

Using the One Dollar Model to Answer the Million Dollar Question, or Assessment of Natural Attenuation Within the Regulatory Framework

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ABSTRACT

Natural attenuation is an important process to be considered when environmental consultants are attempting to establish site-specific soil, groundwater or soil gas criteria at a contaminated site. The methodologies and equations provided in the various regulatory documents to develop site-specific media quality criteria are invariably based on simplified models which use “conservative” assumptions. There are always some gaps (or time lags) between the regulatory approaches and the “state of the practice” techniques which may provide a better representation of natural attenuation but which invariably demand much more data to be collected. With the limits imposed by budget, schedule, and manpower, environmental consultants always face the challenge of making decisions or recommending actions based on limited data and imperfect and/or inexact modelling results. This paper:

- discusses the challenges the environmental consultants face when using simple models to characterize natural attenuation processes under field conditions,
- outlines strategies to effectively use simple models to assist the decision-making process, and
- discusses the important issues of how to assess and communicate the effects of parameter variability, model uncertainty and sensitivity.

Examples are provided to demonstrate an approach, based on Monte Carlo simulation methodology, to quantify the uncertainty/variability in model parameters and to develop remediation guidelines in a situation in which multiple sets of generic soil and water criteria (which are not internally consistent) exist.

Introduction

Natural attenuation (NA), including dilution, dispersion, adsorption and biodegradation, is an important process to be considered when environmental consultants are attempting to establish site-specific soil, groundwater or soil gas criteria at a contaminated site. The current Alberta Environment (AENV) guidelines for petroleum hydrocarbons include generic (Tier 1) criteria which were in part developed using a set of contaminant fate and transport models. The AENV process allows proponents to use site-specific data to modify some of the generic guidelines using the equations provided in the guideline documents (Tier 2). These regulatory models contain various NA components (AENV 2001). Alberta Environment’s approaches are fundamentally consistent with the procedures developed by the Canadian Council of Ministers of the Environment (CCME 2000). The general principles also apply in many other jurisdictions.

The analytical models provided in the regulatory guidelines are based on much simplified geological conditions and contaminant transport and attenuation mechanisms. However, these “simple” models are not necessarily easy to use effectively. Environmental consultants frequently have difficulties applying these models to simulate or account for real field conditions, and some of the problems may be caused by not fully understanding the difference between the regulatory and “textbook” modelling approaches and objectives. This paper discusses:

- the features of the regulatory models,
- the challenges that environmental consultants face when using simple models to characterize natural attenuation under field conditions,
- strategies to effectively use these models to assist the decision-making process, and
- the important issues of how to assess and communicate parameter variability, model uncertainty and sensitivity and how/when to use equivalent parameter values.

Regulatory Models

In the 2001 Alberta guidelines, the model used to evaluate the soil vapour inhalation pathway is a simplified version of the Johnson & Ettinger (1991) model (J&E model; Johnson and Ettinger, 1991, U.S. EPA, 1997). The model uses an attenuation coefficient (λ) to represent the change in the soil vapour concentration associated with vapour phase migration from a subsurface contaminant source into a building. The attenuation coefficient is basically a mixing factor that represents mixing of the contaminant vapour entering the building by diffusion and convection with fresh air entering the building via ventilation and the climate control systems.

In the 2001 Alberta guidelines, the models used to determine the soil and groundwater guidelines to protect the freshwater aquatic life pathway involves the calculation of four dilution factors:

- Dilution Factor (DF) 1 is the ratio of the concentration in soil to the concentration in the leachate/pure water that is in contact with the soil. DF 2 is the ratio of the concentration in the leachate to the concentration in pore water just above the groundwater table. DF2 takes the value of 1 under the conservative assumption that no attenuation takes place during downward migration from the source to the groundwater table.
- DF 3 is the ratio of the concentration in pore water just above the groundwater table, to the concentration in the through-flowing groundwater beneath the source. If the aquifer mixing effect is ignored (a conservative assumption), DF3 also takes on a value of 1.
- DF4 is the ratio of the concentration of a contaminant in groundwater beneath the source, to the concentration in groundwater recharging a surface water body. DF4 is calculated using the Domenico (1987) model:

$$DF4 = \frac{4}{\exp(A)\operatorname{erfc}(B)[\operatorname{erf}(C) - \operatorname{erf}(D)]}$$

$$A = \frac{x}{2D_x} \left\{ 1 - \left(1 + \frac{4L_s D_x}{v} \right)^{1/2} \right\} \quad B = \frac{x - vt \left(1 + \frac{4L_s D_x}{v} \right)^{1/2}}{2(D_x vt)^{1/2}}$$

$$C = \frac{y + Y/2}{2(D_y x)^{1/2}} \quad D = \frac{y - Y/2}{2(D_y X)^{1/2}}$$

$$L_s = \frac{0.691}{t_{1/2}} \exp(-0.07d) \quad v = \frac{V}{q R_s}$$

where x = distance from source to surface water body; D_x = dispersivity in the direction of groundwater flow; L_s = decay constant; v = velocity of the substance in groundwater; V = Darcy velocity of groundwater; q = effective porosity; t = is time since substance release; y = distance to receptor perpendicular to groundwater flow; Y = width of plume in groundwater underneath the source area; D_y = dispersivity perpendicular to the direction of groundwater flow; $t_{1/2}$ = decay half-life of the substance; d = depth to groundwater table; R_s = retardation factor in saturated zone; K_{oc} = organic carbon partition coefficient; and f_{oc} = fraction organic carbon. DF 4 represents attenuation effects caused by adsorption, dispersion, and biodegradation during contaminant migration in groundwater.

The regulatory models listed above are analytical models, and, therefore, require assumptions of uniform geological and hydrogeological properties and regular boundary conditions. The models also simplify (or ignore) certain contaminant fate and transport mechanisms. Most of the model assumptions and simplifications lead to conservative results (that is, they will underestimate contaminant attenuation and will overestimate concentration and risk at the receptor).

One of the major deficiencies of the J&E (1991) model is that it does not include a biodegradation component. A number of studies evaluating vapour migration from the subsurface to indoor air have concluded that biodegradation has a significant effect on the resulting indoor air concentrations of petroleum hydrocarbons originating from a subsurface source (see a summary in DeVaul et al, 2002). Not accounting for biodegradation is considered to be the main reason that models such as J&E typically overestimate petroleum hydrocarbon vapour concentrations in indoor air. The J&E model is a steady-state model, and tends to overestimate the results of soil vapour diffusion which can be a slow process under field conditions. The J&E model further assumes that the contaminant source has infinite size and constant concentration - very conservative assumptions for many contaminated sites.

The Domenico (1987) model is based on the assumption of a semi-infinite contaminant plume, which will overestimate the concentrations at the receptor for many contaminated sites which have plumes of limited size and/or concentration (i.e. where substantial source reduction has been achieved). The Domenico model also does not include a rainfall infiltration component, which can be a significant attenuation factor as a contaminant migrates from a source area to a receptor.

At Tier 2, only a limited number of parameters can be adjusted to reflect site-specific conditions. For example, there is no option to adjust the default building parameters for the J&E model, and the actual house dimensions air exchange rates, etc. at the site cannot be used in the model. Of course, from a regulatory and guideline development standpoint, these restrictions are reasonable, however, they compound the challenge of using these models to simulate site-specific conditions.

Strategies of Using Regulatory Models

As required by the regulators, Tier 2 models should be used strictly for establishing site-specific guidelines or for assessing conservative “yes or no” scenarios. The models are based on a number of conservative assumptions and contain restrictions on which parameter values may be changed (and by how much), that may not be realistic at many sites. Therefore, they should not be used for predictive purposes, except for some simple sites where the conditions happen to approximate the model assumptions. Even if some parameters are based on site-specific data, the models are generally not expected to provide accurate predictions of contaminant fate and transport at the site.

For the same reason, the regulatory models should not be calibrated against field observations. Model calibration is a process to compare model prediction against field observations and determine some parameters that cannot be directly measured in field by other methods. The regulatory models and modelling procedures are not designed for prediction purposes. If model calibration is attempted incorrectly, the resultant calibrated parameter values are meaningless and unlikely to be reasonable.

Input parameters for the regulatory models can be obtained from field tests (i.e. bail tests), laboratory tests on samples (permeameter, foc, moisture, porosity) and literature searches (for most chemical property parameters). For some nonuniform but regular geological and hydrogeological structures, such as layered soil or gradually changing soil moisture content, it is possible to calculate equivalent parameter values. To apply the J&E model to layered soil, an equivalent diffusion coefficient, for example, can be obtained by calculating the harmonic average of the diffusion coefficients of different soil layers (US EPA 1997). In the next section, an example will be presented for the calculation of equivalent permeability for layered soils.

The input parameters obtained from different sources are almost always spatially and/or temporally variable. However, the regulatory models are based on analytical solutions and require a single set of input parameter values. There are many ways to select or calculate a “representative” set of input parameters. Usually the regulators require that a set of parameters to be used that produce conservative results. One of the drawbacks of this approach is that the selected parameter values are often statistical outliers among the data collected and may represent measurement errors or anomalies rather than being representative of the general site conditions. The modeling results may, therefore, be unrealistically conservative. An alternative to calculating a conservative solution using single parameter values is to use a statistical distribution to represent the parameter uncertainty variability and then to select statistically conservative solutions. An example of this approach is presented later in this paper.

Example of Calculation of Equilibrium Parameters

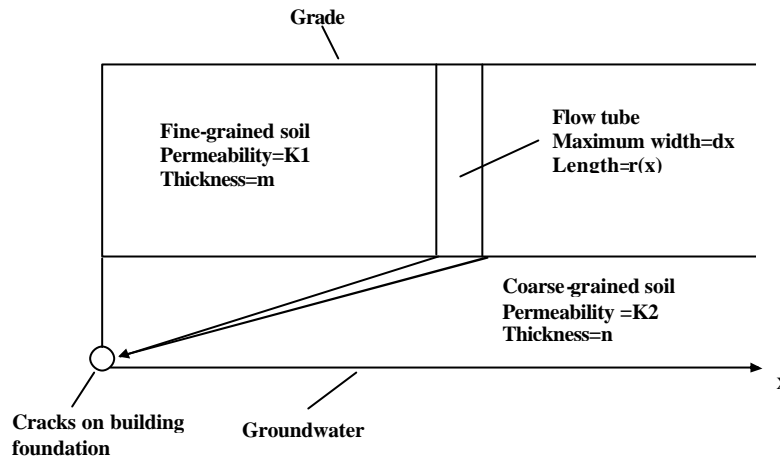


Figure 2: Air flow into building foundation cracks through two layers of soil

This example involves the calculation of an equivalent intrinsic permeability for a site with a layer of fine-grained soil underlain by coarse-grained soil. The groundwater table is encountered in the coarse soils. The calculated equivalent permeability is used in the J&E model to evaluate soil vapour migration into buildings. This example is typical of the geology at a number of petroleum hydrocarbon contaminated sites in central Alberta, where the contaminated groundwater is first encountered a few metres deep in the sand layer and a clayey silt and silty clay layer is present for the first a couple of metres below grade. Without a Tier 2 adjustment, generic inhalation pathway guidelines for coarse-grained soil have to be used since the zone of impact is in the sand layer. However, a Tier 2 calculation will reflect the effect that the shallow fine-grained soil has in reducing the soil vapour flux into the building.

For each of the simplified flow tubes as shown in Figure 1, the average air pressure gradient (J) can be expressed as:

$$J = \frac{\nabla P}{m + r(x)}$$

where: ∇P = the pressure difference between the atmosphere inside the building; m = the thickness of the length of the flow tube in the fine-grained soil layer; $r(x)$ = the average length of the flow tube in the coarse-grained soil layer. The value of $r(x)$ changes with the distance (x) from the building air entry point (foundation cracks) .

If k_1 and k_2 are the permeability of the fine-grained and coarse-grained soils respectively, the average permeability (k_{tube}) for the flow tube is expressed as:

$$k_{tube} = \frac{m + r(x)}{\frac{m}{k_1} + \frac{r(x)}{k_2}}$$

The average width of the flow tube is expressed as:

$$b = \frac{m + \frac{1}{2}n}{m + r(x)} dx$$

where dx is the maximum width of the flow tube.

According to Darcy's law, the flux through the flow tube can be expressed as:

$$q = kJb = \frac{k_1 k_2 \nabla P (m + \frac{1}{2}n)}{[mk_2 + k_1 r(x)][m + r(x)]} dx$$

With the approximation of $dx \approx dr$ (reasonable when for large x values), the total flow rate to the building can be expressed as:

$$\begin{aligned} Q &= k_1 k_2 \nabla P (m + \frac{1}{2}n) \int_n^\infty \frac{1}{[mk_2 + k_1 r(x)][m + r(x)]} dr(x) \\ &= \frac{k_1 k_2 \nabla P (m + \frac{1}{2}n)}{mk_1 - mk_2} \ln\left(\frac{k_1(m+n)}{mk_2 + nk_1}\right) \end{aligned}$$

The equivalent permeability for the whole flow system can be calculated by:

$$k = \frac{Q}{\int_n^\infty Jb dr(x)}$$

where:

$$\begin{aligned} \int_n^\infty Jb dr(x) &= \int_n^\infty \frac{\nabla P}{[m + r(x)]} \frac{m + \frac{1}{2}n}{[m + r(x)]} dr(x) \\ &= \frac{(m + \frac{1}{2}n) \nabla P}{m + n} \end{aligned}$$

and simplified as:

$$k = \frac{k_1 k_2 (m+n)}{m(k_1 - k_2)} \ln\left(\frac{(m+n)k_1}{mk_2 + nk_1}\right)$$

Table 1 shows the calculated equivalent permeability for different combinations of permeability and soil layer thicknesses. The calculated equivalent permeability value is then used to calculate the flux with the J&E model. For comparison, the vapour flux for this 2 layer system was also calculated with Modflow. As shown in the Table, the fluxes calculated using the equivalent permeability and the J&E model are similar to the Modflow results. The fluxes calculated using the J&E model and the permeability of the fine-grained soil or coarse-grained soil are not representative (too high or too low).

Table 1: Soil Gas Flux Calculation Results

k ₁ (cm ²)	k ₂ (cm ²)	m (metre)	n (metre)	Equivalent k (cm ²)	Calculated Flux Using Two Layer Modflow Model (m ³ /day)	Calculated Flux Using J&E Model (m ³ /day)		
						Using k ₁	Using k ₂	Using Equivalent k
1.00E-08	1.00E-06	2	0.3	5.19E-08	0.55	0.08	8.10	0.49
1.00E-08	1.00E-07	2	0.3	2.78E-08	0.19	0.08	0.81	0.26
1.00E-08	1.00E-08	2	0.3	1.00E-08	0.08	0.08	0.08	0.08

Evaluating Modelling Uncertainty: Example

In this real world Ontario example, the regulatory models (Domenico model together with soil/water partitioning calculations) were used to establish site-specific soil and groundwater guidelines to protect offsite surface water. Difficulties were encountered in the selection of model input parameters since the parameters exhibited significant spatial and temporal variation. Moreover, additional uncertainty was introduced by the inconsistency between the regulatory guidelines for soil and groundwater. The background groundwater concentrations, when calculated from the background soil guidelines (Table F value; MOEE, 1997), were lower or higher than the applicable surface water quality guidelines, depending on the soil/water partition coefficients used. A procedure, based on Monte Carlo simulation, was developed to quantify the uncertainty involved and produce statistically conservative site-specific soil and groundwater criteria.

The uncertainty associated with variability in three input parameters (soil/water partition coefficient, hydraulic conductivity, and hydraulic gradient) was evaluated. Parameter ranges rather than single parameter values were used in the model. The distributions of the input parameters were assumed to be uniform. A uniform distribution was chosen in the absence of more specific information regarding the actual nature of the parameter distribution.

Soil/Water Partition Coefficient (K_d)

The reported literature values for the organic carbon partition coefficient (K_{oc}) for many organic constituents of regulatory concern fall within a relatively narrow range. However, the organic carbon content (f_{oc}) in soil can vary substantially for various soil types. In this model, K_d values were calculated for organic constituents using the following equation:

$$Kd = Koc \times foc$$

The maximum and minimum Kd values were determined using the RAIS Koc values (DOE, online) and the minimum and maximum foc values measured in soil samples collected at the site.

Hydraulic Conductivity (K)

In total, twenty-three slug tests were conducted at selected monitoring wells in order to estimate K values. The minimum and maximum calculated K values were used to represent the lower and upper bounds for hydraulic conductivity in the model.

Hydraulic Gradient (I)

Groundwater at the site generally flows toward the lake and river adjacent to the site. However, groundwater flows were observed to be periodically influent during high water level periods in the lake and the river. The lower bound hydraulic gradient value used in the model was assumed to be 0 to conservatively exclude the periods of influent flow. The upper bound hydraulic gradient was assumed to be the maximum hydraulic gradient measured during various monitoring events. The maximum gradient values ranged from 0.001 to 0.005 in different areas of the site.

The site-specific soil and groundwater guidelines were calculated in a 5-step procedure as shown in Figure 2:

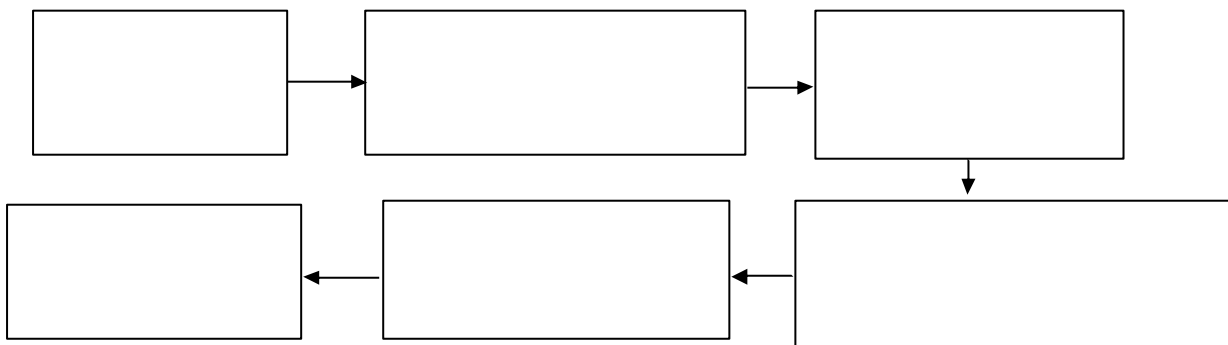


Figure 2: Procedure to calculate groundwater and soil quality guidelines

Point of Exposure (POE) values, defined as the acceptable concentration for each chemical of concern in groundwater reaching the ecological receptor areas, were determined. The POE values were determined by considering the following: (1) surface water quality objectives and; (2) the groundwater concentrations calculated to be in equilibrium with the background soil criteria. The POE values were determined according to Steps 1 through 3 of the flow chart provided in Figure 2. Generally, the larger of the surface water quality objective and the background groundwater value was selected as the governing POE value.

Following Steps 4 through 6, site-specific groundwater and soil guidelines were back-calculated from the POE values for increasing distances from the POE.

To consider the uncertainty/variability associated with some of the input parameters, the input parameters used in the determination of the site-specific criteria consisted of a range of values for parameters such as hydraulic conductivity, hydraulic gradient and Kd. For each constituent and distance from the POE, 1000 iterations of the site-specific groundwater and soil guidelines were calculated, randomly selecting various parameter values from within their range of values. The final site-specific soil and groundwater guidelines were selected to be the lower 90th percentile. The calculations were performed for increasing distances from the POE, resulting in the generation of curves for each constituent illustrating the site-specific soil and groundwater guidelines versus distance from the POE.

Table 2, Figure 3 and Figure 4 provide an example of the site-specific soil and groundwater guideline calculation procedure for toluene at a distance of 1 m from the POE. As shown in Figure 3, for small Kd values, the surface water quality guidelines are less than the calculated background groundwater concentrations, and the governing POE guidelines should be based on the background groundwater concentrations instead. Figure 4 indicates the percentiles of the calculated 1000 soil and groundwater guidelines respectively. To be statistically conservative, the lower 90th percentiles are selected as the site-specific soil and groundwater guidelines. These iterations are repeated for increasing distances from the POE and stop when the calculated site-specific guidelines exceed the maximum concentrations observed at the site (Figure 5).

The procedure demonstrated in this section provides a methodology to account for the uncertainty/variability of multiple model input parameters and the inconsistency between regulatory guidelines for different media. The lower 90th percentile is a subjective choice, but it is an explicit way to choose a statistically conservative site-specific guideline under the conditions of significant data uncertainty. Different percentiles, such as 95th or 85th percentiles, can be used following discussion between the proponents and the regulators. At this site it was not possible to select a single set of parameters, as done in a conventional way, to establish the most conservative guideline because of the interaction between different parameters. Even if such a set of parameters could be found, it was likely to be extremely biased.

Conclusions

The models provided in regulatory documents which are used to calculate and modify generic soil and groundwater guidelines contain some components to account for major natural attenuation processes. However, these models are based on conservatively simple geological situations and contaminant fate and transport mechanisms. Furthermore, only certain parameters may be modified to reflect site-specific conditions. The regulatory models should be used only for establishing site-specific criteria, not for predicting actual contaminant fate and transport at the site. The models typically can not be calibrated or validated (beyond “yes” or “no”).

Calculating equivalent parameter values may help to represent more complex (but still relatively simple) geological conditions in the regulatory models. An example is presented in this paper showing how to calculate an equivalent permeability value which can be used in the J&E model for a two layer soil system.

An example is also provided to demonstrate an approach, using Monte Carlo simulation, to account for the uncertainty in model parameters and find statistically conservative solutions. The example also shows how site-specific criteria may be determined in a situation in which the generic soil and water criteria are not internally consistent.

The regulatory models are irreplaceable tools to establish site-specific criteria following the standard procedures. The models have to be simple and conservative in nature, and cannot include all the “state of the practice” techniques which may provide a better understanding of fate and transport. It is expected that the regulatory models will evolve with the progress in academic research. More frequent communication between the regulators and environmental consultants is helpful for better application of the regulatory models. However, a one-dollar model cannot answer the million-dollar questions (simulate natural attenuation and accurately predict contaminant fate and transport), but it may be the right tool to establish site-specific guidelines and help to make site management decisions.

References

AENV (Alberta Environment), 2001, Alberta Soil and Water Quality Guidelines for Hydrocarbons at Upstream Oil and Gas Facilities, Volume 1, 2 and 3.

CCME (Canadian Council of Ministers of the Environment), 2000, Canada-Wide Standards for Petroleum Hydrocarbons (PHCs) in Soil: Technical Rationale.

Domenico, P., 1987, An analytical model for multidimensional transport of a decaying contaminant species, *J. Hydrology*, 91, 49-58.

DeVaull, G. R., Ettinger, and J., Gustafson, 2002, Chemical Vapour Intrusion from Soil or Groundwater to Indoor Air: Significance of Unsaturated Zone Biodegradation of Aromatic Hydrocarbons. *Soil & Water Contam.*, 11, 625-639.

Johnson, P.C. and , R., Ettinger, 1991, Heuristic Model for Predicting the Intrusion Rate of Contaminant Vapors into Buildings, *Environ. Sci. Technol.* 25 (8), 1445-1452.

MOEE (Ministry of Environment and Energy), 1997, Guideline for Use at Contaminated Sites in Ontario.

U.S. DOE (U.S. Department of Energy), The Risk Assessment Information System (RAIS), online at <http://risk.lsd.ornl.gov/>

U.S. EPA (U.S. Environmental Protection Agency), 1997. User's Guide for The Johnson and Ettinger (1991) Model for Subsurface Vapor Intrusion into Buildings.

Table 2 Example Calculation of Site-Specific Groundwater and Soil Guidelines

Interaction No	Variable Parameter Values			Point of Exposure (POE) Guideline			Calculated Groundwater Guideline (mg/L)	Calculated Soil Guideline (mg/kg)
	Hydraulic Gradient (0 to 0.005)	Hydraulic Conductivity (57 to 6300 m/year)	Soil Partition Coefficient K_d (0.75 to 5.9 L/kg)	Surface Water Quality Objective SWGO (mg/L)	Calculated Table F Groundwater Value (mg/L)	Governing Point of Exposure (POE) Guideline (mg/L)		
1	3.2E-04	498	2.3	0.0008	0.0008	0.0008	2.0E-03	7.4E+05
2	2.1E-03	2789	5.7	0.0008	0.0003	0.0008	4.7E-03	9.0E-02
3	1.3E-03	333	1.6	0.0008	0.0011	0.0011	2.0E-03	1.0E+01
4	4.1E-03	258	3.8	0.0008	0.0005	0.0008	3.2E-03	1.0E+01
5	2.5E-03	2552	4.6	0.0008	0.0004	0.0008	3.9E-03	4.2E-02
6	3.7E-04	205	3.8	0.0008	0.0005	0.0008	3.2E-03	3.2E+07
7	8.0E-04	369	4.7	0.0008	0.0004	0.0008	4.0E-03	3.9E+06
8	4.4E-03	2472	2.7	0.0008	0.0007	0.0008	2.4E-03	6.2E-03
9	5.7E-04	351	4.9	0.0008	0.0004	0.0008	4.1E-03	4.1E+07
10	8.8E-04	131	1.7	0.0008	0.0010	0.0010	2.0E-03	2.1E+06
Continued ...								
995	3.1E-04	179	3.7	0.0008	0.0005	0.0008	3.1E-03	3.1E+07
996	3.0E-03	265	2.2	0.0008	0.0008	0.0008	2.0E-03	2.2E+00
997	5.1E-05	144	3.0	0.0008	0.0006	0.0008	2.6E-03	2.6E+07
998	3.0E-03	5654	5.4	0.0008	0.0004	0.0008	4.5E-03	1.4E-02
999	9.1E-04	160	3.5	0.0008	0.0005	0.0008	3.0E-03	3.0E+07
1000	6.4E-04	570	2.2	0.0008	0.0008	0.0008	2.0E-03	2.1E+02

The 90th Lower Percentile of Calculated Guidelines: 2.0E-03 7.1E-03

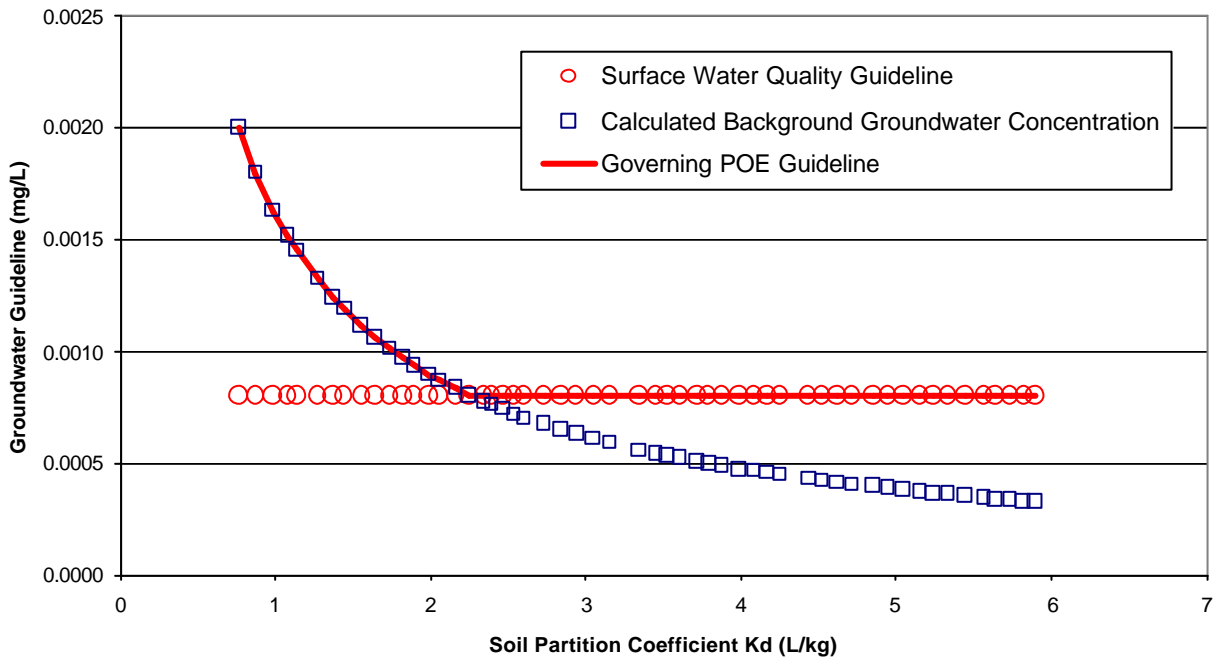


Figure 3 Determine governing point of exposure (POE) guidelines for toluene at 1 m from the river

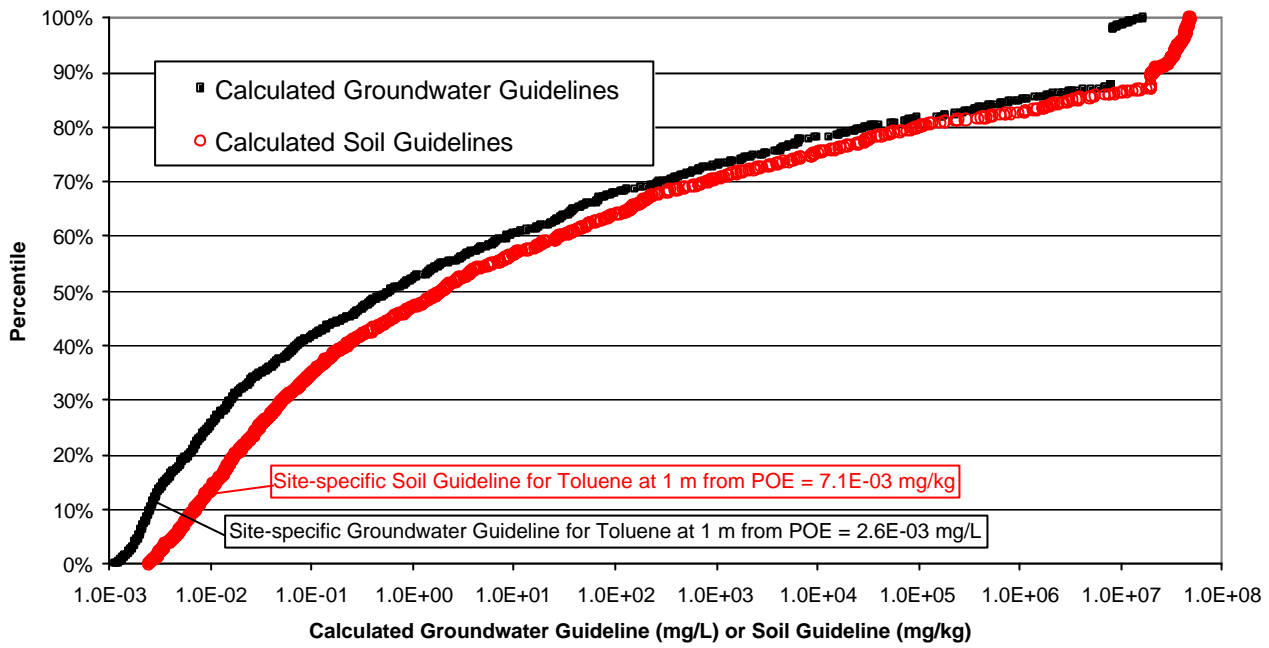


Figure 4 Percentiles of calculated groundwater and soil guidelines for toluene at 1 m from the river

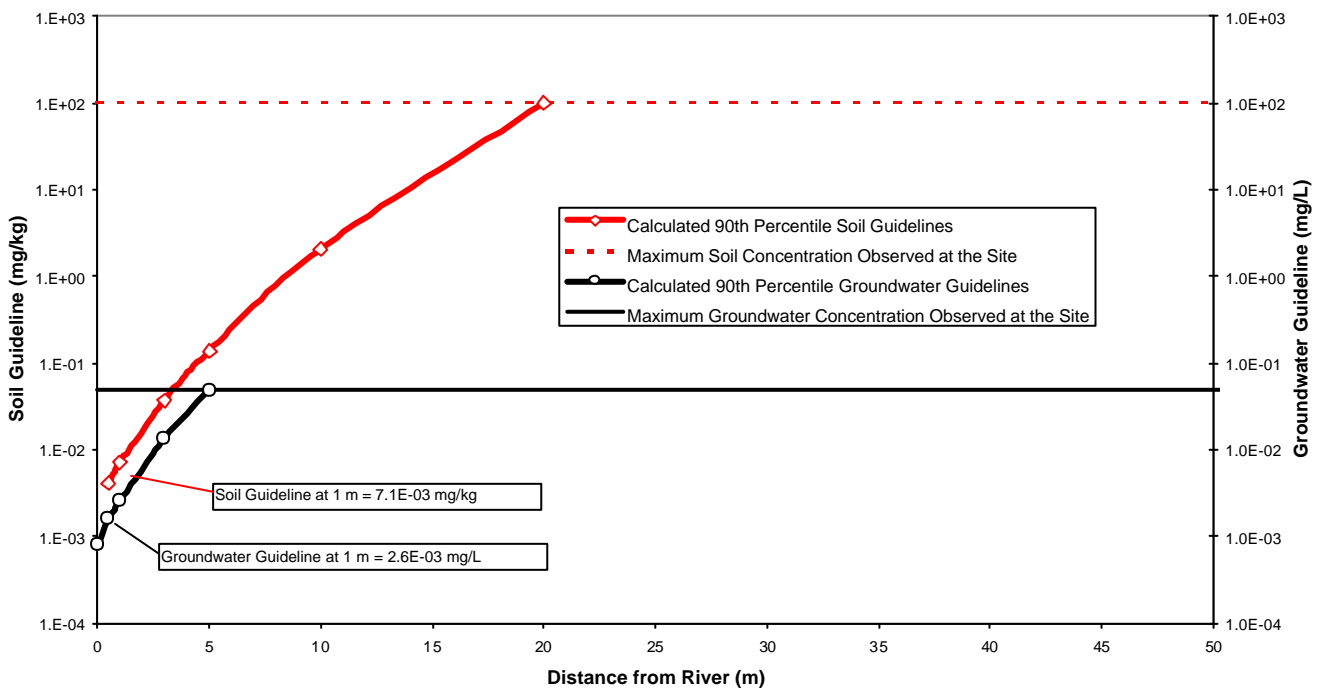


Figure 5 Calculated soil and groundwater guidelines for toluene at increasing distances from the river