Guidance for Selecting Input Parameters for Modeling Pesticide Concentrations in Groundwater Using the Pesticide Root Zone Model

Version 1.0

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U.S. Environmental Protection Agency
Office of Pesticide Programs
Environmental Fate and Effects Division

Health Canada
Pesticide Management Regulatory Agency
Environmental Assessment Directorate

Introduction

EPA's Office of Pesticide Programs (OPP), in coordination with Health Canada's Pesticide Management Regulatory Agency (PMRA), developed this guidance document to help model users select and prepare the appropriate input values for groundwater aquatic exposure modeling. Using this guidance document should improve the consistency in modeling the fate of pesticides in the environment and ultimately the overall quality of risk assessments. The primary sources of input fate parameters that are used in these models include pesticide product chemistry and labeling information as well as sorption coefficients and degradation rates calculated from environmental fate studies that are usually conducted or sponsored by pesticide manufacturers.

This document is intended as guidance for model users. If there is a need to deviate from this guidance during risk assessment, the model user should provide adequate justification for model inputs in the assessment. This guidance document reflects the current policy for groundwater modeling for the OPP and the PMRA.

Summary Guidance Tables for Model Input Parameters

The guidance table listed below contains the parameters, input values, sources of data, and additional explanatory information (notes) for the Pesticide Root Zone Model (PRZM) groundwater (GW) graphical user interface (GUI). More specific information about this groundwater model can be found at the following web site: http://www.epa.gov/oppefed1/models/water/index.htm. If additional guidance is necessary, model users should consult with the appropriate technical advisory group.

PRZM-GW

The following guidance table is for running PRZM-GW, a graphical user interface (GUI) for running PRZM, to estimate exposure in groundwater. The main difference with using GUIs and running the model directly in command line is that GUIs typically require half-lives (in values of days) rather than rate constants (in values of day^{-1}) for metabolism parameters.

Table 2.1 Chemical Input Parameters for PRZM-GW (Version 1.0 October 12, 2012)

Parameter (units)	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Application date(s) (day/mo/yr)	Use the maximum number of applications and minimum application interval for the modeled use.	Product labels or location-specific	The model user should consider location-specific cropping dates and relevant label-specific information. Other relevant information may be obtained from agricultural extension agents, crop experts (land-grant universities, grower groups), and EPA/BEAD. At PMRA, application rate and timing information is provided to EAD by the Re-evaluation and Use Analysis Section (RUAS).
Application rate (kg a.i. ha^{-1})	Use the maximum application rate allowed per application for the modeled use.	Product labels	
Application Method	Cam 1 or 2	Option in GUI	One of two options [bare ground (1) or application to foliage (2)] should be selected.
Hydrolysis half-life (days)	Use the relevant hydrolysis half- life for the aquifer pH.	Hydrolysis data (OPPTS Guideline 835.2120) PMRA DACO 8.2.3.2	Use the maximum hydrolysis half-life value at a pH that represents the scenario to be modeled. If a value at a representative pH is not available, then use the value at pH 7. If no hydrolysis data are available, assume that the compound is stable, *i.e.*, enter zero (0).
Soil Half-life (days)	Use aerobic soil metabolism half -life adjusted to 25ºC	Aerobic soil metabolism data (OPPTS Guideline 835.4100) PMRA DACO 8.2.3.4.2	Adjust half-lives from studies conducted at temperatures other than 25°C to values at 25°C using a Q_{10} of 2 (see **APPENDIX A** for details). If multiple aerobic soil metabolism half-life values are available enter the 90^{th} percentile confidence bound on the mean of the half-lives adjusted to 25ºC. (See Equations 1 and 2 in **APPENDIX A** for instructions.) If a single aerobic soil metabolism half-life value is available, enter 3x the half-life adjusted to 25ºC. (See Equations 1 and 3 in **APPENDIX A**) If no aerobic soil metabolism data are available, assume that the compound is stable to biodegradation under these conditions, *i.e.*, enter zero (0).

Parameter (units)	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Pesticide partition or distribution coefficients ($cm^3\ g^{-1}$)	If sorption is correlated with organic carbon content, use the K_{OC} values. If sorption is not correlated with organic carbon content, use the K_d values. **EPA:** Use the mean of the K_{OC} or K_d values **PMRA:** use the 20th percentile of the K_{OC} or K_d values	Adsorption/ desorption data (OPPTS Guideline 835.1230) PMRA DACO 8.2.4.2	This parameter is calculated differently by EFED/EPA and EAD/PMRA. EFED: Sorption is correlated with organic carbon content if the coefficient of variation (*i.e.*, the standard deviation divided by the mean) for K_{OC} values is less than that for K_d values.[1] Use of the mean K_{OC} may not be appropriate for certain chemicals with binding not correlated with organic carbon content, such as those that are ionic at environmental pH values. In these cases, the model user should document the rationale for the selected model input values. Additional guidance may be sought at the EFED WQTT. EAD: Use K_{OC} values if the correlation between K_d and K_{OC} is less than 0.5. Otherwise use K_d. Consult the Water Modeling Tech Team if there are questions.

[1] Standard methods for calculating sorption coefficients differ for PMRA and USEPA; therefore, input parameters for sorption will be different. A sensitivity analysis should be performed for individual assessments to determine the sensitivity of the sorption parameter on the estimated concentration in groundwater (high, low, mean, median, etc.)

APPENDIX A

Calculations

Calculating the temperature-adjusted degradation half-life

- Prior to using Equations 2 and 3 below, adjust half-lives from studies conducted at temperatures other than 25°C to values at 25°C using Equation 1.

$$t_{adjusted} = \frac{t_{measured}}{Q_{10}^{\left(\frac{T-T_{ref}}{10}\right)}} \quad \textbf{Equation 1}$$

where

$t_{adjusted}$ = half-life adjusted to 25°C [*time*]
$t_{measured}$ = laboratory measured aerobic soil metabolism half-life [*time*]
Q_{10} = factor by which degradation increases for a 10°C temperature rise (use a Q_{10} of 2)
T = temperature of modeled water body [°C] (use a T of 25°C (temperature assumed by PRZM))
T_{ref} = temperature of the laboratory study [°C]

Calculating the 90th percentile confidence bound on the mean half-life value.

- If more than one half-life value is available, use Equation 2 to calculate the 90th percentile confidence bound on the mean half-life value:

$$t_{input} = \overline{t_{1/2}} + \frac{t_{90,n-1}s}{\sqrt{n}} \quad \textbf{Equation 2}$$

where,

t_{input} = half-life input value (*time*)
$\overline{t_{1/2}}$ = mean of sample half-lives (*time*)
s = sample standard deviation (*time*)
n = number of half-lives available (-)
$t_{90,n-1}$ = one-sided Student's t value at $\alpha = 0.1$ (*i.e.*, 1.0-0.9) (-)

This equation does not calculate the 90th percentile of the distribution of half-life values.

Some Student's t values include:

n-1	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	∞
$\mathbf{t_{90}}$	3.078	1.886	1.638	1.533	1.476	1.440	1.415	1.397	1.383	1.372	1.363	1.356	1.282

Student's t values can also be calculated with statistical packages or functions, *e.g.* the Excel TINV function (TINV(0.2, n-2) is equivalent to $t_{90,n-1}$) or the R qt function.

- If only one half-life value is available, multiply the value by 3 (Equation 3) instead of using Equation 2. This is to account for uncertainty in the environmental variability:

$$t_{input} = 3 \times t_{1/2}$$ **Equation 3**