Pesticide Water Calculator 3

User Manual

# Introduction

The 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 earlier PWC versions and should allow for much greater productivity, especially when spatially and temporally comprehensive assessments are desired. To focus on productivity, 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 placed in a secure and less distracting location. PWC3 is also much more computationally efficient as portions of the program have been revised to improve speed and eliminate unnecessary text file read and writes. Massive batch run capabilities that the regulatory community is trending towards have been added. These new capabilities include batch runs with multiple applications methods, various application timings, multiple scenarios, and multiple water bodies. PWC3 addresses the newer ways for conducting regulatory water exposure assessments.

## Conceptual Model Overview

The conceptual model that USEPA uses is shown in Figure 1. A detailed description of the mechanics of the model can be found in Young (2023) and a high-level overview in Young (2019) but briefly, the conceptualizes an agricultural field with a crop and an adjacent water body. After pesticide is applied to a field, subsequent rainfalls or irrigation will transport pesticide to an adjacent waterbody transport by runoff and erosion. Pesticide aerial drift may also apply on the day of application. The model accounts for typical degradation and dissipation process such as metabolism, volatilization, photodegradation, leaching, uptake into sediment, and washout.

Diagram

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Figure . Conceptual Model for PWC3

# Interface Overview

PWC3 inputs are organized by tab pages, with the main pages showing by default at startup. The main tab pages are Chemical, Watershed/Waterbody, Schemes, Applications, and Scenarios. These tab pages are discussed in detail below. At the top of the interface is a menu bar with File and More Tabs. Work can be saved at any time by selecting File then the subitem Save. Likewise previous work can be loaded by selecting File then Retrieve. The More Tabs item gives users the option to open more less frequently needed tabs for advanced work; these tabs are for advanced users and is discussed in detail below. The Calculate button on the bottom right starts the simulation. On the lower left are locations and names of your saved work which become populated after you use File/Save or File/Retrieve. For convenience, you can double clicking on the directory path in the lower left will open that directory in a Windows browser. Your output and input files will be in this directory.

## Saving and Retrieving Work

The File menu item has two subitems Save and Retrieve. Saving work with File\Save will open a standard Windows file browser requesting you to *Save As.* All saves are Save As to help with accidently making unintentional saves. The *Save As* command will specifically request the name you want to use for the file save and will again ask if you are sure about this. Work is saved by default in a file with a PWC extension (e.g., *anyfilename.PWC*). However, it is not necessary to use this extension if a user needs to change it say for some advanced application. Input files are plain text files with a structure detailed in the PWC3 Technical Manual (Young, 2023). Input files can be easily examined or edited with any text reader. External editing though should be done with caution and only by advanced users. Previously saved files can be loaded with File\Retrieve. The default extension is PWC, but PWC3 can read any file as long as it is a text file with the proper structuring. Whenever File\Save or File\Retrieve are used, the directory path at the lower left will be populated with the path corresponding to the Save or Retrieve location. This location is where all output will be delivered at the end of a simulation. A convenient feature is that the path itself can be double clicked so that a user can easily access that location.

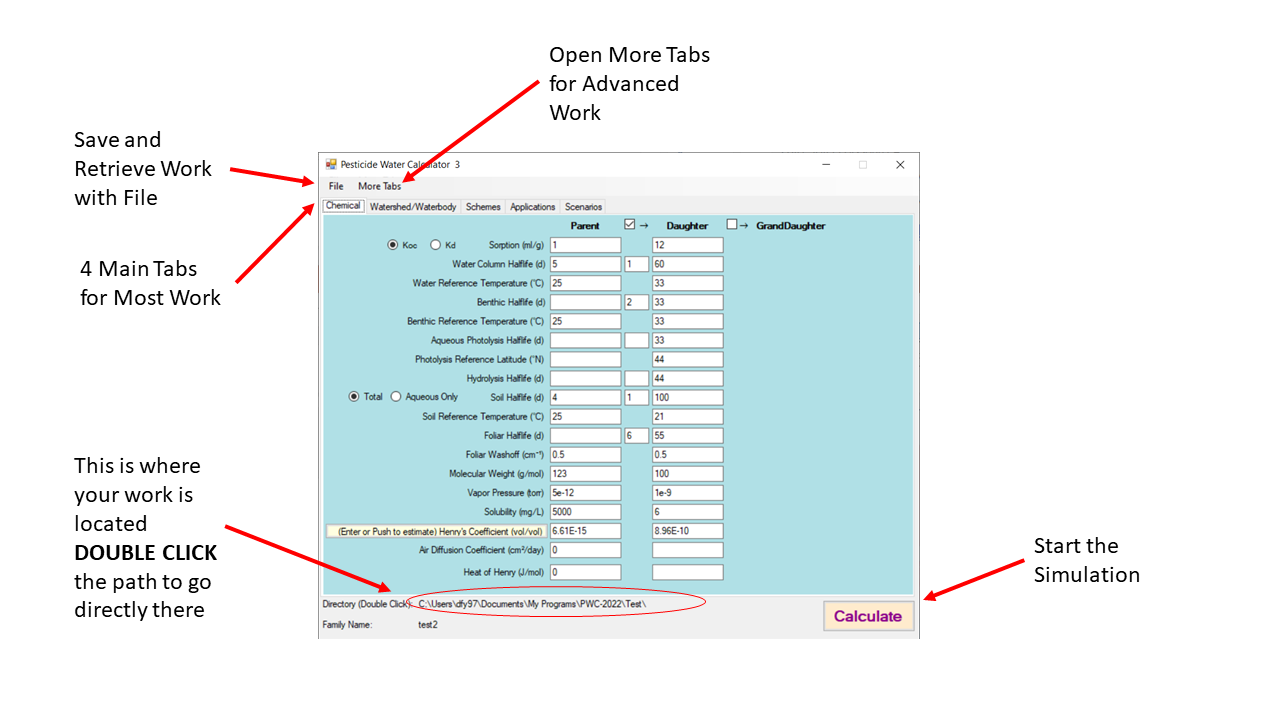


Figure . PWC Main Features

## Chemical Input Tab

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 chemical inputs are as follows:

Table

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Figure . 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. These 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 ass 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 half-life 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 specifies the fractional removal of chemical on foliage that rain removes for every 1 cm of precipitation. PWC suggests a value of 0.5, as this information is typically not readily available. The USEPA has used 0.5 as a default value for the past 30 years in PWC-type exposure assessments.

**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.

Graphical user interface, table

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Figure . Degradate Inputs

## Watershed/Waterbody Tab

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 Pond and the Reservoir. See Figure 4. These two waterbodies can be simulated by checking the respective box. In addition, any number of custom water bodies may be run by selecting the proper file that describes the waterbody. Creation of water body files will be described later. To select waterbodies other than the pond and reservoir, use the *Select Water Bodies* button. This will open a file browser which allows you to choose any number of previously-created waterbody files. Waterbody files all have the extension WAT. These WAT files are plain text files that can be created by means discussed later. Waterbody files can be removed from the list with the self-explanatory Clear Selected and Clear All buttons. Users can select as many hard-coded and custom waterbodies as they need, and all will be processed in a single run.

Graphical user interface, text

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Figure . Waterbody choice

## Schemes

Scheme allow different application types and different scenarios to be simulated and processed in a single run. A scheme is the combination of a specific application schedule along with all the scenarios that it applies to. For example, one scheme could be obtained from a pesticide label that says “Apply 1 lb. per acre to all corn across the continental United States”. Another scheme could be to “Apply 1lb/acre and then 1.5 lb./acre 7 days later to radish in the Southeast”. The number of schemes that can be simulated is unlimited, and rows will appear as needed as rows are populated. By using schemes, all the possible uses of a pesticide can be simulated in a single run.

To create or edit a scheme begin by opening the *Scheme Tab*. Then write a brief description of the scheme you wish to create (see Figure 6) in the *Scheme Description* column of the scheme table. The description has no effect on the program, it is for your reference only. But, the description should provide enough information for you to easily identify its characteristics. This scheme description will remind you on later tabs which scheme you are working on. Scheme descriptions are not recorded in output displays, since the text would be too long; instead, schemes are identified in the output by the *Scheme Numbe*r in the first column.

Checking the edit box will allow you to create and edit the scheme properties on the Applications and Scenarios tabs. The Commit button commits the edits to volatile memory. This means the edits will apply to the current simulation but will not be saved if the program is shut down. To permanently save any work, Use the File\Save command after any commits are made. The *Delete* button removes the scheme from the run. The number of schemes is unlimited, and more rows will appear as needed as rows are populated. *Scheme Number* in the first column simply specifies the numerical order of the schemes in the scheme table.

Any time that a scheme is changed whether on the Scheme Page, the Applications Page or the Scenario Page, you must press the commit button next to the scheme on the Scheme Page to save the changes. **Importantly, 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 save your work to a hard file with the File/Save command.**

All scenarios include reference to a weather file name. Weather files may be located anywhere on your computer network, so the first thing to do is specify the location of the weather files. Click on the Weather Fie Directory button to open a Windows browser, then find the location of your weather files. This only needs to be done once and the location will apply to all schemes.

After entering the scheme description, click the **Edit** box for the scheme. Checking the edit box allows you to enter information for that scheme on the next two tab pages (Applications Tab and Sc4enarios Tab).

Graphical user interface, text, application

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Figure . Schemes summary page

### Application Tab Page

After checking the **Edit** box for the scheme that you want to create or edit, go to the **Applications Tab** (see Figure 7). The **Applications Tab** is the first page for parameter entry for a scheme. At the top on theApplications Tab*,* you will see the *Scheme Number* and the *Scheme Description* that you previously entered. This will remind you of the scheme you are working on. Enter and manipulate application specifics for the pesticide on this tab as follows:

1. Choose the **Application Units** wither lb./acre or kg/ha
2. Choose the appropriate **Dates Relative To** which specifies how relative application dates are referenced or if absolute dates are to be used.
3. Populate **Application Table** as follows:
   1. Date can be the integer number of days after emergence, maturity or harvest. Negative values are used to indicate days before and positive values indicate day after. Absolute dates are specified by the format Mon/Day where Mon and Day are integers (e.g., March 23 is 3/23). Absolute date can be optionally specified with a year as for example 3/23/1991. In this case, the application would only be applied during the year 1991. For all other cases where year is not specified, applications occur every year of the simulation.
   2. Enter the amount of pesticide applied for the application on the respective date. Units depend on the choice from step 1.
   3. Choose the depth that the pesticide penetrates the soil at the time of application. See Appendix A for details on the various application methods.
   4. 0.Select the split for the T-band option if applicable. This specifies what fraction of pesticide resides in the upper 2 cm of the soil during a T-band application.
   5. Choose the Drift Type. The drop-down menu lists the most typical aerial applications for regulatory work. Additionally advanced users can specify custom choices as described later in Watershed/Waterbody file development.
   6. Choose the aerial buffer distance relevant to spray drift. Standard buffer attenuation are pre-calculated in the Watershed/Waterbody file so no additional external work is needed to obtain these values.
   7. Choose the Period of the application. This normally will be set to 1, which means applications occur every 1 year. A value of 3 would mean applications occur once every three years, and so on.
   8. Choose the Lag time. This is the start year for the applications. Normally th lag would be zero which mean that the applications are not lagged and occur on the first year of the simulation. A value of one would mean that application are delayed one year and then start on the second year of the simulation. The combination of Period and Lag allow users to develop more complex application schemes that vary from year to year.
   9. If an application needs to be removed, then push the delete button.
4. The **Clear All** button can be used to easily remove all entries in the Application Table
5. Check the **Use an Application Window** if you want to simulate the impact of application day on the output. This will initiate additional simulations for different application start days. Populate the following:
   1. **Window Span** is the number of days out that the simulation should cover. If you want to simulate the window between June 1 and June 30, enter 30 for the Window Span.
   2. **Step** is the number of days until the next simulation occurring within the Window Spam. For example, if you want to simulate every application start day within the Window Span, then enter 1. If you want simulations only every 3rd day, enter 3, and so on
6. Check the **Adjust Application Dates if Raining** if you want to include a farmer’s potential to consider predicted rainfall on their application date. This routine will adjust the application date according to the weather and the following parameters:
   1. **Intolerable Rain** is the amount of rain that will prevent the farmer from applying pesticide on that day.
   2. **Intolerable Rain Window** is the number of days into the future that the Intolerable Rain should not occur.
   3. **Optimum Application Window** is the number of days around the application date that it is acceptable to apply the pesticide.
   4. **Minimum Days Between Application** is the legal minimum number of days between applications when multiple applications per season are allowed. Note: To get maximum effectiveness from this routine the applications dates in the Application Table should be greater than this minimum.
7. Additional info?

Graphical user interface, application, Word

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Figure . Application Tab for Scheme #1

### Scenarios Page

Th Scenarios Page (Figure 8) is the second part of the scheme. Here you specify all the scenarios that are used with the pesticide application that you specified on the Applications Tab. Scenarios can be added to the scheme by pushing the **Select Scenarios** button. This opens a Widows file browser and scenarios can be selected. Multiple scenarios can be selected using the normal Windows functions with the Control and Shift keys. Scenarios can be removed from the list with the **Clear All** and the **Clear Selected** buttons. Scenario paths and names can also be edited by double clicking on an individual scenario, in which case an edit box opens where edits can be made (Figure 9).

Alternatively, scenarios can be read in from a file with specific formatting and ordering (file structure is given in Appendix B). To use this option, check the box labeled ***Get scenarios from a csv file***. Then, find for the file using the Windows file browser that pops up. This option may be convenient for massive batches of scenarios that have been chosen by procedures external to PWC, as in high resolution spatially explicit assessments.

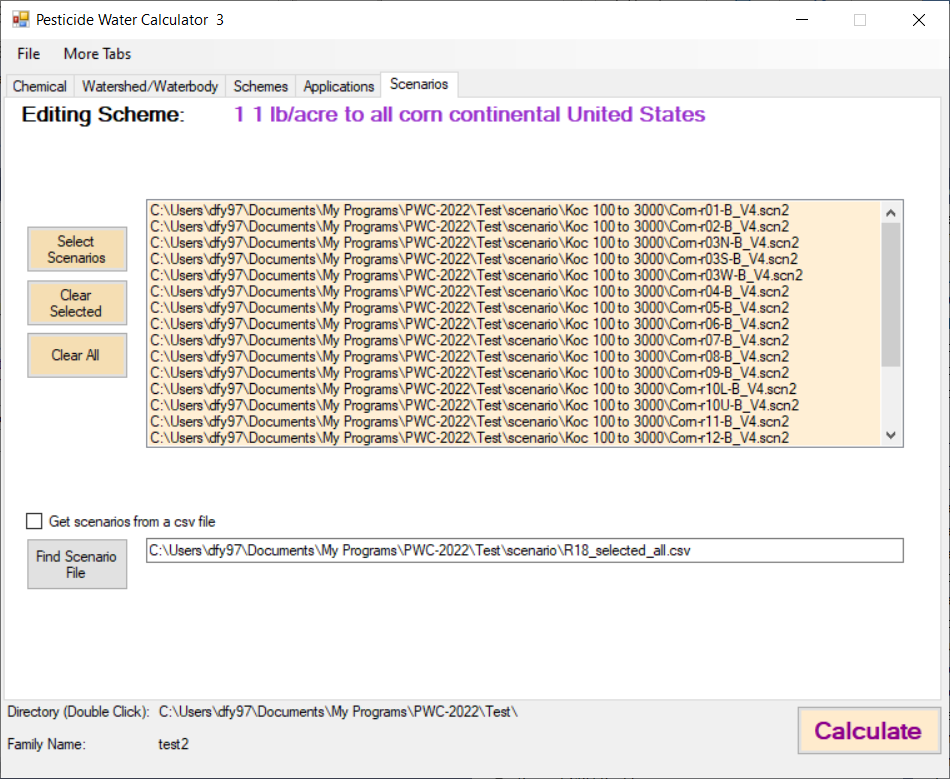


Figure . Scenario Page Tab escribing the scenarios that are used in a scheme.

Graphical user interface, text, application

Description automatically generated

Figure . Double clicking scenario name will bring up an Edit box where file and location name can be changed.

# More Tabs (advance Options)

The menu item at the top of PWC3 labeled More Tabs allows for more advanced work that would not typically be needed for regulatory work. These advanced tab pages can be opened (and closed) by selecting the specific submenu item. The specifics of the advanced tab pages are described in the following:

## Toggle Advanced

This opens and closes a tab page with some features that are not typically used but may be of interest in advanced work. Users of these features should be expertly familiar with the PRZM5/VVWM theoretical documentation. A brief summary of the features are given here:

**Adjust CN for Soil Moisture**- normally in PWC, the curve number is a adjusted for with higher curve numbers occurring as soil moisture increases, but for some validation or sensitivity analyses it may be required to fix the curve number at the known input value. Unchecking this box will fix the daily curve numbers to the input values without further adjustment based on moisture.

**Erosion Model**- by default PWC uses MUSS to calculate erosion. Two other models are available and can be selected by entering the appropriate number.

**Q10**- by default PRZM and VVWM change degradation by a factior of 2 for every 10°C increase in temperature. This Q10 value can be altered by entering a value in this box.

**Use Freundlich Isotherm**- this will allow the use of the Freundlich exponents (N on this same tab page) and nonlinear sorption will be simulated in the PRZM portion of PWC. Non linear sorption is not simulated in VVWM. Use of this feature may thus be most appropriate for groundwater estimates.

**Use Nonequilibrium** - this will allow the use of sorption nonequilibrium routines in PRZM and requires population of the nonequilibrium parameters on this same tab page. Refer to the PRZM/VVWM theoretical documentation for use of this advanced feature. Nonequilibrium sorption is not simulated in VVWM. Use of this feature may thus be most appropriate for groundwater estimates.

**Sub Time Steps**- when using Nonlinear and Nonequilibrium option, the program may become unstable and imprecise if large time steps like for the 1-day default that PRZM uses. This option allow the time step to be subdivided by the factor entered here. By default this value is set to 1, as normal PRZM runs do not have stability problems.

**Lowest Concentration for Freundlich**- because Freundlich isotherms approach to infinite sorption as concentration decreases, a minimum concentration must be given so that the isotherm becomes linear below that value. This prevents program crashes. A value is not need unless Freundlich isotherms are used.

**Nonequilibrium and Freundlich Parameters**- See PRZM/VVWM documentation for explanation of these parameters.

**Pesticide Mass in Nonequilibrium Region** – delivers respective output to output file

**Pesticide Mass in Equilibrium Region**– delivers respective output to output file

**Make HED files**- produces output files for use by HED

**Additional Return Frequencies**- in addition to the default 1-in-10-year output, custom return frequencies will also be produced.

**Subsurface Degradation**- The default degradation profile is set to 10 cm constant degradation that corresponds to the input soil degradation rate. This rate then declines to zero at 200 cm. Actual total degradation will depend on competing degradation processes (i.e., hydrolysis). In addition to the default profile, users can design any ramp-type profile, a constant or an exponentially declining profile. See PRZM/VVWM documentation for details.

## Toggle More Output

This toggles the Optional Output Tab Page. Normally the PWC3 creates a single output file summarizing all batch runs. However, users can find more output by using this tab page. Checking the boxes provides the most common output which appears in a file with a ZTS extension. These are time series files giving daily values for the selected parameters. Additionally more obscure output can be obtained by specifying the parameter fields in the table, which has the same traditional PRZM definitions. See PRZM5/VVWM manual for details. Daily output for the water body appears in its own file that have an ending of *\_wb.OUT* . Separate files will be produced for Degradates.

## Toggle Scenario Examiner

This opens the Scenario Examiner Page. This page allows a user to create or edit or inspect a scenario. To create a scenario, fill out the required fields and then push the **Push Here to Save the Scenario** button. To inspect or edit an existing scenario, push the ***Push Here to Examine Scenario*** button. The scenario will be loaded, and the fields populated. When finished save the scenario with the **Push Here to Save the Scenario** button.

## Toggle Waterbody Examiner

This opens the Waterbody Examiner Page. This page allows a user to create or edit or inspect a waterbody/watershed. To create a waterbody/watershed, fill out the required fields and then push the **Push Here to Save the Waterbody** button. To inspect or edit an existing waterbody, push the ***Push Here to Examine Waterbody*** button. The waterbody will be loaded, and the fields populated. When finished save the waterbody with the **Push Here to Save the Waterbody** button.

Figure 10 shows an example of a loaded watershed file. A brief description of the parameters on this tab page are given here, and details of the parameters including their theoretical basis can be found in the PRZM/VVM documentation (Young, 2023).

***Simulation Type***: this is an indicator for how water flow through the waterbody is simulated.

***Simulation Type 1*** will simulate a varying volume water body where the volume of the waterbody will fluctuate depending on the water amounts entering and exiting the body. Water will overflow and exit the system if the entering water exceeds the **Maximum Depth** (parameterized in the first column of boxes). Water can enter the system by runoff from the adjacent field, direct precipitation, or by **Base Flow** (see box below). Water can exit the system by overflow and evaporation. PRZM/VVWM sets a minimum water depth to 10-8 meters (essentially zero) to prevent numerical errors and divide-by-zero issues.

***Simulation Type 2*** keeps the waterbody at a constant volume and water does not enter or exit the water body. Water losses by evaporation losses also do not occur. Chemical mass associated with any incoming water does enter the system. This could be conceived by assuming that entering runoff and direct precipitation exactly matches the evaporating water, thus keeping volume constant.

***Simulation Type 3*** will keep the waterbody volume constant but will allow flow through the waterbody. Water into the system occurs by runoff. Evaporation, direct precipitation, and base flow are ignored.

**Water Body Area**- area of the water body, necessary for spray drift, evaporation, volatilization, benthic exchange etc.

**Initial Depth** - Depth at the start of the simulation. Specifies the constant depth for Simulation Type 2 and Type 3.

**Maximum Depth** - depth at which water overflows. Only used for Simulation Type 1. Does not impact Type 2 or 3.

**Flow averaging** - For Simulation Type 1 and Type 3, the runoff volumes can be smoothed out by averaging the runoff. This could simulate the effects of a reservoir dam where flow out is buffered or less spiky than the flow in. A value of 0 is a flag to average all flow so that there is a constant daily outflow. A value of 1 means each day’s runoff flows out of the waterbody on the same day. A value of 30 would mean that a day’s runoff entering the waterbody would be evenly distributed in the outflow over the next 30 days.

**Base Flow** – A constant input water flow (without chemical) that applies to Simulation Type 1 and 3

**Field Area** – the area of the adjacent runoff-producing field.

**Flow Length** – the hydrologic length of the field, typically the longest runoff path of the field (square root of field area for a square field would be fine).

**Fractional Cropped Area** – the fraction of field area that is actually treated with pesticide. Output concentrations are reduced proportionately with this value.

**Benthic Depth** – depth of lower compartment in VVWM

**D/dx** – an overall first-order mass transfer coefficient between b4enthic and water column

**Benthic Porosity** – porosity of benthic region

**Benthic Bulk Density** - bulk density of benthic region

**Benthic Foc** – organic carbon fraction of benthic sediment

**Benthic DOC** – dissolved organic carbon in benthic pore water.

**Benthic Biomass** – concentration of benthic biota in pore water

**DFAC** – attenuation parameter for photolysis

**Suspended Solids** – suspended solids concentration in water column.

**Chlorophyll** – chlorophyll concentration in water column

**Water Column Foc** – organic carbon fraction on suspended solids in water column

**Water Column DOC** – dissolved organic carbon in water column.

**Water Column Biomass** – biomass concentration in water column

**Zero Concentration when Water Level Drops Below** – for some simulations it may be desirable to ignore aquatic concentration in VVWM when the water depth are so low that they cannot support life. Concentrations in such cases may be very high, but only microscopic amounts of water exist. In this case, calculations for risk assessments in water may be of more practical use if these concentrations were ignored. Checking this box allows user to specify a depth below which concentrations are ignored only for the sake of output processing and display. Mass balance throughout the simulation is maintained always.

**What Depth?** –specify the depth if the check box above is checked.

**Single Compartment** – not functional yet (for TPEZ inclusion)

**Spray Drift Fractions** –this is a table of spray drift values as determined from Adrift and for which apply to the specific waterbody. The applications in the left column are the most common methods used in exposure assessments and should cover nearly every case. These methods correspond to those on the *Applications Page Tab* in the *Drift Methods* drop down menu. In the Figure 11 table, buffer distances are in the top row. If a user on the Applications Page Tab selects an in-between buffer, 0then

Timely, I’ll forward

Compements of billannouc distance is linearly interpolated.

Graphical user interface

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Figure

Graphical user interface, application, table, Excel

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Figure . Spray Drift Table on Watershed Tab

# Output

Graphical user interface, table

Description automatically generated

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.

Graphical user interface, table

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**Appendix A.**

**Appendix B. Batch scenario csv format**

**Appendix C. Scenario File Format**

**Appendix D. Waterbody/Watershed File Format**