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TECHNICAL MEMORANDUM

CALCULATION OF SOIL AND GROUNDWATER SITE-SPECIFIC SCREENING VALUES FOR 4-METHYLCYCLOHEXANEMETHANOL (MCHM) 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 4-methylcyclohexanemethanol (MCHM). 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 MCHM. 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.

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 MCHM is not sufficiently volatile; as such, the inhalation of volatiles component of the soil equation is not included. The inhalation of particulates component of the equation was included however.

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

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 (cm^2): The SA used in this evaluation is 3,300 cm^2 as presented in the WVDEP Exposure Assumptions Spreadsheet (WVDEP, 2012).

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AF   Adherence Factor (mg/cm^2): The AF used in this evaluation is 0.20 mg/cm^2 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 (m^3/kg): The PEF used in this evaluation is the default value of 1.316 x 10^9 m^3/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/m^3): The derivation of the inhalation reference concentration is described in the following subsection.

2.2 Toxicity Values for MCHM

For the purposes of calculating a site-specific screening value, toxicity values have been developed from the primary scientific research literature for MCHM. All available data were reviewed in order to determine the most appropriate studies to use for reference dose calculations. For the oral reference dose (RfD), the four-week toxicity study by Hosenfeld (1990) was chosen. This study had the longest duration of the applicable studies, and the results were supported by recent studies conducted by the NTP (2014, 2015a). In the Hosenfeld (1990) study, rats were dosed with MCHM in corn oil for five days. Doses were either 200, 400, or 800 mg/kg/day. Results of this study indicate that the lowest-observed-adverse-effect level (LOAEL) was 400 mg/kg-day and the no-observed-effect level (NOEL) was 100 mg/kg-day (Hosenfeld, 1990).

Using the NOEL value of 100 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 0.01 mg/kg-day.

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

$$RfC = RfD \times (BW / IR)$$

Where:

RfC = Reference Concentration (mg/m^3)

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

BW = Body weight (70 kg for an adult)

IR = Inhalation Rate (20 m^3/day for an adult)

Applying these factors, the chronic inhalation RfC for MCHM calculates to be 0.035 mg/m^3.

It should be noted that none of the toxicological studies available are of sufficient duration to accurately simulate lifetime durations of exposure by themselves. In order to address the time duration, an uncertainty factor of 10 which results in an extremely conservative uncertainty factor of 10,000 for the calculation is included in the derivation of the chronic values. Should a chronic study for MCHM become available, the analysis will be revisited.

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 MCHM is calculated to be 8.81E+3 mg/kg.

3.0 SITE-SPECIFIC SCREENING VALUE FOR GROUNDWATER

A site-specific groundwater screening value for MCHM 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 MCHM is not sufficiently volatile, the inhalation component of the groundwater equation is not included.

$$SL\ (ug/L) = \frac{THQ \times AT \times BW \times 1000}{EF \times ED \times (1/RfD \times IRW)}$$

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 MCHM is calculated to be 156 ug/L.

4.0 SITE-SPECIFIC SCREENING VALUE FOR SOIL MIGRATION TO GROUNDWATER

A site-specific migration to groundwater screening value for MCHM was calculated using Equation D-11 of the VRRA 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 156 ug/L (0.156 mg/L) identified above in Section 3.0 and a dilution factor of 20, the target soil/water leachate concentration is 3.12 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.

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

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 3.12 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 Kd value used in this evaluation is 0.068 L/kg.

K_{oc} Soil organic carbon/water partition coefficient (L/kg), chemical-specific. For this evaluation, a K_{oc} value of 34 L/kg was used, which was obtained from the TOXNET Hazardous Substances Data Bank (HSDB) records for MCHM (NIH, 2016).

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 ($n - \theta_w$) 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 $(1-(\rho_b / \rho_s))$ 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 2.62×10^{-4} was used, which was converted from the value of 6.4×10^{-6} atm-cu m/mole presented in the TOXNET HSDB records for MCHM (NIH, 2016).

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 MCHM is calculated to be 0.84 mg/kg.

5.0   SUMMARY

Soil and groundwater *de minimis* values are not available from WVDEP for MCHM. This memorandum presented the calculation of extremely conservative site-specific screening values for this constituent. The non-residential soil site-specific screening value for MCHM is calculated to be 8.81E+3 mg/kg and the groundwater site-specific screening value is 156 ug/L. The site-specific soil migration to groundwater screening value is calculated to be 0.84 mg/kg.

6.0   REFERENCES

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