Review of Approaches for Modelling Vapour Migration into Trenches and Excavations

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1.0 INTRODUCTION

1.1 General

Meridian Environmental Inc. (Meridian) has been contracted by the Canadian Council of Ministers of the Environment (CCME) to conduct a review of potential approaches for modelling vapour migration into trenches and excavations and to recommendat a methodology for calculating management limits for this pathway. This report summarizes that review and provides an illustrative example of the recommended approach.

1.2 Background

A Protocol for the Derivation of Environmental and Human Health Soil Quality Guidelines (CCME, 2006) allows for the derivation of soil quality guidelines for management considerations (SQG_M) to address risks posed by chemicals other than those considered in the human health and environmental guidelines. The companion protocol for groundwater quality guidelines will also allow for management limits.

These management limits can be based on factors not related to toxic effects on human or ecological receptors, such as aesthetic concerns, free product formation, explosive hazards or effects on buried infrastructure. Management limits can also be derived to reflect human or ecological exposure pathways that are either chemical-specific, based on pathways for which standardized methods have not been developed, or are subject to a high level of uncertainty. In most cases it is expected that the management limit would not be the governing exposure pathway; however, in some cases they may be used as “upset limits” in the event that critical human and environmental pathways are inoperative at a site or may aide with the development of site-specific (Tier 2/Tier 3) strategies.

A management limit based on the exposure of workers in trenches was calculated for the Canada-Wide Standard for Petroleum Hydrocarbons in Soil (CCME, 2008) using a modified version of a model developed by the Virginia Department of Environmental Quality (VDEQ); other similar models are available however. The CCME Soil Quality Guidelines Task Group (SQGTG) has determined that a management limit based on effects on workers in trenches may be appropriate for substances that are highly volatile and have high inhalation toxicity to humans, due to the potential for significant exposure in a trench scenario. The purpose of this project is to re-evaluate the VDEQ approach and develop methods for evaluating the exposure of workers in trenches, which could potentially be applied to calculate management limits for the exposure of workers in trenches.

The expected use of this management limit is as a “check” value if other exposure pathways are eliminated or adjusted upwards on a site-specific basis, to ensure that any such site-specific adjustments do not result in risks to other receptors. It is anticipated that a site remediated to meet this guideline value would not result in unacceptable health risks from n-hexane migrating into trenches or excavations during any future site work, but this guideline is not intended to replace appropriate occupational health and safety measures during excavation work at contaminated sites. The approach developed herein is limited to addressing predicted exposures to the substance of concern, and does not address hypoxia caused by contaminant gases or by-products (e.g. CO_2) displacing breathable trench air.

1.3 Scope of Work

This project was conducted in accordance with a Request for Proposals issued by CCME SQGTG. The scope of work includes the following tasks:

1. Review of the Virginia Department of Environmental Quality model that was previously used by CCME (2008), along with other models which are currently available, including US EPA models and a model derived by Ontario Ministry of the Environment. A preliminary review of the models was conducted to determine whether they could potentially be used or adapted for the calculation of management limits, with potentially useful models undergoing a more detailed review.

2. Recommendation of the most appropriate model for the development of a management limit for the exposure of workers in trenches, based on ease of use and application, suitability for evaluating this pathway, and the reliability and scientific defensibility of model predictions. Recommendations are also made with respect to the scenarios to be evaluated, along with appropriate model input parameters and assumptions.

3. Perform illustrative calculations using n-hexane as an example.

2.0 REVIEW OF TRENCH MODELS

2.1 General Model Characteristics and Conceptual Model

Models for the infiltration of contaminant vapours into trenches and excavations share the same general underlying processes, including:

- volatilization of soil and/or groundwater contaminants;
- migration of vapours into the trench;
- mixing of contaminant vapours in the trench; and,
- removal of vapours from the trench via air exchange with outdoor air.

These processes are illustrated in Figure 1.

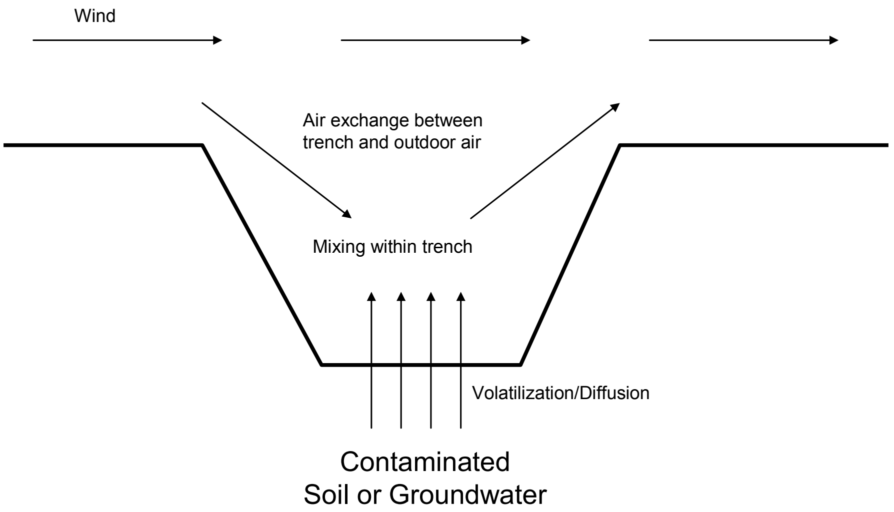

Figure 1: Conceptual Model for Vapour Infiltration into Trenches

2.2 Virginia Trench Model

The Virginia Department of Environmental Quality (VDEQ) published an approach and spreadsheet for predicting exposure of workers to volatiles in construction and utility trenches (VDEQ, 2010). The approach includes two different approaches for estimating volatilization of a contaminant from groundwater to a trench – one based on groundwater pooling in the trench, and the other based on contaminant transport through the vadose zone. A box model is used to estimate dilution within the trench.

The primary equation used is:

$$C_{tremch} = C_{GW} \times VF$$

where:
C_{trench} = concentration of contaminant in trench (µg/m^3)
C_{GW} = concentration of contaminant in groundwater (µg/L)
VF = volatilization factor (see below)

Where groundwater is not in contact with the excavation, the following equation is used to calculate the volatilization factor (certain variables were renamed for consistency with CCME documents):

$$VF = \frac{H \times D_{air} \times \theta_a^{3.33} \times A \times F \times 10^{-3} \times 10^{4} \times 3600}{R \times T \times L_d \times ACH \times V \times n^2}$$

where:

H = Henry's law constant for contaminant (atm-m^3/mol)

D_{air} = diffusion coefficient in air (cm^2/s)

θ_a = volumetric air content in vadose zone (dimensionless)

A = area of trench (m^2)

F = fraction of floor through which contaminant can enter (dimensionless)

R = gas constant (atm-m^3/mol-K)

T = average system temperature (K)

L_d = distance between trench bottom and groundwater (cm)

ACH = air changes per hour (h^{-1})

V = volume of trench (m^3)

n = total soil porosity in vadose zone (dimensionless)

10^{-3} = conversion factor (L/cm^3)

10^4 = conversion factor (cm^2/m^2)

3600 = conversion factor (s/h)

When groundwater is pooling in the trench, the following equation is used instead:

$$VF = \frac{K_i \times A \times F \times 10^{-3} \times 10^4 \times 3600}{ACH \times V}$$

$$K_i = \frac{1}{\frac{1}{k_{iL}} + \frac{R \times T}{H \times k_{iG}}}$$

$$k_{iL} = \left(\frac{MW_{O2}}{MW_i}\right)^{0.5} \times \frac{T}{298} \times k_{L,O2}$$

$$k_{iG} = \left(\frac{MW_{O2}}{MW_i}\right)^{0.335} \times \left(\frac{T}{298}\right)^{1.005} \times k_{G,O2}$$

where:

K_i = overall mass transfer coefficient of contaminant (cm/s)

k_{iL} = liquid-phase mass transfer coefficient (cm/s)

k_{iG} = gas-phase mass transfer coefficient (cm/s)

MW_{O2} = molecular weight of O_2 = 32 g/mol

MW_i = molecular weight of contaminant (g/mol)

$k_{L,O2}$ = liquid-phase mass transfer coefficient of oxygen at 25°C = 0.002 cm/s

$k_{G,O2}$ = gas-phase mass transfer coefficient of oxygen at 25°C = 0.833 cm/s

Based on urban canyon studies and consultation with United States Environmental Protection Agency (US EPA) Region III, an air exchange rate of 2/h is used when the trench depth is greater than the trench width (relative to the wind direction), to reflect circulation cells within the trench limiting gas exchange with the atmosphere. When trench width exceeds the trench depth, air exchange between the trench and atmosphere is considered unrestricted and an air exchange rate of 360/h is used based on the ratio of trench depth to average wind speed.

This model is relatively straightforward and appears to be technically sound. While VDEQ (2010) defines default values for most model parameters, they are readily adjusted. A spreadsheet version of the model is publicly available. It was originally designed for groundwater contamination; the management limits for petroleum hydrocarbons in soil (CCME, 2008) were calculated using a modified version of the model to account for a soil source.

2.3 US EPA Trench Volatilization Factor

US EPA Region 8 published a model describing volatilization of contaminants from groundwater into trenches and excavations (US EPA, 1999):

$$VF = \frac{k_{\mathrm{lg}} \times L \times 1000}{k \times \mu \times H}$$

where:
VF = volatilization factor (mg/m^3 air per mg/L water)
k_{lg} = mass transfer coefficient from liquid to gas phase (assumed to be 3.0x10^{-6} m/s)
L = average trench length
H = average trench depth
μ = average wind speed in excavation (assumed to be 0.45 m/s)
k = air mixing rate between trench and ambient air

Using an assumed 30 m x 3 m trench US EPA (1999) developed a default volatilization factor of 0.133 (L/m^3). The groundwater concentration seeping into the trench is multiplied by this factor to estimate an upper-bound concentration in air in the trench.

This model is limited to scenarios where groundwater is pooling in the excavation.

2.4 American Society for Testing and Materials Model

The American society for Testing and Materials (ASTM, 2004) has published equations to develop risk based screening levels; while the model is designed for outdoor air exposures it could be applied to trench exposure scenarios. Two separate scenarios can be modelled with these equations, one assuming trench surfaces intersect contamination and the second assuming that the trench surface does not come in contact with contamination. Both scenarios require calculation of a dispersion factor for the trench surface which can be adjusted to account for trench dimensions including trench floor and trench wall area, as well as air velocity in the mixing zone (wind speed influences). Separate approaches are used to calculate a volatilization factor from soil to air depending on whether contamination is directly exposed to trench air.

The surface soil model includes the following assumptions:

- The contaminant is uniformly distributed in the affected soils.
- Partitioning between sorbed, dissolved and vapour phases is based on linear equilibrium partitioning.
- The chemical diffuses through the surficial soil layer.
- There is no biodegradation or other loss of the chemical.

- Vapours are well mixed in the atmosphere as modelled by a box model.
- If the time-averaged flux exceeds what would occur if the entire mass of contaminant was volatilized over the averaging time, then the volatilization factor is determined using a mass balance relationship instead.

Depth to source can be adjusted to reflect the depth from the base of the excavation to the source. Alternatively, when groundwater is pooled in the trench a volatilization factor can be calculated accounting for loss from groundwater instead of soil. Risk-based screening levels from soil can be calculated using the volatilization factor and a target concentration in air.

$$DF_{amb} = \frac{U_{Air} \times W \times \delta_{Air}}{A}$$

where:

DF_{amb} = dispersion factor for ambient air from trench surface (cm/s)
U_{Air} = ambient air velocity in mixing zone (cm/s)
W = width of source-zone area (cm)
δ_{Air} = mixing zone height (cm)
A = source-zone area (cm^2)

$$D_{eff-vadose} = D_{air} \times \left(\frac{\theta_{air}^{3.33}}{n^2} \right) + D_{water} \times \left(\frac{\theta_{water}^{3.33}}{H_{eff} \times n^2} \right)$$

where:

$D_{eff-vadose}$ = dispersion factor for ambient air from trench surface (cm^2/s)
D_{air} = molecular diffusion coefficient in air (cm^2/s)
D_{water} = molecular diffusion coefficient in water (cm^2/s)
H_{eff} = effective Henry's Law coefficient (dimensionless)
θ_{air} = volumetric air content of soil (dimensionless)
θ_{water} = volumetric water content of soil (dimensionless)
n = total soil porosity (dimensionless)

VF_{ss} = the lower of $VF_{ss,1}$ or $VF_{ss,2}$:

$$VF_{ss,1} = \frac{\rho_b}{DF_{amb}} \sqrt{\frac{4 \times DF_{eff-vadose} \times H_{eff}}{\pi \times t \times 31536000\ sy^{-1} \times K_d \times \rho_b}}$$

$$VF_{ss,2} = \frac{\rho_b \times L_{ss}}{DF_{amb} \times t \times 3153600\,\mathrm{sec}/yr}$$

where:

VF_{ss} = volatilization factor, surficial soil to ambient outdoor air (g/cm^3)
DF_{amb} = dispersion factor for ambient air (cm/sec)
ρ_b = soil bulk density (g/cm^3)
L_{ss} = thickness of surficial soils (cm)
t = average time for surface emission vapour flux (yrs)
$D_{eff-vadose}$ = dispersion factor for ambient air from trench surface (cm^2/s)
H_{eff} = effective Henry's Law coefficient (dimensionless)
K_d = soil to water partition coefficient (cm^3/g)

$$VF_{sub} = \frac{1}{\left(1 + \frac{DF_{amb} \times L_s}{D_{eff-vadose}}\right) \times \frac{K_d}{H_{eff}}}$$

where:
VF_{sub} = volatilization factor, subsurface soil to ambient outdoor air (g/cm^3)
DF_{amb} = dispersion factor for ambient air (cm/sec)
$D_{eff-vadose}$ = dispersion factor for ambient air from trench surface (cm^2/s)
H_{eff} = effective Henry's Law coefficient (dimensionless)
L_s = depth to subsurface soils (cm)
K_d = soil to water partition coefficient (cm^3/g)

$$RBSL_s = \frac{RBSL_{air}}{VF} \times 10^{-3}$$

where:
$RBSL_s$ = risk-based screening level for soil (mg/kg)
$RBSL_{air}$ = risk-based screening level for air inhalation (mg/m^3)
VF = volatilization factor, soil to ambient air (g/cm^3)

Note: the VF used in the above equation will correlate to either the subsoil or surface soil volatilization; only one will be used to calculate the risk based soil screening level.

This model assumes that vapour concentrations remain constant over the duration of exposure and all inhaled chemicals are absorbed. The calculation of the diffusion coefficient from the vadose zone assumes homogeneous soil layers. These equations published by ASTM (2004) are part of a body of equations used to develop risk-based screening levels and generally have a high level of regulatory acceptance. The application of these equations to a trench exposure scenario can be done through the manipulation of model inputs to reflect the source area and mixing zone of the trench, but are essentially applied without change.

The basis of the equations is not thoroughly documented. There is a reference to the US EPA (1988) Superfund Exposure Assessment Manual, but the specific equations published by ASTM (2004) do not appear to be in that document.

2.5 Jury Model

The original Jury model published in 1983 updated with a simplified equation in 1990, and used to calculate volatilization losses for both infinite and finite sources. In general, both models describe the vapour-phase diffusion of the contaminants to the soil surface and lost by volatilization to the atmosphere, establishing the relationship between vapour and solute diffusion and adsorption by defining total phase concentration partitioning as it relates to the effective diffusion coefficient. Each model predicts an exponential decay curve over time once equilibrium is achieved; determined by the rate at which contaminants diffuse upward. The simplified equation applies the following assumptions (US EPA, 1996):

- uniform soil properties,
- instantaneous linear adsorption,
- linear liquid-vapour partitioning
- contaminants in dissolved phase only; soil concentration is below saturation limit,
- no stagnant air layer, or boundary layer thickness,
- no water evaporation of leaching,
- no chemical reactions including biodegradation or photolysis, and
- diffusion occurs simultaneously across the upper boundary and the lower boundary.

The model is therefore limited to surface contamination extending to a known depth and does not account for subsurface contamination covered by a layer of clean soil. Both models do not account for the high initial rate of volatilization before equilibrium is attained and will tend to under predict emissions during this period (Environmental Quality Management, 1995). The model does also not consider mass flow of contaminants due to water movement in the soil profile, or the volatilization rate of saturated soils or non-aqueous phase liquids.

The US EPA commissioned a study to validate the relative accuracy of the Jury volatilization models using experimental emission flux data (Environmental Quality Management, 1995). From the results of this study, it was concluded that for the compounds included in the experimental data, both models showed good agreement with measured data given the conditions of each test. Each model demonstrated a high agreement with bench-scale measured values, and to a lesser extent the infinite source model showed reasonable agreement with pilot-scale data, and overall these models are expected make reasonable estimates of loss through volatilization at the soil surface given the boundary conditions of each model.

The simplified finite source model as implemented by US EPA (1996, 2002) can be seen below, first calculating the apparent diffusivity followed by contaminant flux. Finally, once the contaminant flux is calculated then a volatilization factor is calculated to give m^3/kg of contaminant released per kg of soil. US EPA has created a publically available model largely based on the Jury model called EMSOFT which could be used to calculate volatilization factors.

$$J_s = C_o \left(\frac{D_A}{\pi t} \right)^{\frac{1}{2}} \left[1 - \exp\left(\frac{-d_s^{\ 2}}{4 D_A t} \right) \right]$$

where:

J_s = contaminant flux at ground surface (g/cm^{2}sec)

C_o = uniform contaminant concentration at t=0 (g/cm^3)

D_A = apparent diffusivity (cm^2/s)

d_s = depth of uniform soil contamination at t=0 (cm)

t = time (seconds)

$$D_A = \frac{\left\lfloor \dfrac{\theta_a^{\;10/3} D_i H' + \theta_w^{\;10/3} D_w}{n^2} \right\rfloor}{\left(\rho_b K_d + \theta_w + \theta_a H'\right)}$$

where:

D_A = apparent diffusivity (cm^2/s)

θ_a = air filled porosity

n = total soil porosity

θ_w = water-filled soil porosity

D_w = diffusivity in water (cm^2/s)

D_i = diffusivity in air (cm^2/sec)

H' = dimensionless Henry's Law constant

ρ_b = soil dry bulk density (g/cm^3)

K_d = soil-water partition coefficient (cm^3/g)

$$VF = \left(\frac{Q}{C}\right) \times \left(\frac{C_o}{\rho_b}\right) \times \left(\frac{1}{J_s}\right) \times 10^{-4}$$

where:

VF = volatilization factor (m^3/kg)

J_s = contaminant flux at ground surface (g/cm^{2}sec)

C_o = uniform contaminant concentration at t=0 (g/cm^3)

ρ_b = soil dry bulk density (g/cm^3)

$\frac{Q}{C}$ = inverse concentration factor for air dispersion (g/m^2 per kg/m^3). If an area emission rate of 1 g/m^{2}s is assumed, then (Js x 10^{-4} cm^2/m^2) = 1, and the equation simplifies to simply the inverse of the maximum contaminant air concentration (kg/m^3).

2.6 Ontario Ministry of the Environment Model

A trench model was developed by staff at the Ontario Ministry of the Environment (OMOE), based on an assumed 13 m long, 1 m wide, 2 m deep excavation through the middle of the contaminated soils. The model starts with the allowable chemical concentration in a trench, back-calculates an allowable flux rate based on an air exchange rate of 2/h, and uses the Jury model (described above) to calculate an allowable soil concentration from the flux rate. The Jury model is used sideways/horizontally in this case, which is considered acceptable since diffusion is isotropic. The model assumes that the trench sidewalls are potentially contaminated rather than groundwater beneath the trench (Goodwin, 2009, personal communication).

The model uses the following equations (Goodwin, 2009, personal communication):

$$J = \frac{C_A \times ACH \times V}{3600 \times A_E \times 10^{12}}$$

where:
J = allowable flux rate (g/cm^2-s)
C_A = allowable concentration in air (µg/m^3)
ACH = air exchange rate (h^{-1})
V = excavation volume (cm^3)
A_E = contaminated soil area exposed (cm^2)

$$D_{eff} = \frac{\theta_a^{3.33} \times D_{air} \times H' + \theta_w^{3.33} \times D_w}{n^2 \times \left(\rho_b \times K_{oc} \times f_{oc} + \theta_w + \theta_a H'\right)}$$

where:
D_{eff} = effective diffusivity (cm^2/s)
θ_a = volumetric air content of soil (dimensionless)
θ_w = volumetric water content of soil (dimensionless)
D_{air} = chemical diffusivity in air (cm^2/s)
D_w = chemical diffusivity in water (cm^2/s)
H' = dimensionless Henry's law constant
n = total soil porosity (dimensionless)
ρ_b = soil bulk density (g/cm^3)
K_{oc} = chemical organic carbon partitioning coefficient (cm^3/g)
f_{oc} = soil organic carbon fraction (g/g)

$$C_s = \left(\frac{J}{C_{t,1} \times P}\right)\left(\frac{1000000}{\rho_b}\right)$$

$$C_{t,1} = \left(\frac{D_{eff}}{\pi \times t}\right)^{0.5}$$

$$P = 1 - \exp(-Q)$$

$$Q = \frac{d^2}{4 \times D_{eff} \times t}$$

where:

C_s = allowable concentration in soil (µg/g)
$C_{t,1}$ = concentration in trench air at time (t) = 1 s
ρ_b = soil bulk density (g/cm^3)
t = time (s) = 1 s
d = average thickness of soil source zone behind trench face (cm)
D_{eff} = effective diffusivity (cm^2/s)
J = allowable flux rate (g/cm^2-s)

This model was specifically designed for a soil source, appears to be technically sound. It has been coded into spreadsheet form.

2.7 Modified Hwang & Falco Model

Another finite source volatilization model was developed by Hwang and Falco (1986) and functions with many of the same assumptions as the Jury model including uniform distribution of contamination across soil depth or the consideration of liquid phase on equilibrium partitioning. A concentration gradient is established across soil depth as emissions occur from the soil surface, and limits the emission rate as time elapses. Therefore a transient volatilization rate at time x is established representing an instantaneous emission rate which decreases as a function of time. Both the Jury model and the Hwang and Falco model would be used to calculate a volatilization factor that would then be used to calculate soil screening levels.

This model is currently used by BC Environment in their calculation of Soil Odour Quality Standards (BC Environment, 1996), and provides default parameter inputs. To derive these standards the Hwang and Falco model is applied in conjunction with physical properties of site contamination like length and area of contamination and could be modified for a trench exposure scenario to consider diffusion height as trench height. Importantly this model also considers the influence of wind; however air exchanges or mixing rates within the trench are not. The equations shown below consider Hwang and Falco model used in the calculation of a volatilization factor as used by BC Environment.

$$VF = \left(\frac{LS \times V \times DH}{A}\right)\left(\frac{\sqrt{\pi\alpha t}}{2D_{eff}\,\theta_{air}K_d \times 10^{-3}\,kg/g}\right)$$

where:
VF = volatilization factor (m^3/kg)
LS = length of side of contaminated area (m)
V = wind speed in mixing zone (m/s)
DH = diffusion height (m)
A = area of contamination (cm^2)
θ_{air} = air filled porosity (dimensionless)
D_{eff} = dispersion factor for ambient air from trench surface (cm^2/s)
D_{air} = chemical diffusivity in air (cm^2/s)
t = time (seconds)
H_{eff} = effective Henry's Law coefficient (dimensionless)
Kd = soil-water partition coefficient (cm^3/g)
C = contaminant concentrations (t=0)

$$\alpha = \frac{D_{eff}\theta_{air}}{\theta_{air} + \frac{\rho_p\left(1-\theta_{air}\right)}{Kd}}$$

where:

α = diffusivity (cm^2/s)
θ_{air} = air filled porosity (dimensionless)
D_{eff} = dispersion factor for ambient air from trench surface (cm^2/s)
D_{air} = chemical diffusivity in air (cm^2/s)
t = time (seconds)
H_{eff} = effective Henry's Law coefficient (dimensionless)
Kd = soil-water partition coefficient (cm^3/g)
ρ_p = particle density (g/cm^3)

$$D_{eff} = D_{air}\frac{\theta_{air}^{3.33}}{n^2}$$

where:

D_{eff} = dispersion factor for ambient air from trench surface (cm^2/s)
θ_{air} = air filled porosity (dimensionless)
D_{air} = chemical specific molecular diffusivity in air (cm^2/s)
n = total soil porosity (dimensionless)

Noteworthy, inconsistencies were discovered in the Hwang and Falco equations in a model validation study contracted by the US EPA (Environmental Quality Management, 1992). Resultant modifications were made to the model, however, the model continued to produce errors. The Hwang and Falco model previously used by the US EPA in soil screening guidance was therefore replaced by the Jury model (US EPA, 1996).

3.0 MODEL EVALUATION AND RECOMMENDATIONS

Several models have been reviewed above; while most were designed primarily for volatilization to outdoor air, they can be adapted for trench exposures with appropriate parameterization.

The underlying principles for the models reviewed are generally similar. The primary differences arise from the calculation of the vapours entering the trench; some models calculate a vapour concentration using equilibrium partitioning and diffusion through soil, while others calculate a rate of vapour emissions from groundwater.

Some of the evaluated models (e.g. Virginia trench model and US EPA volatilization factor) are based on groundwater pooling in the bottom of an excavation. While these models could be used to derive a soil guideline using the soil-water partitioning equation (i.e. effectively calculating a soil guideline for the protection of groundwater pooling in excavations), this approach would not allow for consideration of scenarios where the trench was excavated through shallow contamination and contaminated soils are present along the sidewalls of the trench.

The Jury model (either the original version, the US EPA implementation or the Ontario implementation) and the ASTM model can address the expected scenarios for management limit calculation, since they can be used with a soil source and allow for an excavation directly in contact with contamination along the base, sidewalls or both. The Jury model and ASTM model both have at least some degree of regulatory acceptance and review.

All of these models can be considered to have two main components: a description of the volatilization of contaminants from soil and into air (i.e. the trench) and mixing of the contaminant within the trench air. The approaches these models use for these two components are discussed below.

3.1 Volatilization of Contaminants from Soil to Air

The ASTM model uses 2 equations for volatilization from surface soils, with the lower of the calculated volatilization factors used. The underlying basis for these equations is not clearly documented. The first equation incorporates the rate of volatilization from soil (based on partitioning relationships and diffusivity), and averages the volatilization over a specified averaging time. The second of these effectively assumes that the entire mass of contamination within the specified thickness of contaminated soils enters the air above the soil over the averaging time and is essentially a mass balance check for long-term exposures.

While the specific basis of the ASTM model is not clearly documented, it appears to be based at least in part on an earlier US EPA (1988) approach, which has since been replaced. Furthermore, based on both the use of a time in years in the equation and on information in the US EPA (1988) document, it is likely an approach developed for long-term average emission rates, which may not be appropriate for short-term exposures of workers in trenches.

The Jury model is generally based on similar principles to the ASTM model, including partitioning from soil to pore water and vapour, and diffusivity in soils. The basis for this model is documented in a series of peer-reviewed publications, and it has been adopted by US EPA (1996, 2002). There have been validation tests conducted on the model (Environmental Quality Management, 1995), which generally support the accuracy of the Jury model for predicting contaminant fluxes from soil.

Overall, while both models are similar, the Jury model appears to have more current regulatory acceptance and validation testing. There are also, as discussed above, indications the ASTM model may have been based on long-term releases instead of shorter-term releases appropriate for evaluation worker exposure scenarios.

3.2 Mixing of Contaminants in Air

While the presentation varies, all of the models evaluated use a simple box model to evaluate mixing of contaminants in air. Some modelling approaches presented this box model using a wind speed, while others used an air exchange rate. Mixing in ambient air can be expressed using the equations below:

$$DF_{amb} = \frac{U_{Air} \times W \times \delta_{Air}}{A}$$

Or

$$DF_{amb} = \frac{ACH \times V}{3600 \times A}$$

where:
DF_{amb} = dispersion factor for ambient air from trench surface (cm/s)
U_{Air} = ambient air velocity in mixing zone (cm/s)
W = width of source-zone area (cm)
δ_{Air} = mixing zone height (cm)
A = source-zone area (cm^2)
ACH = air exchange rate (h^{-1})
V = trench volume (cm^3)
3600 = unit conversion (s/h)

The two approaches are functionally the same. It is possible to convert the air exchange rate to a wind speed (or vice versa) by simplifying the equations:

$$U_{Air} = \frac{ACH \times L}{3600} \quad \text{or} \quad ACH = \frac{U_{Air} \times 3600}{L}$$

Overall it makes no difference whether an air exchange rate or a wind speed is used as the basis for evaluating mixing of vapours in the trench, since they can be readily be converted to the other form.

The alternative to using a box model is to couple the volatilization rate from soil with an air dispersion model. However, air dispersion models are generally not designed to reflect air movement within trenches and excavations, and therefore this approach is not expected to be practical for the derivation of soil management limits.

3.3 Recommendations

Based on the above application, the Jury model is recommended for the evaluation of vapour migration into trenches. For simplicity, the analytical solution used by US EPA (1996, 2002) and OMOE is expected to be a practical version that can be readily coded into spreadsheet form.

For mixing in trench air, there is effectively no difference between the approaches applied. Since deep, narrow trenches may behave more like buildings than the atmosphere (VDEQ, 2010), a box model based on an air exchange rate may be easier to work with, but conversion between air exchange rates and wind speeds is simple.

4.0 SENSITIVITY ANALYSIS AND MODEL INPUT PARAMETER RECOMMENDATIONS

Many of the model input parameters are chemical properties or soil properties. Chemical properties should be adopted from reputable sources and, for properties used in other soil guideline calculations, match the values used for the evaluation of other pathways. Soil properties are based on CCME defaults for coarse and fine soils. For the calculations presented herein, n-hexane is used as a case study; the physical-properties of n-hexane specified by CCME (2009 draft) are applied herein.

The other key model parameters are the excavation dimensions, area impacted, air exchange rate and time. In order to evaluate the influence of these parameters, a sensitivity analysis was undertaken.

4.1 Model Sensitivity Analysis

In order to determine the effect of varying key model parameters, the Jury model was encoded into spreadsheet form. The ASTM model was also encoded into the spreadsheet for reference. An initial set of model parameter values was specified as a starting point (based on a trench in coarse-grained soils); these values are summarized in Table 1. The assumed scenario is a trench excavated through contaminated soil, with both sidewalls of the trench contaminated but the base of the excavation uncontaminated. Individual parameters were then adjusted; the results of these adjustments are summarized in Table 2.

Allowable Concentration in Air

The tolerable concentration (TC) for chronic exposure to n-hexane is 0.7 mg/m^3; when adjusted to account for the background atmospheric n-hexane concentration of 0.002 mg/m^3, and for an occupational exposure scenario, the allowable concentration in trench air would be approximately 2.55 mg/m^3.

Management limits calculated using the chronic TC may be very low, however. Concentrations of vapours in trenches with low air exchange may be higher than concentrations in buildings, due to the absence of a concrete foundation slab, and as a result the calculated guidelines may be lower than indoor vapour inhalation guidelines. However, it is expected that exposures in trenches would generally be for an acute or sub-chronic duration rather than chronic. Furthermore, the exposed population would likely be limited to working-age adults. Therefore, it may be appropriate to use an occupational exposure limit instead of a chronic TC (which was the approach used for this pathway for the Canada-Wide Standard for Petroleum Hydrocarbons in Soil). The occupational exposure limit for n-hexane published by the American Council of Government Industrial Hygienists (ACGIH) is 176 mg/m^3 as an 8-hour time-weighted average.

Calculations are provided using both the TC (adjusted for the exposure scenario) and the ACGIH occupational exposure limit.

Time

Time since contamination is a parameter in the model. The models predict that the vapour flux will initially be high, decreasing over time.

While the time since contamination is often unknown, in the case of a trench being excavated through contaminated soil, the time of the excavation can be taken as „time 0'. The time was adjusted from 1 s to 28 800 s (8 h) in the Jury model to evaluate the change in flux over an 8-hour work day, and its associated influence on allowable soil concentrations. The results are provided in Figures 1 and 2. Results calculated using the ASTM model are also provided for reference.

As shown in the figures, if the calculation is based on a worst-case time of 1 s, the resulting allowable soil concentration is very low. There is a rapid initial increase, followed by a gradual levelling off.

The optimum approach for calculating the allowable exposure limit would be to take a time-weighted average over an 8-hour work day. Shorter time frames could also be evaluated (against corresponding short-term exposure limits).

Air Exchange Rate/Wind Speed

The air exchange rate (or wind speed) is a sensitive model parameter. As shown in Table 2, there is a direct linear relationship between air exchange rate and the allowable soil concentration.

Trench Dimensions

The effects of altering trench dimensions are shown in Table 2. The model is sensitive to the trench width, with a doubling of the width resulting in the allowable concentration doubling. Based on a constant air exchange rate, altering the excavation length and depth has no effect on the results. If wind speed was kept constant instead, increasing the excavation length would decrease the air exchange rate, resulting in each doubling of the excavation length decreasing the allowable soil concentration by a factor of 2.

Fraction of Surface Area Exposed

The fraction of surface area exposed represents the proportion of the excavation wall/base area which is open to vapour diffusion and in contaminated soils. The default value of 0.5 was adopted from OMOE, and represents a situation where 50% of the excavation sidewalls are either covered (e.g. by shoring) or uncontaminated (i.e. either contamination does not extend from surface to the full depth of the trench, or one side of the excavation is not in contaminated soils). Since a trench with depth greater than width would normally require shoring under occupational health and safety regulations, and trenches with width greater than depth would have higher air exchange rates than assumed herein, this assumption is considered reasonable. Increasing the fraction exposed to 1 would decrease the allowable soil concentration by a factor of 2.

Thickness of Contamination

As shown in Table 2, adjusting the thickness of contamination beyond the trench sidewalls between 100 cm and 1200 cm had no effect on the allowable soil concentration.

Soil Type

Changing the soil type from coarse-grained to fine-grained, using CCME default soil properties, resulted in a slight increase in the allowable soil concentration, as shown in Table 2.

4.2 Recommended Model Parameters

As discussed above, the sensitive model parameters include the air exchange rate, width of the trench, and time.

The air exchange rate will be lowest (resulting in a lower soil guideline) when the depth of the excavation exceeds the width; the VDEQ (2010) recommended value of 2 air exchanges per hour based on urban canyon studies, which was also applied by Ontario Ministry of the Environment. No other defensible values were identified, but 2 air exchanges per hour is believed to be a conservative value for this scenario and is therefore recommended.

A small trench width is more conservative than a large trench width. A width of 1 m is believed to represent a reasonable worst-case value; narrower excavations are unlikely to be suitable for human entry.

In order to calculate a management limit based on these parameters, the model can be used to calculate the trench air concentration over time using a fixed soil concentration of 1 mg/kg. The time-weighted average air concentration and the allowable air concentration can then be used to back-calculate the allowable soil concentration:

$$C_S = \frac{TRV}{C_{A,Avg}} \times 1 mg / kg$$

Where:

C_S = allowable concentration in soil (mg/kg)
C_A = average concentration in air (mg/m^3) based on 1 mg/kg in soil
TRV = toxicity reference value or allowable air concentration (mg/m^3)

The time-weighted average concentration is, however, dominated by the predicted concentrations from the first few minutes after the trench is excavated. It is unlikely that workers would be present in a trench immediately after excavation, due to the time required to properly shore this type of trench and ensure that entry is safe; furthermore time is required to excavate the full length of the trench, and parts of the trench would likely be exposed for several minutes or even hours, depending on the length, before the trench is completed. Therefore, it is recommended that the first few minutes be excluded from the calculation. If the first 8 minutes are excluded, the 8-hour average air concentration (i.e. from t = 8 minutes to t = 8 hours and 8 minutes) predicted from a soil concentration of 1 mg/kg is 26.781 mg/m^3 for coarse soils or 24.743 mg/m^3 for fine soils.

Additionally, in order to determine the allowable concentration in air, an appropriate exposure scenario must be considered if a chronic toxicity reference value (TRV) is being applied. In most cases exposures in an individual trench or excavation will not be of chronic duration; however, consideration may need to be given to the possibility of a worker being exposed to contamination in several different trenches at different sites over an extended period of time (i.e. repeated subchronic exposures). Therefore, a conservative approach would be to assume a standard CCME industrial exposure scenario. Alternatively, Health Canada can be consulted for their latest approach to evaluating exposures for construction workers. Another potential approach would be to use an occupational health and safety objective instead of a chronic TRV, similar to the approach taken for the Canada-Wide Standard for Petroleum Hydrocarbons in Soil, although the occupational health and safety limits are not strictly intended for this purpose. It is important to note that the approach recommended in this report is intended to address sub-chronic or chronic exposures, and not the acute exposures that may arise if a worker enters a trench immediately after excavation when the flux and resulting contaminant concentrations in air are at their highest; for acute exposures, an acute TRV and time-weighted average concentration for the first 15 minutes (or less) should be used and occupational health and safety regulations should be consulted.

If the Health Canada chronic TRV, adjusted for an industrial exposure scenario (2.55 mg/m^3), is applied, the resulting allowable coarse soil concentration based on an 8-hour averaged exposure would be 0.095 mg/kg. Using the ACGIH limit (176 mg/m^3), an allowable soil concentration of 6.6 mg/kg is calculated. The allowable fine soil concentrations would be 0.10 mg/kg and 7.1 mg/kg.

5.0 CLOSURE

This report was prepared by Meridian Environmental Inc. on behalf of the Canadian Council of Ministers of the Environment, in accordance with an agreed scope of work. The study reported herein is based on a review of readily available information from the scientific literature and regulatory documents. Recommendations included herein are for general guidance only, and do not necessarily apply to any particular site. The report is for the exclusive use of CCME; Meridian does not accept responsibility for use of, or reliance on, this report by any third party.

Respectfully submitted,

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Table 1

Initial Model Parameters

Parameter	**Value**
Trench Characteristics	
Length of trench (m)	13
Width of trench (m)	1
Depth of trench (m)	2
Area of trench exposed (m^2)	52 (based on both sidewalls)
Volume of trench (m^3)	26 (calculated from dimensions)
Fraction of area exposed	0.5
Air exchanges/hour	2
Thickness of contamination (cm)	600
Time (s)	14 400
Soil Properties	
Vapour-filled porosity	0.241
Water-filled porosity	0.119
Total porosity	0.36
Dry bulk density	1.7 g/cm^3
Organic carbon fraction (g/g)	0.005
Chemical Properties (n-hexane)	
Diffusion coefficient in air (cm^2/s)	0.2
Diffusion coefficient in water (cm^2/s)	7.77×10^{-6}
Henry's Law constant (dimensionless)	73.9
Organic carbon partitioning coefficient (cm^3/g)	3410
Molecular weight (g/mol)	86.2

Table 2

Results of Sensitivity Analyses

Parameter Adjustment	Allowable Soil Concentration Using TC (mg/kg)	Allowable Soil Concentration Using Occupational Limit (mg/kg)
Initial model parameters	0.12	8.4
Trench length = 26 m	0.12	8.4
Trench length = 6.5 m	0.12	8.4
Trench width = 2 m	0.24	17
Trench depth = 1 m	0.12	8.4
Air exchange rate = 1/h	0.061	4.2
Thickness of contamination = 100 cm	0.12	8.4
Thickness of contamination = 1200 cm	0.12	8.4
Fine-grained soils (CCME defaults)	0.13	9.1

Figure 1: Allowable soil concentrations based on Tolerable Concentration

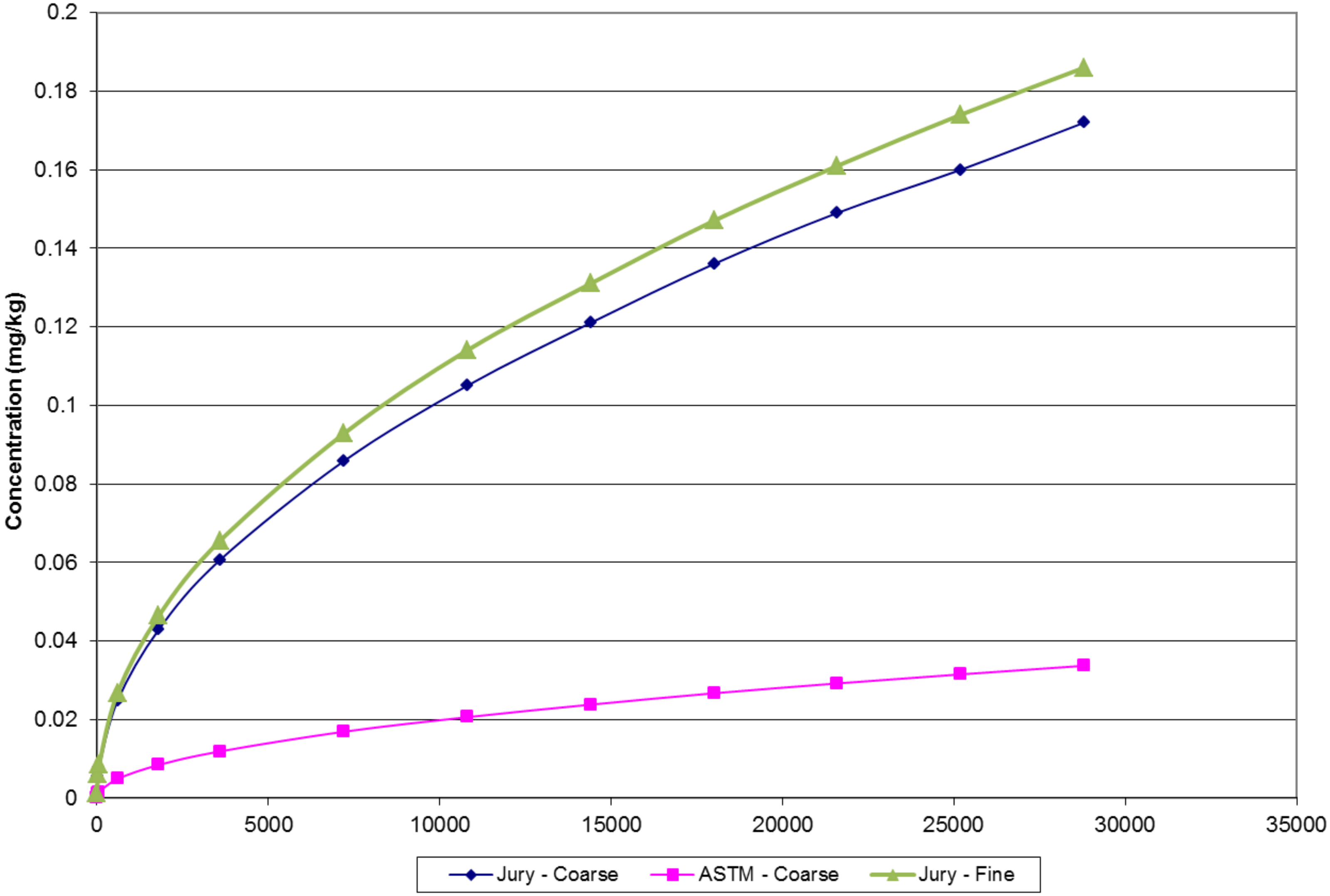

Figure 2: Allowable Soil Concentration based on Occupational Exposure Limit