Spatial Aquatic Model User Manual

(Version: Alpha)

Revision Date: April 21, 2015

Contact Information:
Nelson Thurman
U.S. Environmental Protection Agency
Washington, DC
thurman.nelson@epa.gov

Overview

The Spatial Aquatic Model (SAM) estimates pesticide concentrations for spatially-explicit assessments of human and aquatic species exposure in water. SAM Alpha is publicly available online at http://qed.epa.gov/ubertool/sam with an internet connection and web browser (Figure 1).

Model Disclaimer: Ecological risk calculations contained here should be used for no purpose other than quality assurance and peer review of the presented web applications. This web site is under development. It is available for the purposes of receiving feedback and quality assurance from personnel in the EPA Office of Chemical Safety and Pollution Prevention and from interested members of the ecological risk assessment community.

A brief overview of SAM is provided on the Description tab (Figure 1). Inputs are entered by the user on the Inputs tab, organized into four categories: Chemical, Application, Simulation, and Output (outlined below). The SAM Algorithms, References, QA/QC, and Batch tabs will be updated as the model continues to be developed. The History tab is intended to provide a record of a user's simulation history.

Figure 1. The SAM is available at http://qed.epa.gov/ubertool/sam.

SAM Inputs

1. Chemical Tab

Choose a Scenario: Several chemical-crop scenarios were developed during testing, and can be selected by the user (i.e. Atrazine-Corn, Chlorpyrifos-Corn, Chlorpyrifos-Soybeans, Fipronil-Corn, Metolachlor-Corn). The inputs for these scenarios are set to default values. Selecting "Custom" allows the user to define a custom simulation.

Chemical Name: The name of the chemical being simulated (no specific format) (Figure 2).

Sorption Coefficient (mL/g): The organic carbon partition coefficient. User may enter in terms of K_{oc} or K_d, by selecting corresponding radio button.

Soil Metabolism Halflife (days): The aerobic soil metabolism halflife for the soil system, typically taken from laboratory studies on moist soil. It incorporates both metabolism and hydrolysis, by the nature of aerobic soil metabolism data. A value of zero signals that soil system degradation does not occur for the chemical. Please refer to Input Parameter Guidance (Guideline 162-1) for further information on using the halflife from aerobic soil metabolism studies. Note: Halflife does not include soil photolysis (which usually is not an important degradation pathway), pH-dependent hydrolysis (which can be important for some pesticides, such as organophosphorus or N-methyl carbamates), or foliar interception or dissipation.

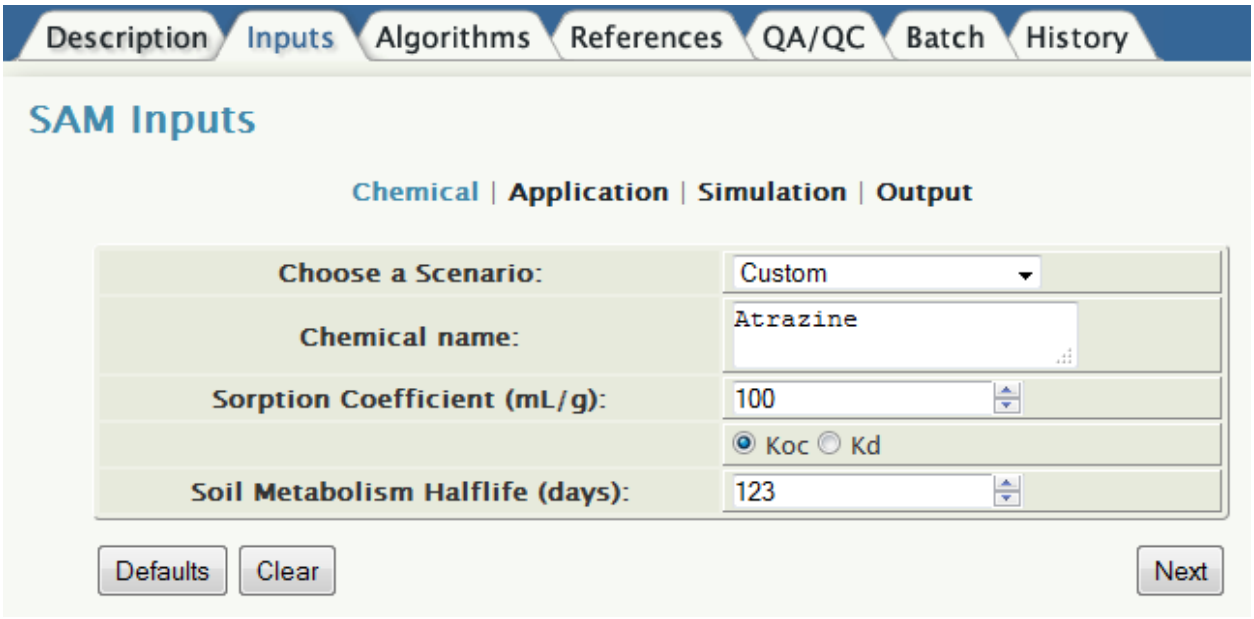


Figure 2. The Chemical tab featuring inputs for scenario, chemical name, sorption coefficient, and soil metabolism halflife.

2. Application Tab

Crop: From the dropdown menu, the crop to be simulated is selected (Figure 3).

Total Number of Crops: The total number of crop groups based on the crop selected is automatically updated. No user input needed.

Number of Applications per Year: The number of applications in each year of the simulation period.

Application Method: From the dropdown menu, the application method for each application is selected (one method selected for each simulation). Additional methods may be added in subsequent versions.

Ground: Distributes chemical under the canopy onto soil with distribution inversely proportional with depth to 4 cm.

Foliar: Chemical is intercepted by foliage in proportion to the foliar aerial coverage at the time of application. Chemical that is not intercepted is treated as a ground application.

Application Rate (kg/ha): The mass of pesticide applied per hectare.

First Application Date: The date of the first application, selected from a dropdown calendar. Based on the pre-processed meteorology in SAM Alpha, the date must be between 1/1/1984 and 12/31/2013, and must be after the Start Date and before the End Date. Subsequent application dates are calculated internally by the model, based on the number of applications per year and the start and end dates.

Refinements: Several application window distribution options are available. These distributions were conceptualized after initial testing showed an instantaneous application (or pulse) of pesticide to a watershed was inconsistent with the temporal distribution of pesticide concentrations in monitoring data (Figure 4).

1) **Uniform application over window**: If selected, the user can define the Time Window (days) over which the daily application rate equals the Application Rate divided by the number of days in the Time Window.

2) **Uniform step application over window**: If selected, the user can define two Time Windows (days) and corresponding Percent Applied (%) during each window (must sum to 100%). The daily application rate in the first window equals the percentage (%) of the total Application Rate divided by the number of days in that window. The remainder of the Application Rate is applied equally across the number of days in the second window.

3) **Triangular application over window**: If selected, the user can define the time window (days) over which the Application Rate is distributed triangularly (symmetric about the midpoint of the Time Window). With this option, the daily Application Rate increases linearly to the midpoint of the window, and then decreases linearly to the end of the window.

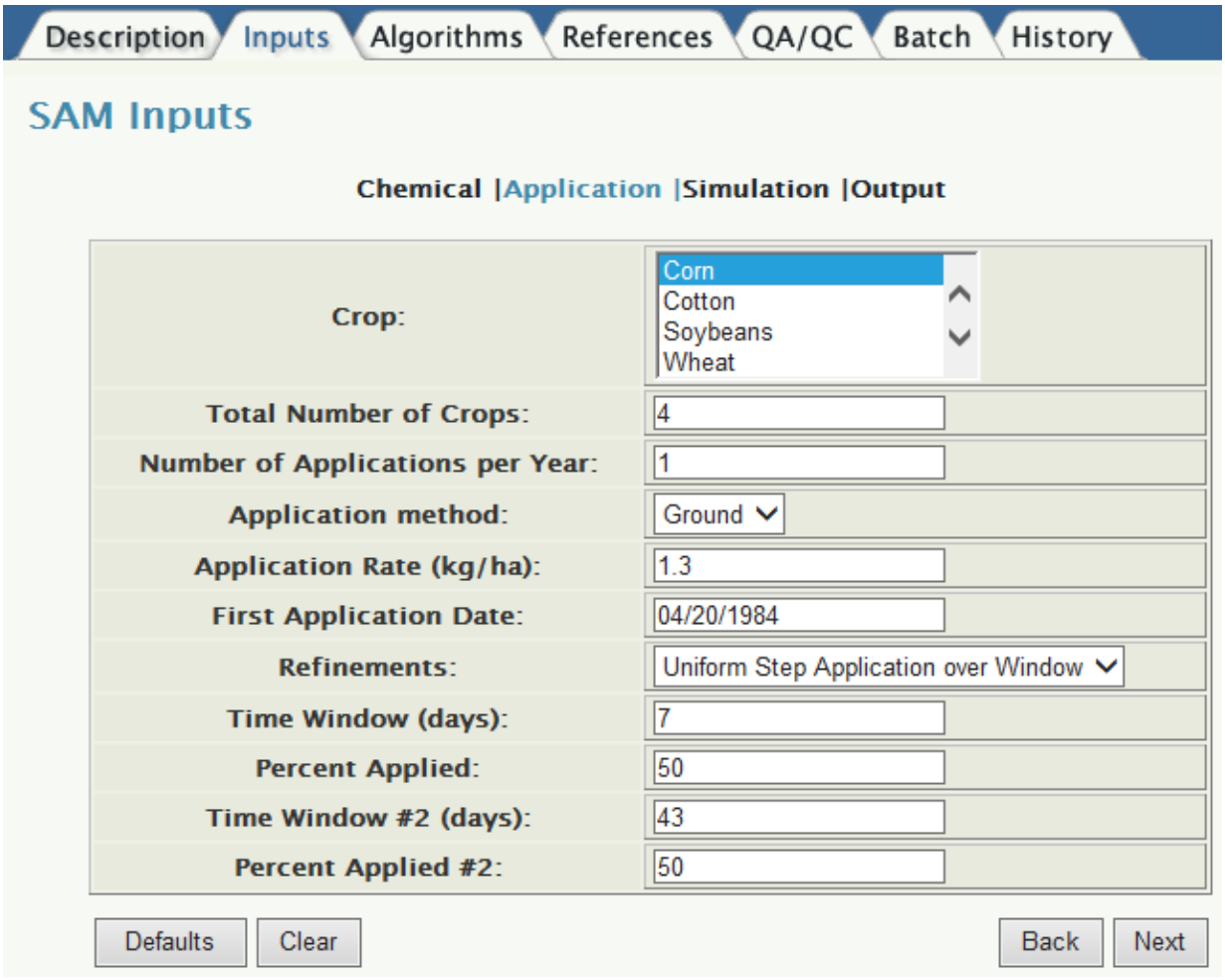
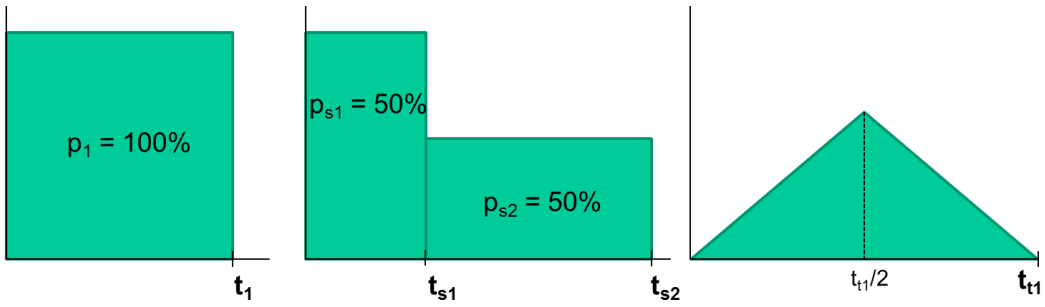


Figure 3. Application tab for entering crop(s) and application details.



Uniform Application Over Window
Time Window, t_1
Percent Applied, p_1

Uniform Step Application Over Window
Time Window #1, t_{s1}
Percent Applied, p_{s1}
Time Window #2, t_{s2}
Percent Applied, p_{s2}

Triangular Application Over Window
Time Window, t_{t1}

Figure 4. Application refinement options in interface.

3. Simulation Tab

State/Region: The state/region of the continental U.S. to be simulated. Ohio Valley is the region available for evaluation in SAM Alpha (Figure 5).

Sim type: One of three simulation types can be selected for each simulation. 'Eco' simulations are used for ecological assessments of water bodies within HUC12 basin units. 'DW Reservoir' simulations are used for assessing non-flowing water bodies (e.g. ponds, lakes, reservoirs) within known drinking water catchments. 'DW Flowing' simulations are used for assessing flowing water bodies (e.g. rivers, streams) within known drinking water catchments. 'Eco' simulations are currently available for evaluation in SAM Alpha.

Start date: The beginning date of the simulation, selected from a dropdown calendar. Based on the pre-processed meteorology in SAM Alpha, the date must be between 1/1/1984 and 12/31/2013, and must be before the End Date.

End date: The last date of the simulation, selected from a dropdown calendar. Based on the pre-processed meteorology in SAM Alpha, the date must be between 1/1/1984 and 12/31/2013, and must be after the Start Date.

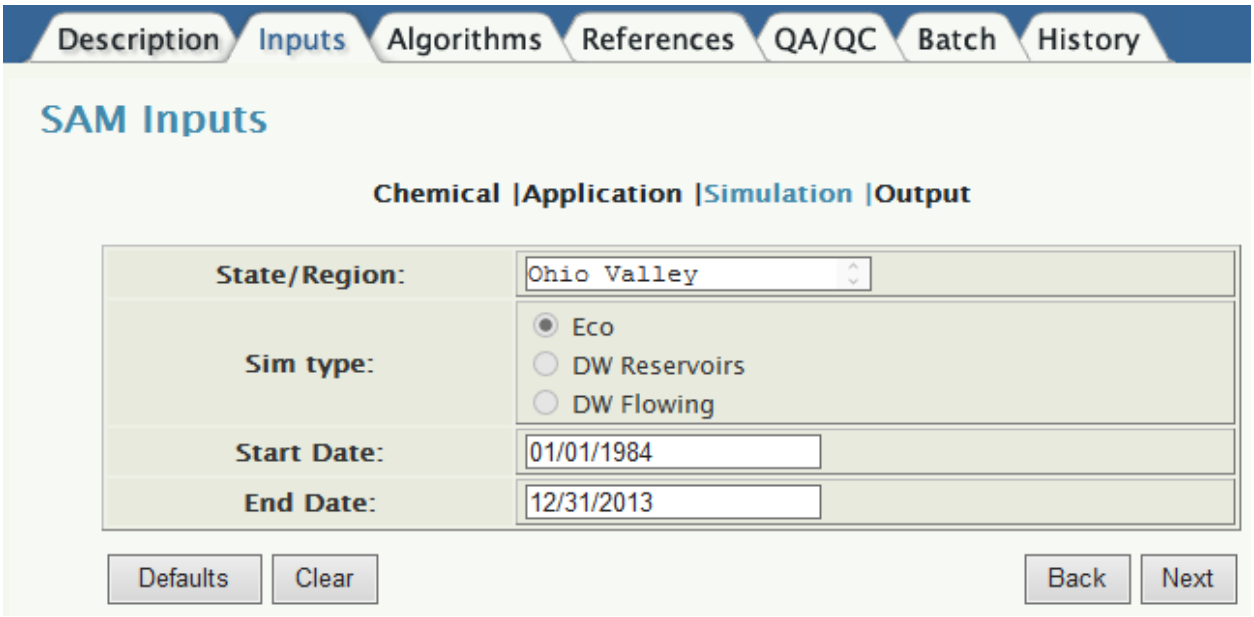


Figure 5. Simulation tab for specifying the region, simulation type, and dates.

4. Output Options Tab

Daily Concentrations: If selected, daily concentrations (µg/L) will be outputted to individual files for each HUC12 or drinking water catchment (Figure 6).

Time-Averaged Results: If selected, time-averaged concentrations or toxicity threshold exceedances will be outputted. Additional options will appear, if the time-averaged results radio button is selected.

> **Averaging Period (days):** The period of days, *n*, used to calculate daily running averages (*n* = 4, 21, 60, 90, or 365 days).

Time-Averaged Concentrations (only select one option below): If selected, one of the following options needs to be chosen:

Daily Time-Average Concentrations: Daily *n*-day average concentrations are outputted to individual files for each HUC12 or drinking water catchment.

Annual Max Time-Average Concentrations: For all simulated years, the annual maximum *n*-day average concentrations are outputted to a summary file (.out) for all HUC12s or drinking water catchments in the simulated state/region.

Toxicity Threshold Exceedances (only select one option below): If selected, the threshold needs to be specified and one of the following options needs to be chosen:

Threshold (µg/L): The *n*-day average concentration above which an exceedance is recorded.

Frequency of exceeding threshold (%), by year: For each of the simulated years, the fraction (0 to 1) of *n*-day average concentration exceedances (of the threshold) are outputted to a summary file (.out) for all HUC12s or drinking water catchments in the simulated state/region.

Frequency of exceeding threshold (%), by month: For each of 12 months, the fraction (0 to 1) of *n*-day average concentration exceedances (of the threshold) are outputted to a summary file (.out) for all HUC12s or drinking water catchments in the simulated state/region.

Average duration of exceedance (days), by year: For each of the simulated years, the average duration of exceedances (of the threshold) are outputted to a summary file (.out) for all HUC12s or drinking water catchments in the simulated state/region.

Average duration of exceedance (days), by month: For each of 12 months, the average duration of exceedances (of the threshold) are outputted to a summary file (.out) for all HUC12s or drinking water catchments in the simulated state/region.

Output Format:

Generate CSVs: Summary tables (comma-separated format) are made available for download.

Generate Map: Summary geospatial maps are displayed and made available for download.

Plots/Histograms: Summary plots/histograms are displayed and made available for download.

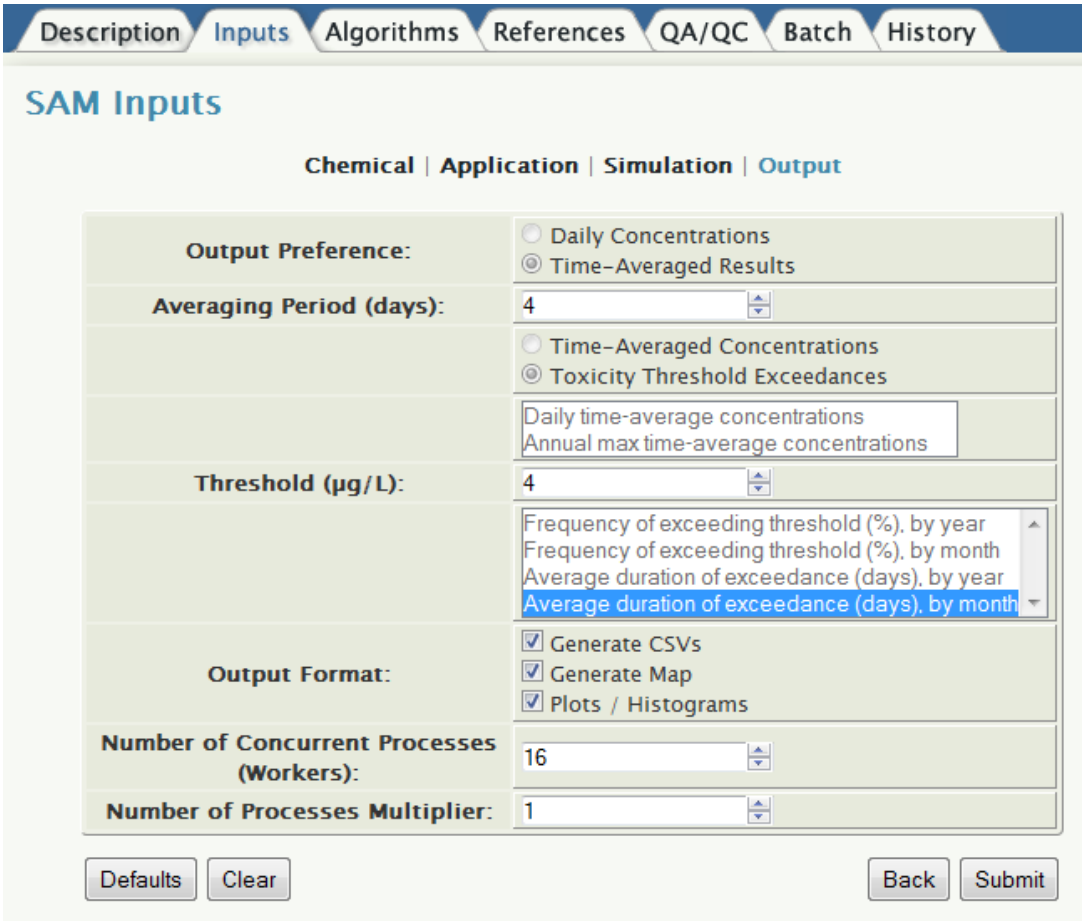


Figure 6. Output tab for selecting the type of output desired (layout in SAM Alpha undergoing updates).

Algorithms

This page will be updated with model theory and key algorithms.

References

This page will be updated with the user manual and supporting documents.

QA/QC

This page is under development. It will be used for selecting standardized simulations for quality control testing.

Batch

This page is under development. It will be used to run several simulations at a time with varying parameters.

History

This page is under development. It currently displays all users' simulation history.

Simulation Example: Inputs and Outputs

1. Inputs

Table 1. Inputs required to run SAM.

Chemical	
Chemical name	Atrazine
K_{oc} (mL/g)	100
Soil metabolism halflife (days)	123
Application	
Crop	Corn
Number of applications per year	1
Application method	Ground
Amount (kg/hA)	1.3
First application date	4/20/1984
Refinements	Uniform Step Application over Window
Time window (days)	7, 43
Percent applied	50%, 50%
Simulation	
Sim type	Eco
State/region	Ohio Valley
Start date	01/01/1984
End date	12/31/2013
Output	
Output preference	Daily concentrations or Time-averaged results
Averaging period (days)	30
Time-averaged concentrations	Daily or Annual maximum
Toxicity threshold exceedances	Frequency by year/month, or Average duration by year/month
Threshold (μg/L)	4
Output format	Table, Map, or Plots/Histograms

2. Outputs

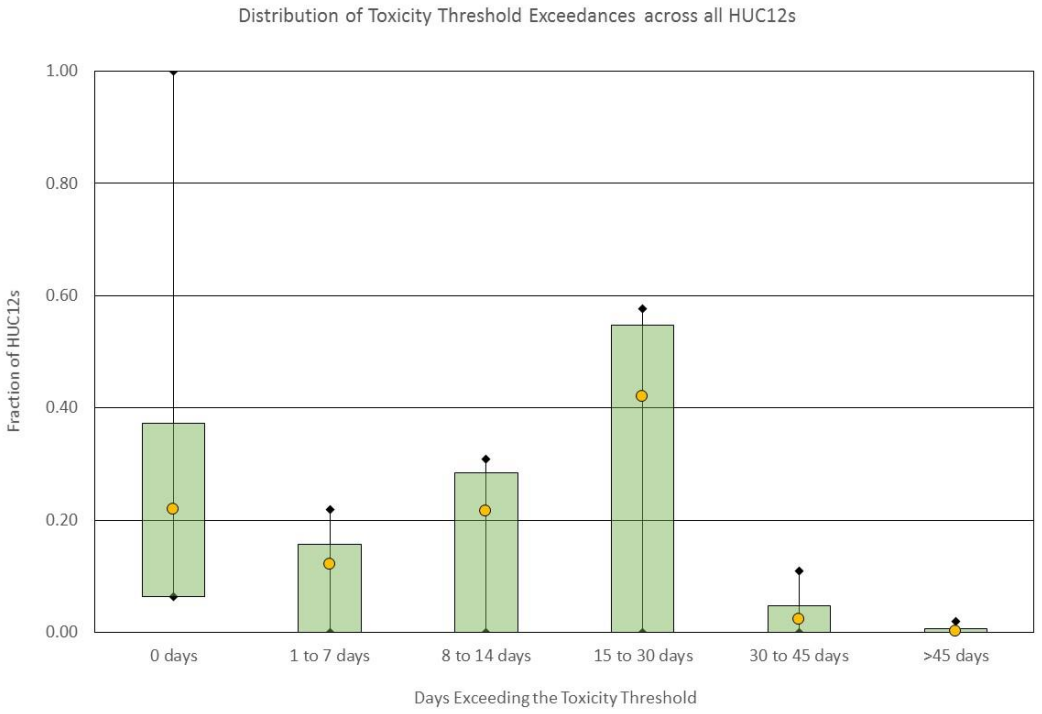
Summary tables can be generated with each model simulation, in comma-separated format. Below is a list of example tables and their contents (Table 2).

Table 2. Output summary tables generated by SAM.

Output summary table	**Contents**
Eco_*000000000000*_daily.out or DW_*0000*_daily.out	*Julian date (since 1900), Daily concentration (μg/L)*: Each basin's daily concentrations
Eco_*000000000000_n*dAvg.out or DW_*0000_ n*dAvg.out	*Julian date (since 1900), n-day average concentration (μg/L)*: Each basin's daily *n*-day average concentrations
Eco_*n*dAvg_AnnMax.out or DW_*n*dAvg_AnnMax.out	*Basin ID, Simulated years (1984-2014*): Each basin's annual maximum *n*-day average concentrations
Eco_ann_toxfreq.out or DW_ann_toxfreq.out	*Basin ID, Simulated years (1984-2014*): Each basin's annual fraction of threshold exceedances for *n*-day average concentrations
Eco_mth_toxfreq.out	*Basin ID, Simulated months (Jan-Dec):*

or DW_mth_toxfreq.out	Each basin's monthly fraction of threshold exceedances for *n*-day average concentrations
Eco_ann_avgdur.out or DW_ann_avgdur.out	*Basin ID, Simulated years (1984-2014):* Each basin's annual average duration of threshold exceedances for *n*-day average concentrations
Eco_mth_avgdur.out or DW_mth_avgdur.out	*Basin ID, Simulated months (Jan-Dec):* Each basin's monthly average duration of threshold exceedances for *n*-day average concentrations

After downloading the .out files, the user can create summary plots offline with Excel or other graphical software (see examples in Figure 7). Geospatial maps can also be generated with each model simulation.



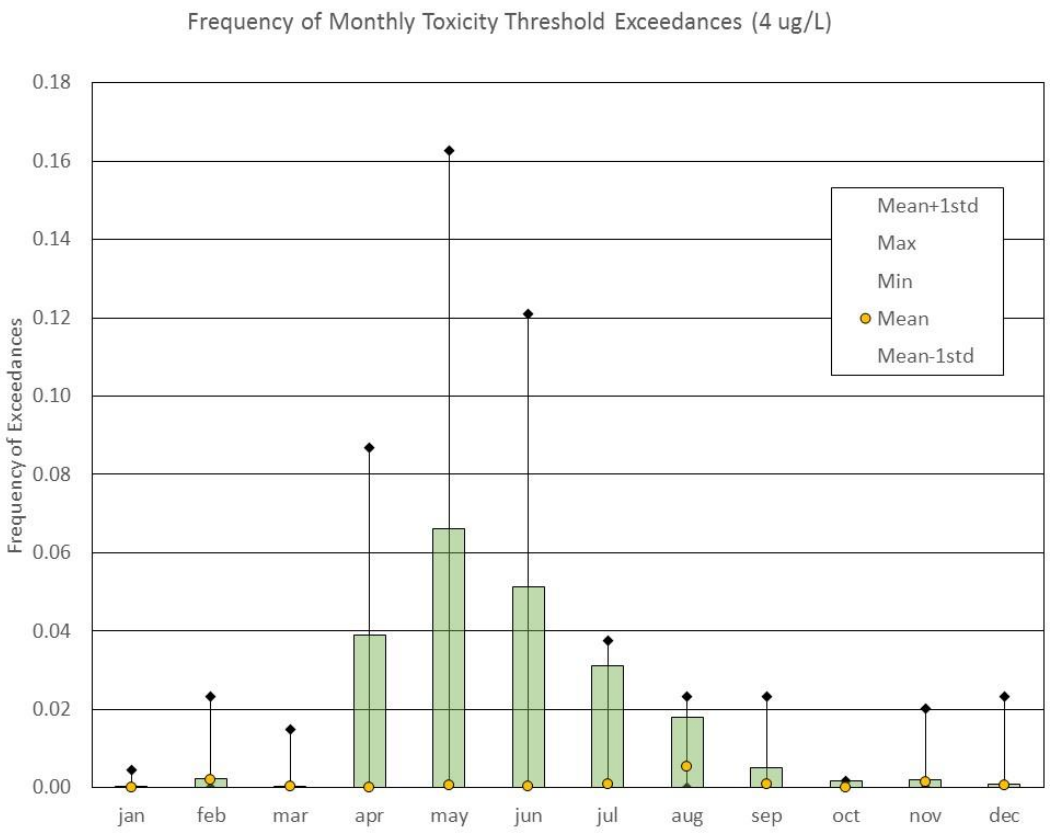


Figure 7. Example box-and-whiskers plots showing the distribution across all HUC12s of the duration of toxicity threshold exceedances (top) and the frequency of monthly threshold exceedances (bottom).

3. Additional Inputs

Chemical			
Chemical name	Metolachlor	Fipronil	Chlorpyrifos
K_{oc} (mL/g)	181	727	6040
Soil metabolism halflife (days)	49	128	109
Application			
Crop	Corn	Corn	A) Corn B) Soybeans
Number of applications per year	1	1	1
Application method	Ground	Ground	Ground
Amount (kg/hA)	1.05	0.1	A) 1.1 B) 1.1
First application date	4/20/1984	4/20/1984	4/20/1984

Refinements	Uniform Step	Uniform Step	Uniform over window
Time window (days)	7, 43	7, 43	A) 30 B) 42
Percent applied	50%, 50%	50%, 50%	--
Simulation			
Sim type	Eco	Eco	Eco
State/region	Ohio Valley	Ohio Valley	Ohio Valley
Start date	1/1/1984	1/1/1984	1/1/1984
End date	12/31/2013	12/31/2013	12/31/2013
Output			
Output preference	Daily concentrations or Time-averaged results	Daily concentrations or Time-averaged results	Daily concentrations or Time-averaged results
Averaging period (days)	30	30	30
Time-averaged concentrations	Daily or Annual maximum	Daily or Annual maximum	Daily or Annual maximum
Toxicity threshold exceedances	Frequency by year/month, or Average duration by year/month	Frequency by year/month, or Average duration by year/month	Frequency by year/month, or Average duration by year/month
Threshold (ug/L)	4	4	4
Output format	Table, Map, or Plots/Histograms	Table, Map, or Plots/Histograms	Table, Map, or Plots/Histograms