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**DRAFT MEMORANDUM**

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**To:** Brian Rakvica, NDEP

**RE:** Supplemental Documentation Supporting Site-Specific Input Parameters for the Johnson & Ettinger Model

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This memorandum provides supplemental documentation supporting the proposed site-specific input parameters for the Johnson & Ettinger (J&E) model described in our January 29, 2010 memorandum (updated February 10, 2010). Specifically, this memorandum documents (1) the calculation of soil water-filled porosity based on data for percent moisture (conducted in support of using a site-specific value for this parameter), the calculation of soil vapor permeability, and (3) the use of a macro to calculate the upper and lower soil vapor screening levels using a standard U.S. EPA J&E modeling spreadsheet.

## Percent Moisture to Soil Water-Filled Porosity Calculations

As noted in the *Site-Specific Input Parameters for the Johnson & Ettinger Model* Memorandum, nearly 300 soil samples collected at the site were analyzed for percent moisture. These data were converted to soil water-filled porosity as a check of the direct measurements of soil water-filled porosity in 16 samples. The following equations/relationships were used to convert percent moisture to soil water-filled porosity.

$$Percent\ Moisture\ \left[\frac{g}{g}\%\right] = \frac{Mass\ wet\ sample - mass\ dry\ sample}{Mass\ wet\ sample} \times 100\%$$
$$= \frac{Mass\ water}{Mass\ Total} \times 100\% = \frac{M_w}{M_t} \times 100\%$$

$$Dry\ Bulk\ Density\ \left[\frac{g}{cm^3}\right] = \rho_d = \frac{Mass\ of\ Soil}{Volume\ Total} = \frac{M_s}{V_t}$$

$$Water\ Filled\ Porosity\ \left[\frac{cm^3}{cm^3}\right] = \theta_w = \frac{Volume\ of\ Water}{Volume\ Total} = \frac{V_w}{V_t}$$

Wet bulk density was estimated as shown below based upon measured values of dry bulk density and water-filled porosity (also called volumetric moisture content[1]) from 16 samples. A site-wide averaged wet bulk density was estimated as the mean of the 16 samples. Results are shown in Table A-2 of the updated *Site-Specific Input Parameters for the Johnson & Ettinger Model* Memorandum.

$$Density\ of\ Water\ \left[\frac{g}{cm^3}\right] = \rho_w = \frac{Mass\ of\ Water}{Volume\ of\ Water}$$

$$Wet\ Bulk\ Density\ \left[\frac{g}{cm^3}\right] = \rho_t = \frac{M_t}{V_t} = \frac{Mass\ of\ Soil + Mass\ of\ Water}{Volume\ Total}$$
$$= \frac{M_s}{V_t} + \frac{M_w}{V_t} = \rho_d + \left(\frac{V_w}{V_t} \times \frac{M_w}{V_w}\right) = \rho_d + (\theta_w \times \rho_w)$$

$$Site\ Wide\ Averaged\ Wet\ Bulk\ Density\ \left[\frac{g}{cm^3}\right] = \rho_{t_{avg}} = \frac{\sum_{i=1}^{16} \rho_{t_i}}{16}$$
$$= \frac{\sum_{i=1}^{16} (\rho_{d_i} + \theta_{w_i} \times \rho_w)}{16}$$

$$Estimated\ Water\ Filled\ Porosity\ \left[\frac{cm^3}{cm^3}\right] = \frac{Percent\ Moisture}{100\%} \times \frac{\rho_{t_{avg}}}{\rho_w}$$
$$= \frac{\frac{M_w}{M_t} \times 100\%}{100\%} \times \frac{\frac{M_t}{V_t}}{\frac{M_w}{V_w}} = \frac{V_w}{V_t}$$

The summary of the results from this calculation are given in Table A-3 of the *Site-Specific Input Parameters for the Johnson & Ettinger Model* Memorandum. The full dataset used is attached to this supplemental memorandum (*MoisturePercent.xlsx*).

[1] Page 52 of J&E Model User's Guide (EPA 2004) uses "volumetric soil moisture content" interchangeably with "soil water-filled porosity".

**Soil Vapor Permeability Calculations**

The procedure used to calculate site-specific soil vapor permeability comes from Section 2.8 of the J&E Model User's Guide (EPA 2004, pg. 26). The results of these calculations are shown in Table S-1.

- The average of the value for Loamy Sand and Sand was used for parameters that are class averages by soil textural classification. These parameters are: saturated hydraulic conductivity ($K_s$), residual water content ($\Theta_r$), and the van Genuchten shape parameter (M). Class average values for $K_s$ are from Table 5 of the J&E Model User's Guide. Class average values for $\Theta_r$ and M are from Table 3 of the J&E Model User's guide.
- Intrinsic permeability ($k_i$) was calculated using Equation 29 in the J&E Model User's Guide (EPA 2004, pg. 28). The inputs are $K_s$, dynamic viscosity of water (.011 g/cm-s at 17°C)[2], density of water (0.999 g/cm$^3$), and acceleration due to gravity (980.665 cm/s$^2$).
- Effective total fluid saturation ($S_{te}$) was calculated using Equation 28 in the J&E Model User's Guide (EPA 2004, pg. 28). The inputs are site-specific soil water-filled porosity (cm$^3$/cm$^3$), site-specific soil total porosity (cm$^3$/cm$^3$) and residual water content, $\Theta_r$ (cm$^3$/cm$^3$). Site-specific values are shown in Table A-2 of the updated *Site-Specific Input Parameters for the Johnson & Ettinger Model* Memorandum.
- Relative air permeability ($k_{rg}$) was calculated using Equation 27 in the J&E Model User's Guide (EPA 2004, pg. 27). The inputs are $S_{te}$, calculated in the previous step, and the van Genuchten shape parameter, M.
- Effective air permeability, also called the soil vapor permeability, is calculated as the product of intrinsic permeability and the relative air permeability at the soil water-filled porosity according to the J&E Model User's Guide (EPA 2004):

$$k_v = k_{rg}(\theta_w) \times k_i$$

[2] 17°C is the average soil temperature for Henderson, NV. See the *Site-Specific Input Parameters for the Johnson & Ettinger Model* Memorandum for more information on average soil temperature.

**Using the J&E Model Macro to Calculate Screening Limits**

The J&E Model upper and lower screening limits were calculated using the EPA's J&E Model Spreadsheet for Soil Gas: *SG-ADV-Feb04_SiteSpecific_Template.xlsx*.

The site-specific input parameters are entered into this workbook on the sheet "DATENTER". A few notes about the parameters on this sheet:

- The soil gas concentration entered in cell F6 is a unit concentration (i.e., 1 microgram per cubic meter [$\mu g/m^3$]) used in the calculations; however, any value could be used to estimate the screening values.
- The site-specific parameters that have been discussed in this supplemental memorandum and the *Site-Specific Input Parameters for the Johnson & Ettinger Model* Memorandum are shaded in grey.
- The Indoor Air Exchange Rate (ER) is either 1/h or 2/h, as discussed in the *Site-Specific Input Parameters for the Johnson & Ettinger Model* Memorandum.
- As discussed in the *Site-Specific Input Parameters for the Johnson & Ettinger Model* Memorandum, the average vapor flow rate ($Q_{soil}$) is either the default (20 L/m) or left blank to have the workbook calculate a site-specific value based on soil vapor permeability. The calculated value can be found on the "INTERCLACS" sheet.

To calculate the lower screening limit, an air exchange rate of 1/h and a $Q_{soil}$ of 20 L/m are entered into the spreadsheet; all other parameters are fixed. To calculate the upper screening limit, an air exchange rate of 2/h is entered in the spreadsheet and the $Q_{soil}$ is left blank. Once the desired input parameters were entered into the EPA's J&E Model Spreadsheet, a macro was used to automatically insert CAS numbers for each chemical analyzed in soil gas on the "DATENTER" sheet and pull out the result from the "RESULTS" sheet. The workbook containing the macro is: *SG_Concentration_Limits_Updated.xlsm*. The "Model" sheet in this workbook is used to run the *JEModel* macro, which will calculate screening values for all chemicals listed on

that sheet.[3] The other sheets are used to store screening results given varying input parameters.

To run the macro, go to the Developer tab[4] in the Excel Ribbon and click on Macros.[5] With *JEModel* highlighted, click on Run. The macro will automatically populate the soil gas concentration screening limits based on 1.00E-06 cancer risk and a hazard index of 1. The macro will also fill in the table to the right showing the key input parameters used in the EPA's J&E Model Spreadsheet to calculate the screening limits. The values in the J&E Model Screening Limit column are taken as the minimum soil gas concentration based on cancer risk and hazard index.

[3] In order for a screening value to be calculated the chemicals must have chemical property information in the EPA's J&E Model Spreadsheet database (found in the "VLOOKUP" sheet). If this information is missing for a given chemical, the macro will show a result of "NA".

[4] To enable the Developer Tab, go to Excel Options. Under the Popular options check the box next to show Developer tab in the Ribbon.

[5] Macros must be enabled in Excel to run a macro. To enable them, go to Excel Options and then select the Trust Center. These instructions are for Excel 2007 and may not be relevant to older versions.



# TABLE S-1
## Soil Vapor Permeability Calculation

| Soil Texture | Saturated Hydraulic Conductivity, $K_s$ (cm/h) | Saturated Hydraulic Conductivity, $K_s$ (cm/s) | Residual Water Content, $\Theta_r$ ($cm^3/cm^3$) | Intrinsic Permeability, $k_i$ ($cm^2$) | Effective Total Fluid Saturation, $S_{te}$ (unitless) | van Genuchten Shape Parameter, M (unitless) | Relative Air Permeability, $k_{rg}$ (unitless) | Effective Air Permeability, $k_v$ ($cm^2$) |
|---|---|---|---|---|---|---|---|---|
| Loamy Sand | 4.38 | 1.22E-03 | 0.049 | 1.358E-08 | 0.257 | 0.427 | 0.832 | 1.130E-08 |
| Sand | 26.78 | 7.44E-03 | 0.053 | 8.305E-08 | 0.295 | 0.685 | 0.652 | 5.419E-08 |
| Site-Specific | 15.58 | 4.33E-03 | 0.051 | 4.832E-08 | 0.279 | 0.556 | 0.754 | 3.645E-08 |