

Notes to Accompany *Risk-Based Concentrations for Individual Chemicals*
Oregon Department of Environmental Quality
Land Quality Division
November 15, 2011

NOTE: This document contains information about the Oregon DEQ spreadsheet entitled *Risk-Based Concentrations for Individual Chemicals*. Section 1 is similar to the Introduction contained in the spreadsheet, which is accessible from the opening screen or the main menu of that document. Sections 2 through 5 are explanations of the notes used on the RBCs, ExpFactors, ChemData, and ToxDa pages of the spreadsheet.

1. INTRODUCTION

This spreadsheet calculates risk-based concentrations (RBCs) for the Oregon Department of Environmental Quality (DEQ) Environmental Cleanup and Tanks Program. It is offered to interested parties as a reference document that contains:

- The Cleanup and Tank Program's generic RBCs for chemical constituents;
- The default exposure factors [ExpFactors], chemical data [ChemData], toxicological data [ToxDa], and Transport factors [Transport] used to calculate the generic RBCs.

For more complete information about the derivation of the RBCs, please refer to Appendix B in *Risk-Based Decision Making for the Remediation of Petroleum-Contaminated Sites* (RBDM Guidance) (DEQ, 2003)¹ and U.S. EPA's Risk Assessment Guidance for Superfund; Volume I-Human Health Evaluation Manual (Part F, Supplemental Guidance for Inhalation Risk Assessment), January 2009.

The default exposure factors, chemical data, and toxicological data in this workbook can be modified to calculate site-specific risk-based cleanup levels. However, depending upon the changes being made, more appropriate models and more effective programs may be available for your purposes.

NOTE: This program is offered for use without warranty or support. It is designed to work with Microsoft® Excel 2007 and may not work properly with other applications, or with older releases of Excel. It is recommended that you have no other files open in Excel when using this program.

Viewing and Printing the Data Files

To view data files, click on the "View Data" button on the [Title] screen or on the [Introduction] page. Each data file is on a separate page, which can be viewed by selecting the appropriate tab located at the bottom of the window – [RBCs], [ChemData], [ToxDa], [ExpFactors], and [Transport]. Each page has been "frozen" so that chemical names and headings remain in view when scrolling through the tables. Explanatory notes and references for each table are provided in other sections of this document.

¹ The equations used to calculate RBCs as shown in DEQ 2003 have been updated for consistency with U.S. EPA's inhalation risk assessment methodology (U.S. EPA 2009). Accordingly, Appendix B of DEQ 2003 is now outdated and does not represent current methodology as described in U.S. EPA 2009, and as implemented in the most recent version of DEQs spreadsheets. Appendix B will be updated as part of the next revision of this guidance. The updated equations used in the 2011 version of DEQs spreadsheet are presented in Appendix C of DEQ's Human Health Risk Assessment Guidance, available at: <http://www.deq.state.or.us/lq/pubs/docs/cu/HumanHealthRiskAssessmentGuidance.pdf>. Comparable equations to those used by DEQ are used by U.S. EPA for residential scenarios and are available at: http://www.epa.gov/reg3hwmd/risk/human/rb-concentration_table/equations.htm

Tables can be printed by selecting the appropriate print command from the "DEQ Risk Calc" menu located on the right end of the main toolbar. The same print options are available on the "Main Menu" which can be accessed from "DEQ Risk Calc" on the Excel ribbon bar. The "Main Menu" also offers additional options, which are described later on this page.

Making Site-Specific Calculations

Although this program is not a sophisticated tool for calculating site-specific risk-based cleanup levels, it can be used to a limited extent for that purpose. Site-specific calculations will usually only involve changes to the default exposure factors. However, changes can also be made to the default chemical data or the toxicity data.

- Make changes to the [ExpFactors], [ChemData], or [ToxData] worksheets by entering new data into any of the existing white data cells. Data cells shown in gray or yellow and cells located outside the body of the table cannot be edited since they contain either formulas or labels or are located outside the boundaries of the work area. (Note: You cannot make any changes to the [RBCs] or the [Transport] worksheets.)
- New data must be the same type as existing data (e.g., don't replace a number with text).
- Data cells must not be left blank unless they are not needed (e.g., a carcinogen does not require RfD tox data).
- Entries for "Risk Type" in the [ToxData] worksheet can be only "c," "nc," or "NA." If "NA" is used that row will be skipped during the recalculation step.
- Entries for "Early Life" in the [ToxData] worksheet can be only "y" or "n," or in the special case of vinyl chloride, "vc."
- Entries for "Breast Feeding" in the [ToxData] worksheet can be only "y" or "n."
- Entries for "Inorganic" in the [ChemData] worksheet can be only "y" or "n."
- After making changes to [ExpFactors], [ChemData], and [ToxData], select "Recalculate" from the "DEQ Risk Calc" menu (or the "Main Menu") to recalculate the RBCs and put the new values in the Table of RBCs.
- Results can be printed by using the Print commands found on the menus.
- To restore DEQ default values to any of the data tables, select "Restore ExpFactors Defaults," "Restore ChemData Defaults," or "Restore ToxData Defaults" from the menu. Then select "Recalculate" to restore defaults in the Table of RBCs.

Adding New Chemicals to the Table

New chemicals can be added to the RBC table using the blank rows provided for this purpose or by replacing any of the existing chemicals.

- First, enter the chemical name(s) and data in the [ChemData] worksheet. Enter the new data on any available blank line or replace the data in a line that is in use. As noted above, enter data only into the white cells; the gray cells will be calculated. Entries for the "Inorganic" column can be only "y" or "n."
- Second, open the [ToxData] worksheet. The new chemical name(s) should be displayed on that page. Add the necessary tox data for the new chemical(s) on the appropriate lines.

Entries for the "Early Life" column can be only "y," "n," or "vc." Entries for the "Risk Type" column can be only "c," "nc," or "NA." Entries for the "Breast Feeding" column can only be "y" or "n."

- Third, select "Recalculate" from the "DEQ Risk Calc" menu or the "Main Menu" and the program will insert RBC values for the new chemical(s) on the [RBCs] page.
- Data can be removed from the [RBCs] page by deleting the [ChemData] and [ToxData] entries and recalculating.

Menu Options

You can use two menus to run this program. The "DEQ Risk Calc" menu is located at the right end of the main menu bar and functions like a standard drop-down menu. It allows you to recalculate RBCs, print out any of the tables, and restore default data to any of the data tables. The "Main Menu" is a floating menu that pops up over the spreadsheet when you select "Main Menu" from the "DEQ Risk Calc" menu, or when you enter [CTRL]-m. The following additional options are available from the Main Menu.

- Show All Values: A number of the RBCs exceed theoretical limits like solubility (S) and soil saturation (C_{sat}). (See Section B.2.1.4 in the RBDM Guidance for more information about this.) If the "Show All Values" checkbox is not selected, "Recalculate" will only display those RBCs that do not exceed these limits. If the checkbox is selected, all RBC values will be displayed upon recalculation, even those that exceed the specified limits.
- Show RBCs in Scientific Notation: If this checkbox is not selected, "Recalculate" will display RBCs in general number format showing two significant figures (e.g., 1.2, 3800, or 0.056). If this checkbox is selected, RBCs will be displayed in scientific notation with two significant figures (e.g., 1.2E+00, 3.8E+03, or 5.6E-02).
- RME Factors or CTE Factors: This determines what default exposure factors are placed in the [ExpFactors] worksheet. If RME Factors is selected, then Reasonable Maximum Exposure values are used. If CTE Factors is selected, then Central Tendency Exposure values are used. (See Appendix H in RBDM Guidance.)
- Chronic RfDs or Subchronic RfDs: This lets you select either chronic reference doses (RfDs) or subchronic reference doses for the RBC calculations. Note that this affects only the RBCs for the Construction and Excavation Worker scenarios.
- New Entries: Table printouts normally include only the default chemicals. To obtain printouts of the optional rows, select the "New RBCs" check box before printing.
- View Screens: Buttons are available here that will allow you to view the "Title Screen" and open the "Introduction" page without having to restart the program.

Restoring Tool Bars and Miscellaneous Options

Because of the size of the tables in this program, most of the typical Excel toolbars are turned off when this spreadsheet is loaded. This provides the maximum area on your monitor to view the data. However, if you prefer to have these toolbars available you can restore them from Excel's menus. Select "View/Formula Bar," "View/Toolbars/Standard" and "View/Toolbars/Formatting" to return the typical toolbars. You can then resize the pages with the percent box to make the tables and text larger or smaller. You can also use "Tools/Options/View/Row & column headers" to restore the standard row and column labels, or the grid lines.

2. RBC TABLE NOTES

RBC values for soil vapor intended for use in assessing vapor intrusion into buildings are included in this table. DEQ has guidance for assessing the vapor intrusion pathway (see <http://www.deq.state.or.us/lq/pubs/docs/cu/VaporIntrusionGuidance.pdf>), which should be consulted when assessing the vapor intrusion pathway at a site. Aside from vapor intrusion investigations, DEQ does not routinely require air (indoor or outdoor) to be tested at cleanup sites due to the great temporal and spatial variability in air concentrations, which makes it difficult to collect representative samples.

The Direct or Indirect Pathway Codes have the following meanings:

DCS means it is a soil direct contact pathway with a limiting value of Csat.

IVS means it is an indirect pathway with a limiting value of Csat.

ILS means it is an indirect pathway with a limiting value of Csat.

DCW means it is a water direct contact limiting value equal to the solubility, S.

IVW means it is an indirect pathway with a limiting value equal to the solubility, S.

DCA means it is an air direct contact pathway with a limiting value at the vapor pressure, Pv.

ICA means it is an air indirect contact pathway with a limiting value at the vapor pressure, Pv.

The symbols in the "Note" columns are explained below. The references can be found in *Risk-Based Decision Making for the Remediation of Petroleum-Contaminated Sites* (DEQ, 2003).

- c This chemical is a known or suspected carcinogen. The RBCs in this row were calculated using equations for carcinogens.
- >Csat This soil RBC exceeds the limit of three-phase equilibrium partitioning. Refer to "ChemData" page for the corresponding value of Csat. Soil concentrations in excess of Csat indicate that free product might be present. See Section B.2.1.4 for additional information.
- L The values for lead reported in this table are not derived from the equations developed in Appendix B. See Section B.3.4 for the source of the lead numbers and information on applying them.
- NA This note is carried over from the ToxData page and issued to skip over calculations in that row. In the 2011 version of the spreadsheet, it is used in two rows, once for lead where the EPA values are used directly without calculation and secondly for trichloroethene, which has calculations performed differently than all other substances in the Table.
- nc This chemical is a noncarcinogen. The RBCs in this row were calculated using equations for noncarcinogens.
- nv This chemical is considered "nonvolatile" for purposes of the exposure calculations.
- >Pv The air concentration reported for the RBC exceeds the vapor pressure of the pure chemical. It can be assumed that this constituent cannot create an unacceptable risk by this pathway. See Section B.2.1.4 for additional information.
- >S This groundwater RBC exceeds the solubility limit. Refer to Appendix D for the corresponding value of S. Groundwater concentrations in excess of S indicate that free product may be present. See Section B.2.1.4 for additional information.
- v This chemical is classified as "volatile" for purposes of the exposure calculations in this document.
- * Leaching-to-Groundwater RBCs are not provided for inorganic chemicals. If this pathway is of concern, then site-specific leaching tests must be carried out.

- When "Show All Values" is not selected on the Main Menu, all RBC values for indirect pathways that exceed a limit (C_{sat}, S, or P_v) are removed from the table and replaced with "-".
- Ψ This chemical has both cancer and noncancer toxicity values and the lowest RBCs (noncancer vs. cancer) vary by medium and exposure scenario. Both should be calculated to ensure the lowest applicable RBC is used. In the Adobe® PDF format table, this is noted as a c*. Because calculation of TCE RBCs was significantly complicated this year (see TCE memo), the cancer-based values were written directly into the spreadsheet and are not calculated in the worksheet. The non-cancer values can be calculated as usual by changing the endpoint. To restore the cancer-based values it is necessary to close without saving and re-open the spreadsheet.
- 1. The Soil Gas RBCs are derived by applying default empirical attenuation factors to the air RBCs. Both the air and soil gas RBCs are rounded to 2 significant digits, before being displayed in the Table. Because the soil gas RBCs are calculated by applying the attenuation factor to the unrounded air RBC, the ratio between the two displayed RBCs is not consistently and exactly equal to the applicable attenuation factor. Rationale for, and derivation of, attenuation factors are provided in Appendix A of DEQ's vapor intrusion guidance.

3. EXPOSURE FACTOR NOTES

The symbols and numbers in the "Note" columns are explained below. The references can be found in *Risk-Based Decision Making for the Remediation of Petroleum-Contaminated Sites* (RBDM) (DEQ, 2003) or are defined below.

- = This exposure parameter is the same as the residential value.
- NA This exposure parameter is not required for any of the RBCs.
- 1. Acceptable risk levels are specified in statute (ORS 465.315) and defined in rule (OAR 340-122-0115).
- 2. EPA (1989)
- 3. EPA (1991b)
 - 3a. Professional judgment: EF for urban resident = 1/2 residential EF
- 4. EPA (1997c)
 - 4a. Incorporates time spent at work (8 hr/24 hr day)
- 5. EPA (2001a)
 - 5a. Mean for residential adult gardener
 - 5b. Mean for commercial gardener used to represent upper end commercial exposure
 - 5c. 95th percentile construction worker
 - 5d. 95th percentile daycare child
- 6. DEQ (2010b). *Human Health Risk Assessment Guidance*. Publication No. 10-LQ-023. October 18, 2010."
- 7. Calculated from equations given in EPA (1998a).
 - 7a. Modified for urban scenario by analogy to equations given in EPA (1998a).
- 8. ASTM (1995b)
 - 8a. *foc* is an average of ASTM (1995b) and EPA (1996b) defaults.
- 9. Calculated from $rs = rb/(1-n)$.

10. Calculated from $na=n-nw$; $nacp=n-nwcap$; $nacr=n-nwcrk$.
 11. $nwcrk$ assumed = nw .
 12. Calculated from $Lv = Lw - Lcap$
 13. EPA (1996b)
 14. Estimated from data reported in Michigan DEQ (1998).
 15. Derived from range of floor-wall seem gaps given in EPA (1997b).
 16. Refer to Section B.3.2.1 in RBDM (DEQ, 2003).
 17. Refer to Section B.3.2.2 in RBDM (DEQ, 2003).
 18. Refer to Section B.3.2.3 in RBDM (DEQ, 2003).
 19. Refer to Section B.3.2.4 in RBDM (DEQ, 2003).
 20. Refer to discussion of Henry's Law Constants in Section B.2.1.2 in RBDM (DEQ, 2003).
 21. EPA (2002c)
 22. Early life-stage factor calculations are based on information provided by EPA in:
 - *Guidelines for Carcinogen Risk Assessment*, EPA/630/P-03/001B, U.S. Environmental Protection Agency, March 2005.
 - *Supplemental Guidance for Assessing Susceptibility from Early-Life Exposure to Carcinogens*, EPA/630/R-03/003F, U.S. Environmental Protection Agency, March 2005.
 - *Memorandum on Implementation of the Cancer Guidelines and Accompanying Supplemental Guidance*, from William H. Farland, Office of the Science Advisor, U.S. Environmental Protection Agency, 14 June 2006.
- For additional information about the vinyl chloride calculation, please see Appendix J in *Risk-Based Decision Making for the Remediation of Petroleum-Contaminated Sites* (RBDM) (DEQ, 2003).
23. DEQ (2010a). *Guidance for Assessing and Remediating Vapor Intrusion in Buildings*. Publication No. 10-LQ-007. March, 25, 2010

4. CHEMICAL DATA NOTES

The symbols and numbers in the “Note” columns are explained below. The references can be found in *Risk-Based Decision Making for the Remediation of Petroleum-Contaminated Sites* (DEQ, 2003).

- * Cyanide is treated as a nonvolatile inorganic and no RBCs are calculated for volatilization pathways. However, toxicity information is based on hydrogen cyanide, which is volatile. If cyanide is an important constituent at your site, please consult with DEQ.
- nv This chemical is classified as “nonvolatile” for purposes of the exposure calculations in this document.
- v This chemical is classified as “volatile” for purposes of the exposure calculations in this document.

PHC/CHC: Petroleum/Organic Hydrocarbon or Chlorinated Hydrocarbon: These categories were differentiated to permit consideration of differing attenuation rates for these classes of compounds, comparing a source area in soil vapor at some distance from a building to vapor immediately underneath a building being assessed. The default attenuation factors assume that vapor samples are collected in the sub-slab under a building and are therefore set to the same value, based on the assumption that little or no additional attenuation that could be attributed to biodegradation of petroleum compounds across the slab. However, soil vapor samples for petroleum compounds collected at some distance from the building may have relatively greater attenuation attributable to biodegradation. If investigating petroleum vapors in soil gas, it's best to consult with DEQ.

1. Volatility is based on EPA (1991a). In previous version of DEQs spreadsheet, a volatile constituent has a Henry's constant $> 10^{-5} \text{ m}^3\text{-atm/mol}$ and a molecular weight $< 200 \text{ g/mol}$. However, in recent years, US EPA has no longer been using the molecular weight criterion, only the Henry's constant. In the 2011 version of DEQs spreadsheet, the molecular weight criterion was eliminated to harmonize with the US EPA definition.
2. Molecular weights can be obtained from many common chemical handbooks and chemistry texts. No specific reference was used here.
3.
 - a. Values from Table 36 (S and H) and Table 37 (Dair and Dw) in EPA (1996b). Note that the value used here for xylene is the average of the values for all three isomers.
 - b. Oak Ridge National Laboratory, The Risk Assessment Information System, Chemical-Specific Parameters, http://rais.ornl.gov/cgi-bin/tools/TOX_search?select=chem_spef
 - c. Syracuse Research Corporation On-Line Interactive Database, <http://www.srcinc.com/what-we-do/databaseforms.aspx?id=386>
4.
 - a. Vapor pressures are calculated from the relationship $P = H * S * 1000000$, where H is the dimensionless Henry's constant, S is the solubility in mg/L, and 1000000 is a conversion factor yielding units of mg/m³ for direct comparison to RBC_{air} values.
 - b. C_{sat} is calculated using Equation [B-21]. See Section B.2.1.4.
5. Kocs are the “Calculated Values” from Table 39 in EPA (1996b).
 - a. This is the average Koc value for the three xylene isomers.
6. Dimensionless Henry's constants are calculated from the relationship $H = KH / R * T$ where KH is the Henry's constant in $\text{m}^3\text{-atm/mol}$, R is the ideal gas law constant ($8.21 \times 10^{-5} \text{ m}^3\text{-atm/K-mol}$), and T is the absolute temperature (293 K).

7. Howard (1993)
8. Dair and Dw are estimated using Equation [B-57]. See Section B.2.3.2.
9. EPA (2002a)
10. The following assumptions are made for inorganics:
 - Volatile pathways are not important, so Dair and K_H are set = 0.
 - Dissolved constituents will have $D_w = 1 \times 10^{-6} \text{ cm}^2/\text{s}$.
 - If the leaching pathway is a concern, leaching tests should be performed. Therefore, Koc values are not required.
11. Lead is a special case since the lead RBCs are not calculated by DEQ. See Section B.3.4.
12. MCPA diffusion coefficient values are assumed to be 1×10^{-2} and 1×10^{-6} .

5. TOXICOLOGICAL DATA NOTES

The symbols and numbers in the “Note” columns are explained below. The references can be found in *Risk-Based Decision Making for the Remediation of Petroleum-Contaminated Sites* (DEQ, 2003).

- c This chemical is a known or suspected carcinogen.
- nc This chemical is a noncarcinogen.
1. The column with the heading of SFi, shows what an inhalation slope factor would be if converted from the inhalation Unit Risk (iUR in ug/m^3)⁻¹ by the following relationship: $\text{SFi} = \text{iUR} * 70 \text{ kg} / 20 \text{ m}^3/\text{day} * 1,000 \text{ ug}/\text{mg}$. This is shown for reference only, and is not used in RBC calculations.
 2. The column with the heading of RfDi, shows what an inhalation reference dose would be if converted from the inhalation reference concentration (RfC in mg/m^3) by the following relationship: $\text{RfDi} = \text{RfC} * 20 \text{ m}^3/\text{day} / 70 \text{ kg}$. This is shown for reference only, and not used in RBC calculations.
 3. U.S. EPA (2010). *Regional Screening Level (RSL) Table, June 2011*.
 4. Trichloroethene: In the 2011 version of DEQs spreadsheet the TCE risk calculation and toxicity values have both been revised. The toxicity values DEQ was relying on previously were withdrawn in 2010 and updates to EPA’s IRIS database are expected. For additional information, see memorandum on the selection of TCE unit risk value on the RBDM web page.
 5. Dermal absorption fraction values are from Exhibit 3-4 in EPA (2001a).
 6. Kp, t, t*, and B are from Exhibit B-3 in EPA (2001a).
 7. Kp, t, t*, and B were calculated from equations given in Appendix A in EPA (2001a).
 8. DAw is calculated from equations given in EPA (2001a). See Section B3.3.4.
 9. NA : These data are not available and are not used in RBC calculations.
 10. ORNL (2010). http://rais.ornl.gov/cgi-bin/tools/TOX_search?select=chem.
 11. US EPA IRIS Database, September, 2011.
 12. For cadmium, two noncancer toxicity values are available, one for dietary and one for water. DEQ elected to use to water-based value as most appropriate for groundwater pathways. Use of the dietary Oral RfD will result in somewhat higher RBCs for the soil direct contact pathways. See U.S. EPAs notes on cadmium for more details.
 13. Residential and infant risk adjustment factors (IRAF) from DEQ (2010b). *Human Health Risk Assessment Guidance*, Publication No. 10-LQ-023, October 18, 2010. Urban residential IRAF values calculated by DEQ.
 - a. When the breastfeeding pathway is included, the RBC spreadsheet will show the lowest RBC from either the adult (or adult/child receptor) or the breastfeeding infant receptor. For this reason, IRAFs less than 1 are replaced with 1 in the RBC calculations.
 - b. Because of the short exposure duration for construction and excavation workers, consideration of bioaccumulation for the breastfeeding pathway is inappropriate, and the pathway is not included in the calculation of RBCs for these receptors.
 - c. In cases where the urban residential breastfeeding pathway RBC is less than the residential breastfeeding pathway RBC, the urban residential breastfeeding pathway RBC is replaced with the residential breastfeeding pathway RBC.