Pesticide Water Calculator 3

User Manual

Diagram

Description automatically generated

Figure

# Introduction

Pesticide Water Calculator 3 (PWC3) is a tool for calculating pesticide concentrations in waterbodies for use in risk assessments, as typically used in government regulatory work. PWC3 is a major upgrade from previous PWC versions and should allow for much greater productivity, especially when spatially and temporally comprehensive assessments are desired. The user interface is streamlined with only the most necessary inputs brought forward for user interactions. Parameters that are seldomly altered and those that should not be altered for standard risk assessments are places in a more secure location. The mathematical portion of the program has been revised to greatly improve speed by eliminating unnecessary text file read and writes. Massive batch run capabilities have been added to enhance analysis of multiple applications methods, various application timings, multiple scenarios, and multiple water bodies. It is designed to address the newer ways that risk assessors are conducting regulatory water exposure assessments.

## Conceptual Overview

## Model Interface Overview

Graphical user interface, table

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# Running the Model

PWC3 is organized by tabs with the most primary inputs ordered from left to write—Chemical, Watershed, Schemes, Applications, Scenarios. Each of these pages as well as some hidden advanced pages are covered in the following sections.

## Chemical Inputs

When the program starts up, the input screen will appear as in Figure 2. There is a column of chemical inputs that will be used for every simulation in a run. These inputs are for the primary (or parent) compound, that is it is for the chemical that will be directly applied to the field. Degradate properties will be discussed later in this document. Most properties can be left blank if information is unknown, in such cases, the function will be disabled for that process. For example, if hydrolysis is left black, the effective degradation rate for hydrolysis will be zero (i.e., infinite half-life). For the case where a parameter must be populated, the program will alert the user to enter a value. Details of the cemical inputs are as follows:

Table

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Figure 2. chemical inputs for parent

**Koc or Kd** – choose Kd if the sorption input is the standard sorption coefficient referenced to total solid mass. Choose Koc if the sorption input is referenced to organic carbon mass. Theses are well-known standard definition available in any environmental chemical transport reference.

**Sorption (mL/g)** this is the value of either Kd or Koc

**Water Column Half life (d)** – this is a value for water column degradation that acts on all phases of the compound. The water column, as described elsewhere, contains suspended solids and other material that can sorb the chemical. This water column degradation parameter will act on these sorbed chemical phases as well as any dissolved in the water phase.

**Water Column Reference Temperature (°C)** This is the temperature at which the Water Column Half-life was obtained. This temperature is used as a reference when adjusting the degradation as environmental temperatures change during a simulation.

**Benthic Half life (d)** – this is a value for benthic degradation that acts on all phases of the compound. The benthos, as described elsewhere, contains solids that can sorb the chemical. This benthic degradation parameter will act on all chemical phases in the benthos.

**Benthic Reference Temperature (°C)** This is the temperature at which the Benthic Half-life was obtained. This temperature is used as a reference when adjusting the degradation as environmental temperatures change during a simulation.

**Aqueous Photolysis Half-Life (d)** This is the near surface half-life due to photolysis of the chemical dissolved in water. It should be the overall daily average value optimally best representing the daylight hours when the pesticide is most actively in the environment, but 12 hours of light would be a fine assumption.

**Photolysis Reference Latitude (°N)** This is the latitude that the photolysis study is meant to represent. This latitude is used as a reference when adjusting the degradation for different locations.

**Hydrolysis Half life (d)** – this is a value for degradation by hydrolysis. This parameter acts only on the aqueous phases in the model. It is effective in both the water column and the benthic region. There are no temperature adjustments on this parameter.

**Soil Half life (d)** – this is a value for total soil degradation. Depending on the radio button that follows, this can act on all phases of the compound (water and sorbed) or just on the water phase.

**Total or Aqueous** Determines whether the soil degradation wass calculated as a total degradation rate or as an aqueous-only rate.

**Soil Reference Temperature (°C)** This is the temperature at which the Soil Half-life was obtained. This temperature is used as a reference when adjusting the degradation as environmental temperatures change during a simulation. (IS it on or off?)

**Foliar Half life (d)** – this is the degradation half life of chemical that is on the foliage. This is chemical halflife and should not include washoff due to precipitation. It could include dissipation due to volatilization if that information is available.

**Foliar Washoff (cm-1)** Washoff coefficient that species the fractioanal removal of chemical on foliage that is removed for every 1 cm of precipitation.

**Molecular Weight (g/mol)** common molecular weight

**Vapor Pressure (Torr)** vapor pressure of compound (preferably at standard temperature, 25°C)

**Solubility (mg/L)** solubility of compound (preferably at standard temperature, 25°C)

**Henry’s Coefficient (vol/vol)** volumetric Henrys coefficient (preferably at standard temperature, 25°C)

**Air Diffusion Coefficient (cm2/d)** Diffusion coefficient of the chemical in air

**Heat of Henry (J/mol)** Enthalpy of phase change from water solution to air solution

### Daughter and Granddaughter

Checking the daughter and the granddaughter boxes will allow entry and calculation of direct degrates of the parent chemical as shown in Figure 3. Definitions of inputs are the same as for the parent. For each degradation process there is an entry required to specify how many moles of the degradate is produced per mole degrading of the preceding chemical. For example, if hydrolysis of one mole of parent produces 2 moles of daughter, then the box between parent and daughter on the hydrolysis row should be populated with 2.

Table

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Figure . Degradate Inputs

## Watershed/Waterbody

This tab specified the type of waterbodies that receive the chemical coming off the field. PWC 3 has 2 hard-coded waterbody systems that are standard for USEPA risk assessments—the Farm P and the Reservoir. See Figure 4. These two waterbodies can be simulated by checking the respective box. Both system can be run together in a single run as explained later. In addition, any number of custom water bodies may be run by selecting the appropriate file that describes the waterbody. Creation of water body files will be described later. Users can select as many hard-coded and custom waterbodies as they need, asnd all will be processed in a single run. Buttons are provided to populate the custom water body selection. The selection button opens a standard Window browser that enables standard file searching and filtering. Waterbody files all have the extension WAT.

Graphical user interface, application

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Figure . Waterbody selection

## Schemes

Number of Schemes is unlimited. The table will expand to accommodate any number of schemes. The scheme description is used only for user notes.

A scheme can be edited by checking the respective edit box. When checked, the next two pages are available to specify scheme characteristics.

Any time that a scheme is changed, you must press the commit button next to the scheme in order to save the changes. Note that commits are saved in volatile memory for the duration of the session (just like any text box). If you want to permanently save the commits (or any text box changes), then the file must be saved to a hard file as usual with the File/Save command.

Graphical user interface, table

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Figure . Schemes

# Output

Graphical user interface, table

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Figure

Scenario Input Files are now separated in a manner that makes multi-runs easier. Inputs are separated into field inputs and watershed inputs

## Field Input Files

Scenario input contain all intrinsic properties of the field. These include all area-independent parameters. Because these files are completely independent of the waterbody and extrinsic watershed properties, they can be used with any waterbody.

## Waterbody/Watershed Input Files

This file defines the extrinsic properties of the watershed. These include scale dependent parameters such as field size, hydraulic length, waterbody size, and drift parameters.