

TECHNICAL MEMORANDUM

CALCULATION OF SOIL AND GROUNDWATER SITE-SPECIFIC SCREENING VALUES FOR PROPYLENE GLYCOL PHENYL ETHER (PPH) FREEDOM INDUSTRIES SITE - CHARLESTON, WEST VIRGINIA

January 20, 2016

1.0 INTRODUCTION

This technical memorandum has been prepared by RBR Consulting, Inc. for the Freedom Industries site located in Charleston, West Virginia (site). Specifically, this memorandum presents the calculation of soil and groundwater site-specific screening values for propylene glycol phenyl ether (PPH). The site-specific screening values are incorporated into the non-residential human health risk assessment of the site.

2.0 SITE-SPECIFIC SCREENING VALUE FOR NON-RESIDENTIAL SOIL

A *de minimis* value for industrial soil is not available for PPH. Therefore, a standard was calculated for this constituent using the outdoor worker soil land use equation as presented in Section 4.3.1 of the United States Environmental Protection Agency (USEPA) Regional Screening Level Table User's Guide (USEPA, 2015), which applies to non-carcinogenic constituents. The USEPA equations are used to be consistent with current recommendations from WVDEP. It should be noted that PPH is highly degradable in the environment (OECD, 2004) and its inclusion in a quantitative human health risk assessment is likely to result in overestimates of the potential for adverse effects.

2.1 Equation and Input Assumptions

The equation below was used to calculate a site-specific screening value for non-residential soil. The input factors and exposure assumptions used in the calculation are based on WVDEP (2012) recommended values. Toxicity values were derived as described in Section 2.2 below. The equation was modified to account for the fact that PPH is not sufficiently volatile; as such, the inhalation of volatiles component of

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the soil equation is not included. The inhalation of particulates component of the equation was included however.

SL (mg/kg) =	1		
	$\frac{EF \times ED \times (1/RfD \times IR \times 1E-6)}{THQ \times AT \times BW}$	+	$\frac{EF \times ED \times (1/RfD \times GIABS \times SA \times AF \times ABS \times 1E-6)}{THQ \times AT \times BW}$
		+	$\frac{EF \times ED \times (ET/24 \times 1/RfC \times 1/PEF)}{THQ \times AT}$

Each of the input factors included in this equation is described below.

- SL** Screening level in soil (mg/kg).
- THQ** Target Hazard Quotient (unitless): The THQ is the default value of 1 as per the WVDEP (1997).
- BW** Body Weight (kg): The default value for the average body weight of an adult is 70 kg based on WVDEP (2012).
- AT** Averaging Time (days): The doses for noncarcinogenic health effects are averaged over the specific period of exposure for a given receptor. Noncarcinogenic averaging times are, therefore, calculated by multiplying the exposure duration for the receptor by 365 days/year. For this evaluation the exposure duration is 25 years, resulting in an averaging time of 9125 days (WVDEP, 2012).
- EF** Exposure Frequency – occupational (days/yr): Default exposure factors for industrial workers are provided by WVDEP (2012). Exposure frequency for the worker is 5 days per week for 50 weeks a year, or 250 days per year.
- ED** Exposure Duration – occupational (yrs): The exposure duration for industrial workers is 25 years (WVDEP, 2012).
- IR** Soil Ingestion Rate – occupational (mg/day): The WVDEP (2012) recommended value of 50 mg/day is used to describe soil ingestion for a worker not involved in construction or intrusive activities.
- RfD** Oral Reference Dose (mg/kg-day): The derivation of the RfD in units of (mg/kg-day) is described in the following subsection.

- GIABS** Gastrointestinal Absorption Factor (unitless): The GIABS is the default value of 1 as per USEPA (2015).
- SA** Surface Area (cm²): The SA used in this evaluation is 3,300 cm² as presented in the WVDEP Exposure Assumptions Spreadsheet (WVDEP, 2012).
- AF** Adherence Factor (mg/cm²): The AF used in this evaluation is 0.20 mg/cm² as presented in the WVDEP Exposure Assumptions Spreadsheet (WVDEP, 2012).
- ABS** Absorption Factor (unitless): The ABS is the default value of 0.1 for semivolatiles as per USEPA (2015).
- PEF** Particulate Emission Factor (m³/kg): The PEF used in this evaluation is the default value of 1.316 x 10⁹ m³/kg as presented in Appendix D of the WVDEP (2001) Guidance Manual and the Exposure Assumptions Spreadsheet (WVDEP, 2012).
- ET** Exposure Time (hrs): Inhalation exposures are calculated over the specific daily amount of time during which the receptor is exposed to airborne concentrations of constituents. The industrial worker is assumed to be present and subject to inhalation exposure from soil for 8 hours (WVDEP 2012). In the equation, this value is divided by 24 hours/day.
- RfC** Inhalation Reference Concentration (mg/m³): The derivation of the inhalation reference concentration is described in the following subsection.

2.2 Toxicity Values for PPH

For the purposes of calculating a site-specific screening value, toxicity values have been developed from the primary scientific research literature for PPH. All available data were reviewed in order to determine the most appropriate studies to use for reference dose calculations. For the oral reference dose, the toxicity study determined to be most appropriate was that conducted by ECHA (2014). In this study, Wistar rats were continuously administered PPH in drinking water for 90 days at concentrations of 0, 500, 2000, and 6000 ppm (0, 35/46, 146/177, and 429/486 mg/kg-day bw in males/females). The no-observed-adverse-effect level (NOAEL) in this study was 146 mg/kg-day (2000 ppm group), based on body weight changes in males and discoloration of urine in both males and females seen in the next highest dose group of 6000 ppm (429/486 mg/kg-day bw in males/females), which was the highest dose tested.

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Using the NOAEL value of 146 mg/kg-day and dividing by an extremely conservative uncertainty factor of 10,000 based on the following rationale:

- 10 for interspecies variability;
- 10 for intraspecies variability (human-to-human and consideration of the possible effects on sensitive subpopulations);
- 10 for database incompleteness; and
- 10 for the use of a subchronic study to model a potential chronic exposure

results in a chronic oral RfD of 0.015 mg/kg-day.

The inhalation reference concentration (RfC) was derived using the following equation presented by USEPA (2009):

$$\text{RfC} = \text{RfD} \times (\text{BW} / \text{IR})$$

Where:

RfC = Reference Concentration (mg/m³)

RfD = Oral Reference Dose (mg/kg-day)

BW = Body Weight (70 kg for an adult)

IR = Inhalation Rate (20 m³/day for an adult)

Applying these factors, the chronic inhalation RfC for PPH calculates to be 0.053 mg/m³.

It should be noted that the study duration of 90 days on which the toxicity values are based is a less than lifetime duration. There is uncertainty associated with applying less than lifetime study results to a simulation of a lifetime exposure. However, in the absence of a longer or more appropriate study, the data from ECHA (2014) were considered to be the most suitable. An uncertainty factor of 10 which results in an extremely conservative uncertainty factor of 10,000 for the calculation was included in the derivation to account for the study duration.

2.3 Final Non-Residential Soil Site-Specific Screening Value

The toxicity values presented in Section 2.2 and the WVDEP exposure factors described in Section 2.1 were incorporated into the outdoor worker soil land use equation as presented in Section 4.3.1 of the USEPA Regional Screening Level Table User’s Guide (USEPA, 2015). The resulting non-residential soil site-specific screening value for PPH in soil is calculated to be 1.32E+4 mg/kg.

3.0 SITE-SPECIFIC SCREENING VALUE FOR GROUNDWATER

A site-specific groundwater screening value for PPH was calculated using the tapwater equation as presented in Section 4.8.1 of the USEPA Regional Screening Level Table User’s Guide (USEPA, 2015), incorporating the toxicity values described above in Section 2.2. Consistent with WVDEP protocol, the dermal pathway component of the groundwater equation is not included. Additionally, to account for the fact that PPH is not sufficiently volatile, the inhalation component of the groundwater equation is not included.

SL (ug/L) =	THQ x AT x BW x 1000
	EF x ED x (1/RfD x IRW)

The parameters THQ and RfD were described previously in Section 2. The additional input factors included in this equation are described below.

- SL** Screening level in water (ug/L).
- EF** Exposure Frequency – residential (days/yr): Exposure frequency for a residential child is 350 days per year (WVDEP, 2012).
- ED** Exposure Duration – residential (yrs): The exposure duration for a residential child is 6 years (WVDEP, 2012).
- AT** Averaging Time (days): Because the exposure duration for a resident is 6 years, the averaging time is 2,190 days (WVDEP, 2012).
- IRW** Water Ingestion Rate – child (L/day): The WVDEP (2012) recommended ingestion rate for a residential child is 1 L/day.

The toxicity values and WVDEP exposure factors were incorporated into the tapwater equation as presented in Section 4.8.1 of the USEPA Regional Screening Level Table User's Guide (USEPA, 2015). The groundwater site-specific screening value for PPH is calculated to be 235 ug/L.

4.0 SITE-SPECIFIC SCREENING VALUE FOR SOIL MIGRATION TO GROUNDWATER

A site-specific migration to groundwater screening value for PPH was calculated using Equation D-11 of the VRRRA Guidance Manual (WVDEP, 2001). This equation is consistent with the Method 1 partitioning equation for migration to groundwater as presented in Section 4.12.3 of the USEPA Regional Screening Table User's Guide (USEPA, 2015).

First, a target soil leachate concentration must be calculated by multiplying the acceptable groundwater concentration (i.e., calculated site-specific groundwater screening value) by the dilution factor. The WVDEP (2001) default value of 20 was used for the dilution factor. Using the calculated site-specific groundwater screening value of 235 ug/L (0.235 mg/L) identified above in Section 3.0 and a dilution factor of 20, the target soil/water leachate concentration is 4.7 mg/L.

The partition equation (Equation D-11) below was then used to calculate the total soil concentration corresponding to the soil leachate concentration identified above.

$$\text{Screening Level in Soil (mg/kg)} = C_w \left[K_d + \frac{(\theta_w + \theta_a H')}{\rho_b} \right]$$

Each of the input factors included in this equation is described below.

- C_w** Target soil leachate concentration (mg/L). The target soil leachate concentration is 4.7 mg/L as calculated above.
- K_d** Soil/water partition coefficient (L/kg). The value for K_d is calculated using the equation (K_{oc} x f_{oc}) based on WVDEP (2001). Using the K_{oc} and f_{oc} values below, the calculated K_d value used in this evaluation is 0.04 L/kg.
- K_{oc}** Soil organic carbon/water partition coefficient (L/kg), chemical-specific. For this evaluation, a K_{oc} value of 20 L/kg was used, which is the midpoint of the range of estimated values presented in the Material Safety Data Sheet (MSDS) (Dow, 2013).

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- F_{oc}** Fraction organic carbon in soil (g/g). The default value for F_{oc} is 0.002 g/g based on WVDEP (2001).
- θ_w** Water-filled soil porosity (L_{water}/L_{soil}). The default value for θ_w is 0.3 L_{water}/L_{soil} based on WVDEP (2001).
- θ_a** Air-filled soil porosity (L_{air}/L_{soil}). The value for θ_a is calculated using the equation (n - θ_w) based on WVDEP (2001). Using the calculated n value below and the default θ_w value identified above, the calculated θ_a value used in this evaluation is 0.13 L_{air}/L_{soil}.
- ρ_b** Dry soil bulk density (kg/L). The default value for ρ_b is 1.5 kg/L based on WVDEP (2001).
- n** Soil porosity (L_{pore}/L_{soil}). The value for n is calculated using the equation (1 - (ρ_b / ρ_s)) based on WVDEP (2001). Using the default values for ρ_b and ρ_s, the calculated n value of 0.43 L_{pore}/L_{soil} is used in this evaluation.
- ρ_s** Soil particle density (kg/L). The default value for ρ_s is 2.65 kg/L based on WVDEP (2001).
- H'** Dimensionless Henry's law constant, chemical-specific. For this evaluation, a H' value of 1.81E-5 was used, which was converted from the value of 4.41E-7 atm·m³/mol presented in the MSDS (Dow, 2013).

The input factors above were incorporated into the Equation D-11 of the WVDEP (2001) Guidance Manual. The site-specific soil migration to groundwater screening value for PPH is calculated to be 1.13 mg/kg.

5.0 SUMMARY

Soil and groundwater *de minimis* values are not available from WVDEP for PPH. This memorandum presented the calculation of extremely conservative site-specific screening values for this constituent. The non-residential soil site-specific screening value for PPH is calculated to be 1.32E+4 mg/kg and the groundwater site-specific screening value is 235 ug/L. The site-specific soil migration to groundwater screening value is calculated to be 1.13 mg/kg.

6.0 REFERENCES

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