr. Mesard has extensive experience as a hydrogeologist, engineering geologist, and civil engineer. His principal area of specialization is environmental release reconstruction and source identification (environmental forensics), including chemical-characteristic analysis (chemical fingerprinting), the dating of chemical releases, and chemical fate and transport. Mr. Mesard has assisted his clients on various CERCLA, RCRA, and state-equivalent sites, to identify and quantify the contributions of specific sources, evaluate the technical appropriateness and costs associated with remedial actions, and assess the consistency with state and federal regulations. Mr. Mesard also has expertise in quantifying the flux, timing, and extent of chemical releases for dose reconstruction estimates related to toxic tort claims. Mr. Mesard's areas of interest include risk management and decision analysis in assisting financial, legal, insurance, and commercial clients in quantifying and assessing the risks and costs associated with environmentally distressed properties, and in allocating environmental responsibilities and costs among responsible parties in cost-contribution and cost-recovery efforts.

