

# **Surface Water Concentration Calculator User Manual**

**USEPA/OPP 734F14001**

June 12, 2014

Meridith Fry, Karen Milians, Dirk Young, He Zhong  
Environmental Fate and Effects Division  
Office of Pesticides  
United States Environmental Protection Agency  
Washington, DC 20460

Technical Contact Information:  
Dirk F. Young  
U.S. Environmental Protection Agency  
Washington, DC  
[young.dirk@epa.gov](mailto:young.dirk@epa.gov)

## Overview

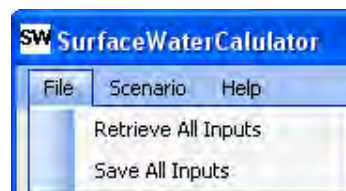
The Surface Water Concentration Calculator (SWCC) estimates pesticide concentrations in water bodies that result from pesticide applications to land. The SWCC is designed to simulate the environmental concentration of a pesticide in the water column and sediment and is used for regulatory purposes by the USEPA Office of Pesticide Programs (OPP). The SWCC uses PRZM version 5.0+ (PRZM5) and the Variable Volume Water Body Model (VVWM), replacing the older PE5 shell (last updated November 2006), which used PRZM3 (Carousel et al., 2005) and EXAMS (Burns, 2003). This updated model will improve users' interactions with the program and facilitate maintenance and operation of the software.

## Installation and Launching

The SWCC can be installed by obtaining the installation file (SWCC.msi) from an appropriate location. Internet users can access SWCC at: ([http://www.epa.gov/pesticides/science/models\\_db.html](http://www.epa.gov/pesticides/science/models_db.html) while EFED personnel can also go to the G drive Model Repository. Clicking on the msi file will install all necessary components of the SWCC. The SWCC should be installed to a directory where the user has administrative rights. After installation, SWCC can be launched by double-clicking on the SurfaceWaterGUI icon, which is saved in the model setup directory.

## Menu

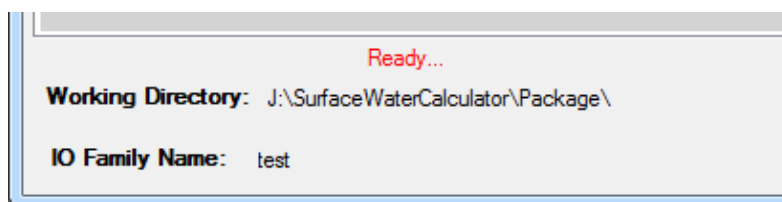
File manipulations in the SWCC are performed from the top Menu bar.



### File

- *Retrieve All Inputs* will open a file browser and allow the user to upload a previously created input file (\*.SWI) into the user interface. All information necessary for a simulation is recorded in the input file, including the scenario and pesticide information. The input files are text files that can be created either within the interface or within a text editor.
- *Save All Inputs* will open a file browser and allow the user to select a directory to save the inputs from the interface to a text file (Note: Output files will be saved in the same directory).

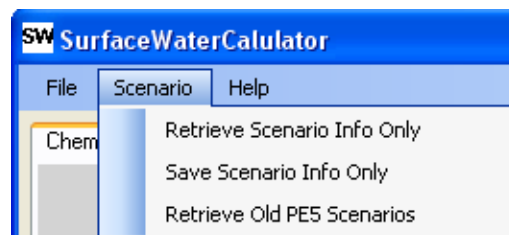
**Note 1: Using File Save and File Retrieve will automatically specify the working directory where the output file will be saved. Always save your work to the directory where you wish the output to be located. The working directory and name of the output files are given in the status section of the SWCC at the bottom left side as shown below.**



**Note 2: The File Save routine stores information for a simulation in a text file (\*.SWI). Users do not need to interact with these text files to run the SWCC. However, users wishing to externally manipulate these files for advanced processing can find the structure of the \*.SWI file in Appendix A.**

## Scenario

- *Retrieve Scenario Info Only* will load only the scenario information from a scenario file (\*.scn). Scenario filenames should be a maximum of 50 characters.
- *Save Scenario Info Only*. Scenarios created within the SWCC interface can be saved with this menu option.
- *Retrieve Old PE5 Scenarios* will load scenario files (tab-delimited text files) that are in the PE5 format. This feature maintains backward compatibility.



**Note : Scenario files are stored as text files. Users do not normally need to interact with these files as the SWCC creates them for you. However, users wishing to externally manipulate these files for advanced processing can find the structure of the \*.SCN file in Appendix B.**

## Help

*Help* contains this guidance and the developer's contact information.

## Chemical Tab

### For Parent Compound:

**Sorption Coefficient (mL/g):** Enter the value of the sorption coefficient in this text box, and then select whether it is a  $K_{oc}$  or  $K_d$  value.

- **$K_{oc}$  (mL/g):** Selecting the  $K_{oc}$  radio button indicates to the program that the partitioning coefficient ( $K_d$ ) is to be calculated by multiplying the *sorption coefficient* by the OC content of each horizon (see Scenario: Crop/Land tab).
- **$K_d$  (mL/g):** Selecting the  $K_d$  radio

button indicates to the program that the sorption coefficient is the  $K_d$  value entered directly into the program without adjustment. All soil layers will have the same  $K_d$  with this option.

**Water Column Metabolism\* Half-life (days):** This input represents a degradation half-life that applies to all forms of the chemical in the water column (typically the aerobic aquatic metabolism half-life in an OPP/EFED assessment). This includes forms sorbed to suspended solids and dissolved organic carbon (DOC) as well as dissolved forms of the chemical. The half-life that is entered should correspond to the water column reference temperature entered below. A value of zero or a blank is a signal to the program that this degradation process does not occur for this chemical.

**Water Reference Temperature (°C):** This value is the temperature at which the water column degradation applies. During a simulation, the degradation rate will change according to a Q10 assumption, with the entered temperature and degradation half-life as the references. Q10 is the factor by which degradation changes over 10°C.

**Benthic Metabolism\* Half-life (days):** This input, also known as the metabolism rate representative of the sediment (e.g., anaerobic aquatic half-life), represents a degradation half-life that applies to all forms of the chemical in the benthic layer. This includes forms sorbed to sediment and DOC, and dissolved forms of the chemical in pore water. The half-life entered should correspond to the benthic temperature reference entered below. (See note below regarding the use of the word *metabolism*.) A value of zero or a blank is a signal to the program that this degradation process does not occur for this chemical.

\*Note that the word *metabolism* is used in these descriptions because in a typical USEPA regulatory application these inputs would correspond to the bacterial metabolism degradation studies; however, these inputs can be used to represent any degradation that occurs in the compartment —benthic or water column— on all forms of the chemical.)

**Benthic Reference Temperature (°C):** This number is the temperature at which the benthic degradation half-life applies. During a simulation, the degradation rate will change according to a Q10 assumption, with the entered temperature and degradation half-life as the reference points.

**Aqueous Photolysis Half-life (days):** This input represents the 24-hour average near-surface photolysis rate as typically derived from photodegradation in water studies submitted to OPP. A value of zero or a blank is a signal to the program that this degradation process does not occur for this chemical.

**Photolysis Reference Latitude (°):** This value is the latitude at which the photolysis test was designed to represent (e.g., 40°).

**Hydrolysis Half-life (days):** This value represents the relevant hydrolysis half-life in the water body (the hydrolysis rate is not applied to the field degradation). Typically, the hydrolysis rate for pH 7.0 is used for standard EPA water bodies. If a non-standard water body with a different pH is used, users may enter the relevant hydrolysis rate that corresponds to the appropriate pH.

A value of zero or a blank is a signal to the program that hydrolysis does not occur for this chemical. The hydrolysis rate only applies to the top aqueous-phase compound. (Although the term *hydrolysis* is used here, this degradation input could be used for any degradation that is believed to occur only in the aqueous phase; i.e., this is a straight-forward rate with no manipulations to the input for temperature, pH, or any other environmental factor.)

**Surface Soil Half-life (days):** This input represents the total system half-life, typically obtained from a degradation test conducted on moist soil (aerobic soil metabolism). The program applies the associated degradation rate to both the soil and aqueous phases. If the soil temperature simulation option is used, then this degradation rate should correspond to the rate conducted at the temperature entered as the *Soil Reference Temperature* (see below). If the temperature simulation option is not used, then the soil degradation rate is constant for the entire simulation. Entering a zero or a blank indicates to the program that soil degradation does not occur.

**Soil Reference Temperature (°C):** This number is the temperature at which the soil degradation half-life applies. If the PRZM temperature simulation option is used during a simulation, the degradation rate will change according to a Q10 assumption, with the entered temperature and degradation half-life as the reference points. The Q10 assumption is based on an equation which corrects for temperature dependent degradation; a factor for rate increase when temperature increases by 10°C.

**Foliar Degradation Half-life (days):** This value represents the half-life of a pesticide on foliage. Entering a zero or blank signals to the program that foliar degradation does not occur.

**MWT (g/mol):** This input represents the molecular weight of the chemical. It is used in the water body volatilization routine and in the degrade production routine.

**Vapor Pressure (torr):** This value is the vapor pressure of the chemical and is used only in the volatilization calculations for the water body.

**Solubility (mg/L):** This input is the solubility of the chemical in water and is used only in the volatilization calculations for the water body. The program does not limit the pesticide concentration in water; the solubility limit can be exceeded.

**Degradate 1 Check Box:** Checking this box allows for the simulation of a daughter degradate of the parent. Chemical properties of the degradate should be entered as described above for the parent.

**Degradate 2 Check Box:** (Note: This box is only available if the Degradate 1 Check Box is checked). Checking this box allows for the simulation of a daughter degradate of degradate 1 (granddaughter of parent). Chemical properties of this degradate should be entered as described above for the parent.

**Molar Conversion Factors:** These factors are the ratios of moles of degradate produced to moles of parent degraded for each of the processes. For example, if one parent molecule breaks

down and produces one degradate, then the ratio is 1. If the process does not produce the degradate of interest, then the ratio is zero.

## Applications Tab

**Number of Applications:** Up to 50 pesticide applications per year can be specified. When the number of applications is altered, the user must click the *Update Applications* button, and then only the relevant applications will be shown. The number of rows in the table will equal the number of applications (Note: The number of applications will also be registered at run time if the *Update Applications* button is not pressed). Unless otherwise specified, these applications will repeat for every year of the simulation.

**Absolute and Relative Application Dates:** By selecting the appropriate radio button, pesticide application dates can be entered as absolute dates by specifying the day and the month (e.g., Day =31 Mon =1 for January 31), or as dates relative to the emergence date (e.g., 10 days since emergence).

**Specify Years:** This checkbox will reveal another set of text boxes that allows a user to specify the exact year at which the application occurs. This may be used, for example, in validation studies where the exact date is known.

**Amount:** This value refers to the applied mass of the pesticide in kg/ha.

**Application Method:** The application method specifies the way in which the pesticide is applied. There are 5 methods available:

1. Ground (entirely surface applied, distributed linearly decreasing to 4 cm in the profile),
2. Foliar (Pesticide is distributed to the canopy in proportion to its areal coverage, the remainder is applied as a ground application as above),
3. Incorporate (uniform incorporation into the soil to a user-specified depth),
4. @Depth (placed entirely in a single compartment at a user-specified depth),
5. T-Band (a fraction of the chemical is applied in the top 2 cm, and the remainder is applied uniformly between 2 cm and the user-specified depth).

**Depth (cm):** This number refers to the depth of pesticide incorporations for the *Incorporate*, *@Depth*, and *T-Band* application methods (see above).

**T-Band Split:** This input is the fraction of the application rate that will be applied to the top 2 cm in a T-band application.

**Eff.:** This value is the efficiency, which is a multiplier of the application rate in PRZM. It is used to reduce the actual applied mass to the field, without changing the input application rate (has utility when performing spray drift applications). The efficiency does not affect spray drift calculations.

**Drift:** The spray drift fraction is used to calculate drift loading. Typically for aquatic ecological exposure assessments (pond), use 0.05 for aerial spray, 0.01 for ground spray, or 0.03 for orchard air blast. In drinking water assessments (Reservoir), use 0.16 for aerial spray, 0.064 for ground spray, or 0.063 for orchard air blast. Refer to Input Parameter Guidance for more information (USEPA, 2006)

**Custom, Reservoir, or Pond:** Drift and efficiency are water-body specific parameters according to OPP/EFED policy. Therefore, the SWCC allows each type of water body (Pond, Reservoir, or Custom) to be parameterized differently with respect to drift and efficiency. Using the radio buttons above the *Eff* and *Drift* labels (see adjacent figure) allows the user to enter different values for each water body.

	Eff.	Drift
1.0	0.03	
.99	0.05	
.98	.01	
.97		

### Application Refinements:

**Applications occur:** This input includes user-specified frequency of applications (every number of years) and the interval. Interval is defined as year 1 to any number of years less than what is in the meteorological file. The word *last* represents the last year in the meteorological file. For example, a simulation could be run in which applications of pesticide occurred only for the first 15 years, and then no more applications were made for the remaining years. This could be done by entering *1* into the "from year" box and *15* into the "to year" box. If applications were to occur for every year of that 15-year period, a 1 would be entered into the "Applications occur every years(s)" box. Such an example could show the environmental recovery time after a pesticide use had ceased.

### Application Window Batch Analysis:

**Apply Pesticide Over a Time Window:** Selecting this check box will initiate a batch run of simulations with different application dates as specified by Window (days) and Skip (days). Output is delivered to a summary file in the Working directory.

☐ Specify Years

**Application Refinements**

Applications occur every  Year(s)

Applications occur from year  to year

**Application Window Batch Analysis**

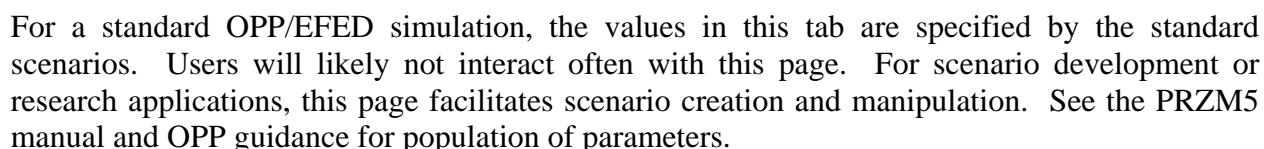
☒ Apply Pesticide over a Time Window

Window (days)

Step (days)

**Step:** When using the time window, *step* specifies how many days are between each of the batch runs. For example, if the window is 10 days and the step is 2 days, then 6 batch simulations would occur for applications on 0, 2, 4, 6, 8, and 10 days added to the original application date.

### ***Crop/Land Tab***



## Growth Descriptors

**Day Month Emerge:** Enter the day and month when the crop emerges from the ground.

8



This value is the start day for canopy and root development.

**Day Month Mature:** Enter the day and month when the crop reaches its maximum size. This number is the day when the maximum root depth and the maximum canopy coverage are attained.

**Day Month Harvest:** Enter the day and month when the crop is removed. This value is the day when the root depth and the canopy coverage are returned to zero.

**Root Depth (cm):** Enter the maximum root depth of the crop. Root depth is used in evapotranspiration calculations and in the irrigation calculation. Any depth can be used, but because of the vertical discretization scheme, root depth should be rounded to the nearest centimeter for depths up to 20 cm and then to the nearest 20 cm for root depths greater than 20 cm (i.e., 20, 40, 60 cm).

**Canopy Cover (%):** Enter the maximum areal coverage of the crop canopy. Canopy coverage affects the amount of pesticide that is directly applied to the ground when pesticides are applied over the canopy. Canopy coverage also has a small effect on the amount of rainfall that reaches the ground.

**Canopy Height (cm):** Enter the height of the crop at maturity. This value is used only for PRZM volatilization calculations. However since field volatilization is not operational in this SWCC version, the canopy height parameter has no effect on output).

**Canopy Holdup (cm):** This parameter along with the canopy cover (%) determines how much water can be stored in the canopy.

#### **Hydro Factors:**

**Pan Factor:** Values for the vast majority of the U.S. range from 0.7 to 0.8. PRZM multiplies the pan evaporation values in the weather file by the Pan Factor to estimate potential evapotranspiration (See the PRZM5 manual for typical values).

**Snowmelt Factor (cm/°C/day):** This value is the amount of accumulated snow that melts per °C above 0° C. Typical values for open agricultural areas are in the range of 0.4 to 0.5 (See Table 5.1 of Carousel et al., 2005 for more detailed values).

**Evaporation Depth (cm):** This parameter is the minimum depth of the soil that can be used to satisfy the potential evapotranspiration. If the root depth is greater than this value, then PRZM uses the soil water up to the root depth to satisfy evapotranspiration. If the root depth is less than this depth, then PRZM uses this minimum value. Generally, the evaporation depth ranges from 10 to 35 cm, depending on location (See Figure 5.2 of Carousel et al., 2005 for details).

Hydro Factors

<input type="text"/>	Pan Factor
<input type="text"/>	Snowmelt Factor
<input type="text"/>	Evaporation Depth (cm)

#### **Post-Harvest Foliage:**

Post-Harvest Foliage

☒ Surface Applied  
☐ Removed  
☐ Left as Foliage

For a foliar applied pesticide, determine how the pesticide remaining on the foliage is to be handled. It can be handled in one of the following ways:

**Surface Applied:** Pesticide remaining on the foliage is applied to the ground. ?

**Removed:** Pesticide remaining on the foliage is removed from the simulation.

**Left as Foliage:** The pesticide remains in the simulation as attached to foliage and can be washed off even after harvest.

### **Irrigation (auto-populated):**

**Irrigation Type:** Choose one of the three irrigation types: None (no irrigation, default selection), Over Canopy irrigation, or Under Canopy irrigation.

**Extra Water Fraction:** Enter the amount of extra water for leaching (as a fraction of the demand) beyond that which is required to meet the crop demand. Out of the total water required to satisfy the demand, some fraction of additional water may be desirable to wash out salts.

**Allowed Depletion:** Enter the degree (%) to which the available water in the active root can be depleted before irrigation is required.

**Irrigation**

☒ None
 ☐ Over Canopy
 ☐ Under Canopy

Extra Water Fraction: 
 Allowed Depletion: 
 Max Rate:

**Max Rate of Water Supplied (cm/hr):** Enter the limit to the amount of water that can be supplied. Because PRZM operates on a daily time scale, this value should be adjusted to account for the fact that this rate will be applied over the entire 24-hour period. For example, if 1 cm of water is applied per day, then the max rate should be 0.042 cm/hr (1/24), regardless of how fast the actual delivery equipment can produce for short periods.

### **Soil Layers:**

**Soil Layers**

Number of Horizons:   ☐ Simulate Temperature

Thick	$\rho$	Max. Cap.	Min. Cap.	O.C.	N

**Number of Horizons:** Enter the total number of soil horizons and click the *Update Horizons* button. The user can define the soil properties in each horizon by the following parameters:

**Thick:** thickness of the compartments in the horizon (Thick, cm)

**p:** effective porosity in the horizon ( $\rho$ ),

**Max Cap:** maximum water holding capacity for the tipping bucket method. For lack of a better parameterization, the USEPA has historically used field capacity for this value ( $\text{cm}^3 \text{cm}^{-3}$ ).

**Min Cap:** minimum capacity. The USEPA has traditionally used the wilting point for this value ( $\text{cm}^3 \text{cm}^{-3}$ ).

**O.C.:** organic carbon in the horizon (%)

**N:** number of compartments in the horizon.

**Simulate Temperature:** The user can decide whether to include a temperature simulation, in which case additional soil properties need to be entered.

## Runoff Tab

**Day Mon CN C N Table:** These values specify the day, month, curve numbers, and USLE erosion parameters (universal soil loss cover management factor [C] and manning's n factor [N]) for up to 50 times per year.

Chemical Applications Crop/Land <b>Runoff</b> Watershed Batch Runs Out						
No. of Time-Varying Factors	Day	Mon	CN	C	N	
26	1	16	2	89	.188	.011
	2	1	3	89	.190	.011
	3	16	3	89	.191	.011
<input type="checkbox"/> Specify year	4	1	4	89	.527	.011
	5	16	4	89	.558	.011
	6	1	5	89	.569	.011
	7	16	5	94	.572	.011
	8	1	6	94	.574	.011
	9	16	6	94	.575	.011

**USLE K:** Specifies the universal soil loss equation of soil erodibility. See PRZM manual.

**USLE LS:** Specifies the universal soil loss equation topographic factor. See PRZM manual.

**USLE P:** Specifies the universal soil loss equation practice factor. See PRZM manual.

**IREG:** Specifies location of NRCS 24-hour hyetograph. See PRZM manual.

**Slope:** Specifies the slope of the hydraulic flow path. See PRZM manual.

<input type="text"/>	USLE K
<input type="text"/>	USLE LS
<input type="text"/>	USLE P
<input type="text"/>	IREG
<input type="text"/>	Slope

**Specify Years:** This checkbox will reveal another set of text boxes that allows a user to specify the exact year during which the event occurs. This number may be used for example in validation studies where the exact date is known.

### **PRZM Runoff and Erosion Extraction (New For PRZM5):**

**R-Depth (cm):** Enter the lowest depth at which runoff interacts with the soil.

**R-Dcline (1/cm):** Enter the exponential decline of runoff interaction as a function of depth.

**Efficiency:** Enter the amount of runoff that interacts with the soil.

**E-Depth (cm):** Enter the lowest depth at which erosion interacts with the soil.

**E-Dcline (1/cm):** Enter the exponential decline of erosion interaction as a function of depth.

PRZM5 Runoff & Erosion Extraction	
Distribution of Runoff in Surface	Distribution of Eroded Solids
R-Depth (cm) <input type="text" value="2.0"/>	E-Depth (cm) <input type="text" value="0.1"/>
R-Dcline (1/cm) <input type="text" value="1.55"/>	E-Dcline (1/cm) <input type="text" value="0"/>
Efficiency <input type="text" value="0.266"/>	

## ***Watershed Tab***

**Simulation Type:** Users can select the EPA Pond, EPA Reservoir, and user-defined custom water body in the same run. Users can choose among three different types of custom runs: varying volume with flow through, constant volume with flow through, or constant volume without flow through. Users also have the option to choose a reservoir with user-specified flow-through averaging as does PMRA Health Canada.

**Sediment Accounting:** The default setting is for no sediment burial, but the user may select sediment burial. This input allows for a first-order solute removal mechanism based on the sediment delivery rate to the benthic region.

**PRBEN:** This value specifies how the pesticide associated with eroded solids is distributed between the water column and the benthic regions. The default value of 0.5 specifies that half is placed in the benthic region and half in the water column. A value of one distributes all into the benthic region, whereas a value of zero places all in the water column.

Chemical Applications Crop/Land Runoff V

Simulation Type

☒ EPA Pond

☒ EPA Reservoir

☐ Use Flow Averaging (days)

User-Defined Water Body  
(Choose one or none):

☒ Varying Volume & Flowthrough

☐ Constant Volume No Flowthrough

Sediment Accounting

☒ No Burial

☐ Burial

PRBEN

**Watershed and Water Body Dimensions:** The watershed and water body dimensions are given here for the selected water bodies. A Cropped Area Fraction can be entered and represents

the fraction of the watershed that actually receives pesticide. Default values for the EPA Pond and the EPA Reservoir cannot be changed.

Watershed and Water Body Dimensions			
	EPA Pond	EPA Reservoir	User Defined
Field Area (m <sup>2</sup> )	100000	1728000	10000
Water Body Area (m <sup>2</sup> )	10000	52600	12
Initial Depth (m)	2	2.74	4.2
Max Depth (m)	2	2.74	4.8
Hydraulic Length (m)	356.8	600	600
Cropped Area Fraction	1	1.0	1.0

### **Water Body Physical Parameters**

The physical parameters are the same as those defined in the VVWM documentation. Checking the USEPA/OPP defaults box will reset all values to the standard water body parameters and will lock them.

Water Body Physical Parameters			
<input type="checkbox"/> USEPA/OPP defaults			
Water Column Parameters		Benthic Parameters	
DFAC	1.19	Benthic Depth (m)	0.05
Water ColumnSS (mg/L)	30	Benthic Porosity	0.5
Chlorophyll (mg/L)	0.005	Bulk Density (g/cm <sup>3</sup> )	1.35
Water Column foc	0.04	Benthic foc	0.04
Water Column DOC (mg/L)	5	Benthic DOC (mg/L)	5
Water Column Biomass (mg/L)	0.4	Benthic Biomass (g/m <sup>2</sup> )	0.006
		Mass Xfer Coeff. (m/s)	1E-08

### ***Batch Runs Tab***

Multiple scenarios can be run if desired. The buttons on this tab open a file browser so that users can select specific scenarios for batch runs. Typical Windows-type file selection methods can be used to select specific sets. For example, using “\*CA\*” in the file browser for *file* will select all California scenarios, whereas “\*corn\*” will select all corn scenarios. Multiple files can be selected using the standard browser functions associated with the Shift and Ctrl keys.

<input type="checkbox"/> Do a Batch Run
Select Scenarios for Batch Runs
Clear Selected
Clear All

Output is delivered to a summary file. Users can analyze the summary file and identify scenarios in need of more analysis. Information presented in the summary file should be sufficient to identify problematic scenarios.

## Output Tabs

**Out: Pond:** This output tab gives results for the EPA Pond and user-defined water bodies.

**Out: Reservoir:** This output tab gives results for the EPA Drinking Water Reservoir.

**Out: Custom:** This output tab gives results when not using the EPA Pond and EPA Drinking Water Reservoir.

The graphs on these two output tabs show annual peaks for the water column and benthic pore water.

## Concentrations:

**Absolute Peak = 0.0**

**Water Column 1-in-10 year Conc. (ppb)**

Peak	<input type="text"/>	4-day Avg	<input type="text"/>
365-day Avg	<input type="text"/>	21-day Avg	<input type="text"/>
Entire Mean	<input type="text"/>	60-day Avg	<input type="text"/>

**Absolute Peak:** Highest peak of the entire simulation (ppb).

**Peak (acute):** Upper 90<sup>th</sup> ranked annual peak of the simulation (ppb).

**4-day:** Upper 90<sup>th</sup> ranked annual 4-day average of the simulation (ppb).

**21-day:** Upper 90<sup>th</sup> ranked annual 21-day average of the simulation (ppb).

**60-day:** Upper 90<sup>th</sup> ranked annual 60-day average of the simulation (ppb).

**365-day Avg (chronic):** Upper 90<sup>th</sup> ranked annual average of the simulation (ppb).

**Simulation Average:** Mean value of all daily concentrations in the simulations.

**1-in-10 Benthic Peak:** Upper 90<sup>th</sup> ranked annual benthic pore water peak of the simulation (ppb).

**Total/Dry Sed:** Concentration in sediment (ppb).

**1-in-10 Benthic 21-day:** Upper 90<sup>th</sup> ranked annual 21-day average of benthic pore water for the simulation (ppb).

**Benthic 1-in-10 Yr Conc. (ppb)**

	Pore Water	Total/Dry Sed
Peak	<input type="text"/>	<input type="text"/>
21-day Avg	<input type="text"/>	<input type="text"/>

**Sediment Bioavailable Fraction**

**Total/Dry Sed:** Concentration in sediment (ppb).

**Sediment Bioavailable Fraction:** Fraction of total chemical in the benthic region that resides in the pore water.

**Relative Transport:**

**Runoff:** This value is the fraction of pesticide mass that moved to the water body by runoff (pesticide moved to water body by runoff / pesticide that entered water body by all means) It is calculated over the entire simulation.

**Erosion:** This input is the fraction of pesticide mass that moved to the water body by erosion. It is calculated over the entire simulation.

**Drift:** This value is the fraction of pesticide mass that moved to the water body by drift. It is calculated over the entire simulation.

Relative Transport	
Runoff	<input type="text"/>
Erosion	<input type="text"/>
Drift	<input type="text"/>
Fraction from Field to Water	
<input type="text"/>	

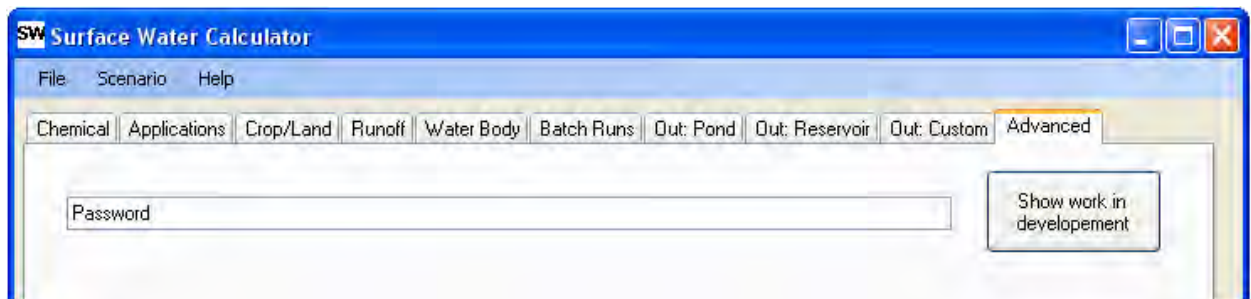
**Fraction from Field to Water:** This input is the fraction of the pesticide applied to the field that moved into the water body.

**Effective Half-lives:** These values report the effective half-life of each of the processes (days). The total values represent the overall effective half-life of the respective compartment (i.e., water column or benthic).

Effective Water Column Halflives (day)	Effective Benthic Halflives (day)
Washout <input type="text"/>	Burial <input type="text"/>
Metabolism <input type="text"/>	Metabolism <input type="text"/>
Hydrolysis <input type="text"/>	Hydrolysis <input type="text"/>
Photolysis <input type="text"/>	Total <input type="text"/>
Volatilization <input type="text"/>	
Total <input type="text"/>	

**Advanced Tab**

This tab is primarily used by the developers and will change frequently as developer needs arise. For more information, contact the developer, whose information is supplied in the *Help* menu and on the first page of this document.







## APPENDIX A: Surface Water Input File Format

Input files for the SWCC (\*.SWI files) are created by the interface and store all of the information needed for a SWCC simulation. There is no required format or positioning of the values within the lines. However, lists of numbers on the same line must be comma-delimited. The line location for the information stored is as follows:

- Line 1. Chemical ID info (text)
- Line 2. Number of parent and degradates (1 to 3 values)
- Line 3. True if  $K_{oc}$ ; false if  $K_d$
- Line 4. Sorption coefficient values, mL/g, (Parent, Degradate 1, Degradate 2)
- Line 5. Water metabolism half-life, days, (Parent, Degradate 1, Degradate 2)
- Line 6. Water metabolism reference temperature, °C, (Parent, Degradate 1, Degradate 2)
- Line 7. Benthic metabolism half-life, days, (Parent, Degradate 1, Degradate 2)
- Line 8. Benthic metabolism reference temperature, °C, (Parent, Degradate 1, Degradate 2)
- Line 9. Aqueous photolysis half-life, days, (Parent, Degradate 1, Degradate 2)
- Line 10. Photolysis reference latitude, degrees, (Parent, Degradate 1, Degradate 2)
- Line 11. Hydrolysis half-life, days, (Parent, Degradate 1, Degradate 2)
- Line 12. Soil half-life, days, (Parent, Degradate 1, Degradate 2)
- Line 13. Soil reference temperature, °C, (Parent, Degradate 1, Degradate 2)
- Line 14. Foliar half-life, days, (Parent, Degradate 1, Degradate 2)
- Line 15. Molecular weight, g/mol, (Parent, Degradate 1, Degradate 2)
- Line 16. Vapor pressure, torr, (Parent, Degradate 1, Degradate 2)
- Line 17. Solubility, mg/L, (Parent, Degradate 1, Degradate 2)
- Line 18. Water Column Metabolism Molar Conversion Factor (Parent to Degradate 1, Degradate 1 to Degradate 2)
- Line 19. Benthic Metabolism Molar Conversion Factor (Parent to Degradate 1, Degradate 1 to Degradate 2)
- Line 20. Photolysis Molar Conversion Factor (Parent to Degradate 1, Degradate 1 to Degradate 2)
- Line 22. Hydrolysis Molar Conversion Factor (Parent to Degradate 1, Degradate 1 to Degradate 2)
- Line 22. Soil Molar Conversion Factor (Parent to Degradate 1, Degradate 1 to Degradate 2)
- Line 23. Foliar Molar Conversion Factor (Parent to Degradate 1, Degradate 1 to Degradate 2)
- Line 24. Unused.
- Line 25. Unused
- Line 26. Unused
- Line 27. Q10 factor
- Line 28. Number of pesticide applications
- Line 29. List of comma-delimited days of month of the applications
- Line 30. List of comma-delimited months of the applications
- Line 31. List of comma-delimited application rates, kg/ha (count = Line 28)
- Line 32. FALSE if years are not explicitly entered; TRUE if the years of applications are specified;
- Line 33. List of comma-delimited years of the applications (Required if Line 32 is TRUE)

Line 34. List of comma-delimited application methods (integer representations)  
 Line 35. List of comma-delimited efficiency for custom applications (fraction)  
 Line 36. List of comma-delimited drift for custom applications  
 Line 37. List of comma-delimited efficiencies for pond applications (fraction)  
 Line 38. List of comma-delimited drift for pond applications  
 Line 39. List of comma-delimited efficiency for reservoir applications (fraction)  
 Line 40. List of comma-delimited drift for reservoir applications  
 Line 41. List of comma-delimited depths of incorporations, cm  
 Line 42. List of comma-delimited relative application days  
 Line 43. TRUE if application dates are absolute; FALSE if they are relative to planting  
 Line 44. List of comma-delimited T-band depths  
 Line 45. Unused  
 Line 46. Unused  
 Line 47. Unused  
 Line 48. Scenario ID (string)  
 Line 49. Full path and file name of the weather file  
 Line 50. Unused  
 Line 51. List of Boolean indicators for the simulations to be bunned: EPA Reservoir, EPA Pond, VVWM, VVWM Constant Volume w/Flow, VVWM Constant Volume w/o Flow.  
 Line 52. TRUE if Reservoir averaging is used, number of averaging days  
 Line 53. TRUE if burial ; FALSE if no burial  
 Line 54. Field area for custom water body, m<sup>2</sup>  
 Line 55. Waterbody area for custom water body, m<sup>2</sup>  
 Line 56. Initial depth for custom water body, m  
 Line 57. Maximum depth for custom water body, m  
 Line 58. Mass transfer coefficient, m/s  
 Line 59. PRBEN  
 Line 60. Benthic depth, m  
 Line 61. Benthic porosity  
 Line 62. Bulk density g/mL  
 Line 63. Benthic foc  
 Line 64. Benthic DOC, mg/L  
 Line 65. Benthic biomass  
 Line 66. DFAC  
 Line 67. SS  
 Line 68. Chlorophyll  
 Line 69. Water column foc  
 Line 70. Water column DOC  
 Line 71. Water column biomass  
 Line 72. Use EPA defaults for physical parameters (Boolean)  
 Line 73. Fraction Cropped Area Reservoir, Fraction Cropped Area Custom  
 Line 74. Unused  
 Line 75. Emergence day of month  
 Line 76. Emergence month  
 Line 77. Maturity day of month  
 Line 78. Maturity month

Line 79. Harvest day of month  
 Line 80. Harvest month  
 Line 81. Root depth, canopy height  
 Line 82. Canopy cover  
 Line 83. Canopy holdup  
 Line 84. Post-harvest foliage 1,2,3  
 Line 85. PFAC  
 Line 86. SFAC  
 Line 87. Evaporation depth  
 Line 88. Flag: 0= No irrigation; 1= Over canopy; 2= Under canopy  
 Line 89. Extra leaching water fraction  
 Line 90. Allowable depletion for irrigation  
 Line 91. Maximum irrigation rate ( average daily in cm/hr)  
 Line 92. USLE K  
 Line 93. USLE LS  
 Line 94. USLE P  
 Line 95. IREG  
 Line 96. Slope  
 Line 97. Hydraulic length for custom waterbody  
 Line 98. Number of soil layers  
 Line 99. List of comma-delimited thicknesses  
 Line 100. List of comma-delimited bulk densities  
 Line 101. List of comma-delimited maximum capacities  
 Line 102. List of comma-delimited minimum capacities  
 Line 103. List of comma-delimited organic carbon percentages  
 Line 104. List of comma-delimited numbers of increments in layers  
 Line 105. List of comma-delimited sand percentages  
 Line 106. List of comma-delimited clay percentages  
 Line 107. Albedo  
 Line 108. Temperature at lower boundary, °C  
 Line 109. TRUE to simulate temperature; FALSE for no temperature simulation  
 Line 110. Number of erosion /runoff factors  
 Line 111. List of comma-delimited days of month for the runoff/erosion event  
 Line 112. List of comma-delimited months for the runoff/erosion event  
 Line 113. List of comma-delimited curve numbers for the runoff/erosion event  
 Line 114. List of comma-delimited C factors for the runoff/erosion event  
 Line 115. List of comma-delimited Manning's n values for the runoff/erosion event  
 Line 116. Runoff interaction depth (cm), decline (1/cm), bypass  
 Line 117. Erosion interaction depth (cm), decline (1/cm)  
 Line 118. TRUE if specific years used for erosion/runoff; FALSE if the events occur every year  
 Line 119. List of comma-delimited years for the runoff/erosion event (used if Line 112 is TRUE)

## Appendix B: Scenario File Format

The Scenario file (\*.SCN) is exactly the same as the SWI file, starting at line 48 of the SWI File. The SCN File line number format is therefore as follows:

- Line 1. Scenario ID (string)
- Line 2. Full path and file name of the weather file
- Line 3. Unused
- Line 4. List of Boolean indicators for the simulations to be bunned: EPA Reservoir, EPA Pond, VVWM, VVWM Constant Volume w/Flow, VVWM Const Volume w/o Flow.
- Line 5. TRUE if Reservoir averaging is used, number of averaging days
- Line 6. TRUE if burial ; FALSE if no burial
- Line 7. Field area for custom water body, m<sup>2</sup>
- Line 8. Waterbody area for custom water body, m<sup>2</sup>
- Line 9. Initial depth for custom water body, m
- Line 10. Maximum depth for custom water body, m
- Line 11. Mass transfer coefficient, m/s
- Line 12. PRBEN
- Line 13. Benthic depth, m
- Line 14. Benthic porosity
- Line 15. Bulk density g/mL
- Line 16. Benthic foc
- Line 17. Benthic DOC, mg/L
- Line 18. Benthic biomass
- Line 19. DFAC
- Line 20. SS
- Line 21. Chlorophyll
- Line 22. Water column foc
- Line 23. Water column DOC
- Line 24. Water column biomass
- Line 25. Use EPA defaults for physical parameters (Boolean)
- Line 26. Unused
- Line 27. Unused
- Line 28. Emergence day of month
- Line 29. Emergence month
- Line 30. Maturity day of month
- Line 31. Maturity month
- Line 32. Harvest day of month
- Line 33. Harvest month
- Line 34. Root depth, canopy height
- Line 35. Canopy Cover
- Line 36. Canopy holdup
- Line 37. Post-harvest foliage 1,2,3
- Line 38. PFAC
- Line 39. SFAC
- Line 40. Evaporation depth

Line 41. Flag: 0= No irrigation; 1= Over canopy; 2= Under canopy  
 Line 42. Extra leaching water fraction  
 Line 43. Allowable depletion for irrigation  
 Line 44. Maximum irrigation rate ( average daily rate in cm/hr)  
 Line 45. USLE K  
 Line 46. USLE LS  
 Line 47. USLE P  
 Line 48. IREG  
 Line 49. Slope  
 Line 50. Hydraulic length for custom waterbody  
 Line 51. Number of soil layers  
 Line 52. List of comma-delimited thicknesses  
 Line 53. List of comma-delimited bulk densities  
 Line 54. List of comma-delimited maximum capacities  
 Line 55. List of comma-delimited minimum capacities  
 Line 56. List of comma-delimited organic carbon percentages  
 Line 57. List of comma-delimited numbers of increments in layers  
 Line 58. List of comma-delimited sand percentages  
 Line 59. List of comma-delimited clay percentages  
 Line 60. Albedo  
 Line 61. Temperature at lower boundary, °C  
 Line 62. TRUE to simulate temperature; FALSE for no temperature simulation  
 Line 63. Number of erosion /runoff factors  
 Line 64. List of comma-delimited days of month for the runoff/erosion event  
 Line 65. List of comma-delimited months for the runoff/erosion event  
 Line 66. List of comma-delimited curve numbers for the runoff/erosion event  
 Line 67. List of comma-delimited C factors for the runoff/erosion event  
 Line 68. List of comma-delimited Manning's n values for the runoff/erosion event  
 Line 69. Runoff interaction depth (cm), decline (1/cm), bypass  
 Line 70. Erosion interaction depth (cm), decline (1/cm)  
 Line 71. TRUE if specific years used for erosion/runoff; FALSE if the events occur every  
         year  
 Line 72. List of comma-delimited years for the runoff/erosion event (used if Line 112 is  
         TRUE)