

**BACKGROUND DOCUMENT IN SUPPORT OF THE  
MEETING OF THE FIFRA  
SCIENTIFIC ADVISORY PANEL**

**ON THE**

**DEVELOPMENT OF A SPATIAL AQUATIC MODEL (SAM)  
FOR PESTICIDE ASSESSMENTS**

**SEPTEMBER 15-18, 2015**

**US EPA Office of Pesticide Programs  
Environmental Fate and Effects Division**



# **Development of a Spatial Aquatic Model (SAM) For Pesticide Assessments**

## **Background Paper for the September 15-18, 2015, FIFRA SAP**

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## Acronyms and Abbreviations

<b>Abbreviation</b>	<b>Description</b>
AEEMP	Atrazine Ecological Exposure Monitoring Program, conducted by Syngenta Crop Protection in the midwestern US
AMP	Atrazine Monitoring Program, conducted by Syngenta Crop Protection
CDL	Cropland Data Layer, provided by USDA National Agricultural Statistics Service
CN	Curve Number, used in runoff calculations
CPR	Crop Progress Reports, provided by USDA National Agricultural Statistics Service
CREM	USEPA's Council for Regulatory Environmental Modeling
CSTR	Completely Mixed Stirred Tank Reactor, used in SAM to calculate pesticide concentrations in water
EEC	Estimated Environmental Concentration(s)
EFED	USEPA OPP's Environmental Fate and Effects Division
ESRL	NOAA Earth System Research Laboratory
EXAMS	Exposure Analysis Modeling System
FEMVTF	FIFRA Environmental Modeling Validation Task Force
FFDCA	Federal Food, Drug, and Cosmetic Act
FIFRA	Federal Insecticide, Fungicide, and Rodenticide Act
GDD	Growing degree day
GUI	Graphical user interface
HUC/HUC12	Hydrologic Unit Code
IRF	Impulse response function, used to describe the response of a water body to a pulse input
MLRA	Major Land Resource Area
MUKEY	Map Unit Key, a unique identifier of soil map units used in SSURGO
MUSS/MUSLE	Modified Universal Soil Loss Equation
NASS	USDA National Agricultural Statistics Service
NAWQA	USGS National Water Quality Assessment program
NCDC	NOAA National Climatic Data Center
NCEP/NCAR	National Centers for Environmental Prediction and Atmospheric Research
NHDPlus	National Hydrography Dataset Plus, the geospatial hydrologic dataset developed by USEPA and USGS. Version 2 is used in the model.
NOAA	National Oceanic and Atmospheric Administration
NRCS	USDA Natural Resources Conservation Service
NWIS	National Water Information System, maintained by USGS
OPP	USEPA Office of Pesticide Programs
ORD	USEPA Office of Research and Development
PHZ	Plant Hardiness Zone (USDA map)
PRZM / PRZM5	Pesticide Root Zone Model / version 5 (the current version)
SAM	Spatial Aquatic Model

<b>Abbreviation</b>	<b>Description</b>
SAMSON	Solar and Meteorological Surface Observation Network
SSURGO	Soil Survey Geographic database, the geospatial soil dataset developed by the USDA Natural Resources Conservation Service
SWCC	Surface Water Concentration Calculator
USDA	United States Department of Agriculture
USEPA	United States Environmental Protection Agency
USGS	United States Geological Survey
USLE	Universal Soil Loss Equation
VVWM	Variable Volume Water Model
WARP	Watershed Regression on Pesticides, USGS model

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## **Executive Summary**

As a part of the requirements for pesticide registration and registration review, the US Environmental Protection Agency Office of Pesticide Programs (USEPA OPP) conducts aquatic exposure assessments to determine whether pesticides that are applied according to label directions can result in water concentrations that may adversely impact human health or aquatic organisms. To do this for the hundreds of registration and registration review actions each year, USEPA OPP uses a model that estimates pesticide concentrations in water that accounts for a combination of soil, weather, hydrology, and management/use conditions that are expected to maximize the potential for pesticides to move into water. If these resulting high-end exposures are less than the various toxicity endpoints of concern (for fish, invertebrates, plants, or humans consuming drinking water), then USEPA OPP can conclude that the pesticide is unlikely to pose adverse risks to humans or aquatic organisms based on its labeled uses.

However, if the estimated pesticide concentrations from these high-exposure conditions exceed one or more of the toxicity endpoints, then USEPA OPP may need to determine how likely these estimated concentrations are to occur, how often they may exceed toxicity thresholds, where areas of greatest concern occur, and how confident we are in the exposure assessment. To do this, USEPA OPP has used a number of approaches, including modeling a wider range of conditions, including more typical use patterns, trying to identify the most vulnerable areas, and evaluating pesticide monitoring data. These approaches, however, require a lot of time and resources and do not capture the full range of potential conditions affecting how much pesticide moves from the field to water bodies that occur throughout the country. While USEPA OPP uses monitoring data to get snapshots of actual pesticide concentrations in water, most monitoring studies do not sample water frequently enough to capture every peak that occurs in water (e.g., samples taken every two weeks are unlikely to capture the maximum daily concentration that may occur during that time); nor do the studies cover the full extent of the pesticide use area or the range in vulnerability.

Because of an increasing need for more spatial specificity in our aquatic exposure assessments both for human health (from drinking water) and aquatic organisms for ecological assessments, USEPA OPP needs a tool that adds both a spatial context for the diversity of conditions affecting pesticide movement to water, and a time aspect for when and how frequently pesticide concentrations may exceed toxicity endpoints of concern. Given the number of risk assessments completed each year (on the order of hundreds), the tool needs to provide results in an efficient, consistent, and understandable way.

To address this need, USEPA OPP has developed an alpha version of a Spatial Aquatic Model (SAM), focusing first on the Ohio River basin. The intent of this alpha model was to evaluate the feasibility of pulling together spatial data that captures the diversity of soil, land cover, weather, hydrology, and crop conditions/management practices as they occur across the

country to generate daily estimates of pesticide concentrations over a number of years for a wide variety of streams, rivers, lakes, and reservoirs. This involved making some changes in the conceptual approach USEPA OPP uses to estimate aquatic exposures, as described in Section 1. USEPA OPP is asking this Scientific Advisory Panel (SAP) to comment on the clarity of this conceptual watershed modeling approach and its strengths and limitations for estimating pesticide concentrations over time across the country.

One of the challenges in developing SAM was to make sure the model could process the large datasets needed for a national scale assessment, simulate the key fate, transport, and hydrologic processes that drive pesticide movement to water, and generate outputs in a concise and timely manner (on the order of minutes to hours rather than days to weeks). USEPA OPP has taken several steps to make this possible. First, the model processes were streamlined to reduce redundant calculations and focus on the main processes that drive pesticide fate and transport (these have been identified through a long history of pesticide modeling and analyses to determine the inputs that most influence pesticide movement to water). Second, those processes that are not impacted by pesticide applications – daily runoff and erosion – have been processed ahead of time. Finally, SAM will run as a web application to take advantage of cloud-based data storage and parallel processing across multiple computers.

The current “alpha” version of SAM (Section 2) focuses on the pesticide runoff routines in a dominantly corn-soybean-small grains agricultural setting. USEPA OPP has included initial comparisons with a set of monitoring data on atrazine to help identify areas for further model development and improvement. The atrazine studies provide some of the most intensive sampling (with daily to weekly frequency targeted to high use areas) available for pesticides. USEPA OPP is also looking for similarly intensive monitoring for other pesticides for further model testing. For this SAP consultation, we are asking for panel feedback on the model design, the streamlined pesticide transport calculations, and methods for calculating pesticide concentrations in water.

This alpha version does not yet take into account pesticide loadings from sediment transport or spray drift; nor does it account for pesticide fate in the water body (degradation, sorption to sediment). USEPA OPP plans to add these processes to future versions of the model. In the meantime, we are asking the panel for recommendations on how best to account for sediment transport and pesticide fate in water bodies.

In Section 3, USEPA OPP describes what we believe are the best available national data sets for soil, land cover, weather, crop characteristics and management practices, and hydrology. We also describe how these diverse data sets are organized as soil-land cover-weather combinations (scenarios) for inputs to the model and to reflect the spatial diversity in conditions. USEPA OPP is asking the SAP to comment on the approach used to aggregate spatial inputs across varying scales.

With an eye toward optimizing data storage and processing requirements for large national datasets, USEPA OPP evaluated an approach to reduce the total number of soil-land cover-weather combinations (scenarios) by grouping individual soil map units based on similarities in properties that influence chemical transport to water (runoff potential, erosion potential, surface organic matter content, and slope). Section 3 includes a comparison of results from the grouping approach in support of a charge question on the implications of aggregating model input parameters using soil water quality classes.

The alpha version of SAM calculates daily pesticide concentrations in water based on daily runoff and pesticide mass loads aggregated across the entire watershed area. While this may be a viable option for small watersheds, it does not account for differences in the time it takes pesticide loads from the upper end of a larger watershed to reach the outlet, compared to pesticide loads from fields near the outlet. The larger the watershed, the more spread out the pesticide loads in water are likely to be. This is likely to result in lower peak concentrations of pesticide at the outlet, but a longer duration of exposure. Section 4 describes an approach USEPA OPP is testing to account for differences in time of travel. Results have improved estimated concentrations in comparison to monitoring data across a range of watershed sizes and water body types. In the charge questions, USEPA OPP is asking the SAP to comment on the proposed approach, its adaptability across a range of watershed sizes, and the potential to adept this to reactive and/or sorbing chemicals.

In initial model comparisons to monitoring data, USEPA OPP noticed that, in some years, the time of occurrence of pesticides in water estimated using SAM did not always correspond well with the timing of the pesticides in monitoring data for the same sites. The timing of pesticide applications is a key driver in determining the timing and amount of pesticides that reach water. However, detailed spatial information on the timing and amount of pesticide applied across the country is not readily available. USEPA OPP is exploring some approaches to estimate the potential pesticide application window based on crop planting and crop growth information in Section 5. Preliminary tests using atrazine on corn showed that accounting for year-to-year variations in planting and emergence dates (using crop progress reports) resulted in better correspondence between estimated concentrations and monitoring data for both the timing and magnitude of concentrations in water. While this approach may not be applicable to all types of pesticides or crops, USEPA OPP is asking the SAP for feedback on these options for linking the timing and duration of pesticide applications to USDA crop progress reports and/or crop growth models, or for recommendations on other methods for defining pesticide application windows in the absence of usage information.

USEPA OPP appreciates the opportunity to consult with this SAP on these issues as it moves forward in developing the Spatial Aquatic Model for pesticides.

## A Note on Model Versions

USEPA OPP developed an alpha version of the Spatial Aquatic Model (SAM), using the Ohio River Basin, to develop and refine the conceptual model, evaluate key model components and data compilation methods, and test the feasibility of running the model on a national scale. This version of SAM focuses on hydrology and pesticide runoff routines in a dominantly corn-soybean-small grains setting. It does not yet take into account pesticide loadings from sediment transport or spray drift; nor does it account for pesticide fate in the water body (degradation, sorption to sediment). These will be included in future iterations of the model.

Because of the deployment cycle for SAM to the public, we are presenting results from two versions of SAM exist. The first alpha version (SAM alpha 1.0), which is available on the übertool site (<http://qed.epa.gov/ubertool/sam>), calculates concentrations for each HUC-12 unit based on volumes and flow rates for the immediate (local) HUC-12. Such estimates do not account for contributions from upstream HUC-12 units and the results could be misleading. Adjustments will be made to this model based on feedback from the SAP.

Since this initial development, USEPA OPP replaced the HUC-12 units with National Hydrography Dataset (NHDPlus) catchments for individual reaches (SAM alpha 2.0). The NHDPlus reaches, which are at a more detailed scale than HUC-12 units, provide a more efficient framework for modeling mass movement downstream and accounting for upstream contributions. Although results from SAM alpha 2.0 are presented to the SAP, this version is not publicly available.

Based on model evaluations discussed in Section 2.4, USEPA OPP has proposed updates and refinements to the test version of SAM for SAP consideration: re-distributing daily pesticide loads from individual catchments based on their travel time to receiving water bodies in larger drainage networks (Section 4) and defining application windows (Section 5).

Additional improvements to the model are under consideration to address several limitations of the test version. This section describes additions that USEPA OPP is evaluating for future versions of SAM. As part of the peer review process, USEPA OPP welcomes recommendations and feedback on these and other model improvements. Recommendations will be considered based on their scientific merit, ease of incorporation into the model, and the availability of intensive monitoring data for validation.

After this SAP consultation and consideration of panel recommendations, USEPA OPP will incorporate these components into a new test version of SAM on the übertool site.

## **Introduction**

The US Environmental Protection Agency (USEPA) Office of Pesticide Programs (OPP) has developed a Spatial Aquatic Model (SAM) for pesticides to address the goals and objectives of aquatic exposure assessments that are a part of the pesticide registration and registration review process. In developing SAM, USEPA OPP focused on improving the existing aquatic modeling approach in order to provide a higher-tiered assessment to use in regulatory decision making under the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) and the Federal Food, Drug, and Cosmetic Act (FFDCA). This background document describes the conceptual model for SAM (Section 1), the core model components (Section 2) and data used in the model (Section 3), a method for taking into account time of travel for pesticide loadings in water as the watershed size and travel time increase (Section 4), and a proposed approach to define pesticide application windows on a watershed scale based on crop growth (Section 5). Specific charge questions for this FIFRA Scientific Advisory Panel (SAP) focus on the information provided in each section.

The model described here is an alpha version that focuses on key components for which USEPA OPP is soliciting comment from the SAP:

- the watershed-based conceptual model;
- a streamlined framework that captures main drivers for pesticide fate and transport to water;
- runoff, mass transport, and water concentration estimations, particularly for flowing water bodies;
- best available methods for aggregating spatial data of varying scales for model inputs;
- methods to account for time of travel differences for pesticide loadings in water across larger watersheds; and
- an approach for varying pesticide application windows in response to crop growth and year-to-year variations in weather;

The primary goal of this consultation is to get feedback on the scientific strengths and limitations of the model for predicting pesticide concentrations in surface water on a watershed basis across the U.S., and to seek recommendations on improving the model.

## **Objectives of OPP's Pesticide Aquatic Exposure Assessments**

As a part of its requirements for pesticide registration and registration review, USEPA OPP conducts aquatic exposure assessments to determine whether pesticides that are applied according to label directions can result in concentrations in water that may adversely impact human health or aquatic organisms. If estimated aquatic exposures indicate a potential for adverse effects, the assessment may need to characterize the likelihood of occurrence, including the range in magnitude of exposure, the frequency of exceeding toxicity thresholds,

the likely locations of exposures that exceed the thresholds, and the degree of certainty in the risk assessment.

Currently USEPA OPP estimates aquatic exposures using the Pesticide Root Zone Model (PRZM version 5) and Variable Volume Water Model (VVWM<sup>1</sup>), which is based on the Exposure Analysis Modeling System (EXAMS). These models are linked with a user interface in the Surface Water Concentration Calculator (SWCC)<sup>2</sup>. As a part of its tiered screening approach, USEPA OPP uses standard crop-specific scenarios to represent combinations of soil, crop, weather, and hydrological factors that are expected to contribute to high-end pesticide concentrations in water. The PRZM portion of the SWCC simulates pesticide sorption to soil, in-field decay, and runoff from an agricultural field/drainage area following pesticide application(s). The VVWM simulates resulting concentrations in an adjacent surface water body (a “standard” pond for aquatic organisms or an “index reservoir” for drinking water) receiving the pesticide loading.

For ecological assessments for aquatic species, USEPA OPP compares the 1-in-10 year return frequency concentration for either single-day (peak concentrations for estimating acute exposures) or time-averaged concentrations of different durations (for estimating chronic exposures) to relevant toxicity endpoints of concern. Drinking water assessments for human health risk assessments make use of the full distribution of simulated daily concentrations for acute toxicity concerns. This approach is intended to screen out pesticides (and/or specific uses) that are not likely to be of potential concern, but does not provide estimates of how pesticide concentrations vary across different watersheds in the pesticide use areas<sup>3</sup>.

For pesticides that do not clear these screens, refinements to incorporate spatial and temporal details, when needed, require considerable time and resources, and have not yet been automated to consistently capture the extent of potential variability in exposures. Examples of pesticide risk assessments that have incorporated spatial refinements include drinking water assessments for organophosphate and N-methyl carbamate cumulative risk assessments, which focused on regional high-exposure areas<sup>4</sup>, and the proposed reassessment of ecological risks

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<sup>1</sup> The documentation for the 2004 FIFRA Scientific Advisory Panel on Refined (Level II) Terrestrial and Aquatic Models for Probabilistic and Ecological Assessment of Pesticides provides more information on the VVWM and the use of these models for aquatic exposures, at [http://www.epa.gov/scipoly/sap/meetings/2004/033004\\_mtg.htm](http://www.epa.gov/scipoly/sap/meetings/2004/033004_mtg.htm)

<sup>2</sup> Models and documentation are available through the USEPA OPP Water Models web site at <http://www.epa.gov/oppefed1/models/water/>. The models and approaches have been subject of a number of FIFRA Scientific Advisory Panel consultations. A link to relevant SAP sessions related to aquatic modeling can be found at [http://www.epa.gov/oppefed1/models/water/sap\\_sessions.htm](http://www.epa.gov/oppefed1/models/water/sap_sessions.htm).

<sup>3</sup> A more detailed description of USEPA OPP’s ecological risk assessment process can be found in the 2004 Overview of OPP’s ecological risk assessment process, available at <http://www.epa.gov/oppfead1/endanger/consultation/ecorisk-overview.pdf>.

<sup>4</sup> Information on assessing pesticide cumulative risk, including links to the Organophosphates and N-Methyl Carbamates assessments, can be found at [http://www.epa.gov/pesticides/cumulative/common\\_mech\\_groups.htm](http://www.epa.gov/pesticides/cumulative/common_mech_groups.htm).

for atrazine that will use a combination of spatially-linked modeling and monitoring data<sup>5</sup>. For example, assessments under the Endangered Species Act often would benefit from estimates of the spatial and temporal distributions of pesticide concentrations, and where these distributions may overlap with the ranges of listed species (NRC, 2013).

USEPA OPP needs a tool to meet the increased demand for spatially-resolved human health (drinking water) and ecological aquatic exposure assessments. Such a tool should add both spatial and temporal contexts to aquatic exposures in an efficient, consistent way, ideally while minimizing the demand for extra work on the part of risk assessors.

## **Objectives of SAM**

The goal of SAM is to improve on OPP's existing aquatic exposure assessments by providing more systematic spatial- and temporal-contexts for aquatic exposure assessments for both human health (drinking water) and aquatic organisms. Such contexts are needed to address common risk management questions regarding the likelihood of exposures that may exceed toxicity thresholds of concern and, should such exposures occur, how often, how long, and where adverse impacts from pesticides in water overlap with populations (human and ecological) at potential risk.

A spatial model is possible because key factors that drive pesticide concentrations in water occur in predictable patterns in time and space. These factors include pesticide use intensity, rainfall timing and intensity, soil factors related to runoff and/or erosion vulnerability, land cover type, and landscape/ hydrologic factors related to runoff. Evidence supporting this concept include data collected through the US Geological Survey's (USGS) National Water Quality Assessment (NAWQA) program (Gilliom et al, 2006; see the Pesticide National Synthesis Project website at <http://water.usgs.gov/nawqa/pnsp/> for further studies), the development of the Watershed Regression on Pesticides (WARP) model (Stone and Gilliom, 2009, 2012; Stone *et al*, 2013), and analyses presented at several FIFRA SAPs on atrazine monitoring studies (USEPA OPP, 2007, 2009a, 2010a, 2010b, 2011, 2012). While neither SAM nor other pesticide models include every possible variable that may impact pesticide concentrations in water, SAM simulates the major known drivers (described in Sections 2 and 3) to illuminate exposure patterns in time and space, so that risk assessors can understand and account for them and better inform risk managers.

Though a number of runoff, erosion, and pesticide fate and transport algorithms used in SAM are similar to those used in USEPA OPP's traditional field-based water models mentioned above, SAM brings a new spatial approach to modeling the fate and transport of pesticides and expansion to watershed-scale processes and outputs. Section 1 highlights differences in the

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<sup>5</sup> See the June 2012 FIFRA SAP on Problem Formulation for the Reassessment of Ecological Risks from the Use of Atrazine, available at <http://www.epa.gov/scipoly/sap/meetings/2012/061212meeting.html>.

conceptual approaches moving from field- to watershed-scale models. As with USEPA OPP's current aquatic modeling approach, SAM will generate daily concentrations and distributions for a variety of human health and ecological toxicity endpoints. However, instead of providing estimates for a single pond or index reservoir representative of expected high-exposure conditions, SAM will provide distributions for a variety of water body types across the country. Ideally, the model should be capable of providing relatively quick turnarounds on national-scale assessments and require little or no calibration.

Once fully developed and evaluated, USEPA OPP intends to use SAM in regulatory assessments, primarily for pesticides that do not pass lower-tiered screening assessments. SAM will improve upon OPP's current capacity by adding more spatial and temporal contexts to aquatic exposure assessments. No model can accurately predict patterns in contaminant concentrations at all spatial and temporal scales; SAM is intended to provide concentration estimates that realistically reflect ranges in magnitude that can occur while nonetheless minimizing Type II or "false negative" errors (i.e., systematically underestimating actual exposures).

## Preliminary Model Development

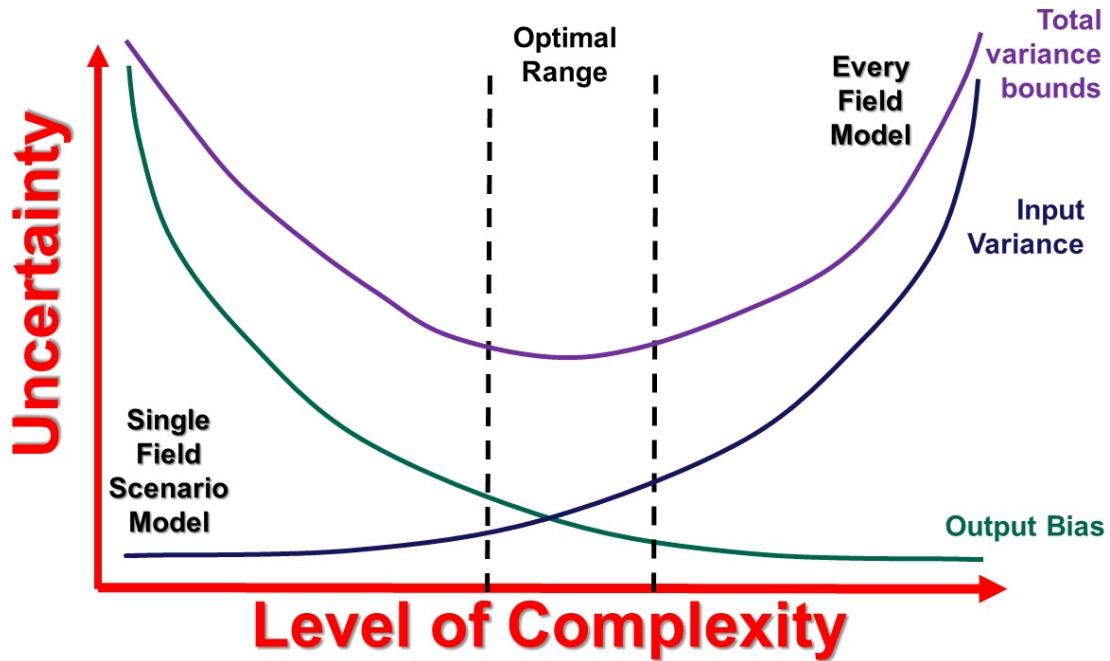
In developing SAM, USEPA OPP started with key, well-known hydrology/runoff and pesticide fate/transport algorithms that represent the movement of pesticides from landscapes to receiving waters (Section 2). Section 3 describes the key inputs used by these algorithms in the model. One goal for increasing the level of complexity in a model is to reduce uncertainty and increase accuracy in model outputs, thereby moving estimates closer to actual or known values (to the extent that such values can be reliably measured).

Adding complexity to a model entails bringing in additional routines and/or inputs, which can increase the variability of model outputs. Where inputs aren't readily available or have a high degree of inherent uncertainty and/or variability, the resulting increased uncertainty in model output may negate any potential increase in accuracy. Of course, not all potential model inputs exert equal influence over pesticide fate and transport.

In model development, we ideally consider the uncertainty implications of all input sources (Figure 1). The single-field/drainage area approach used in USEPA OPP's current screening assessments is low in complexity, but high in uncertainty with respect to capturing the full range of potential pesticide exposures. Nonetheless the approach is useful because if resulting high-exposure estimates do not exceed toxicity thresholds of concern, then no further modeling is necessary.

At the other end of the complexity spectrum would be to model pesticide applications to every field and simulate pesticide movement by every transport pathway into and through every drainage way from headwater reaches to the mouth of large rivers. Not only would such an approach be data- and computationally-intensive, but the uncertainty in required modeling

inputs and the adequacy of algorithms to represent processes across a range of scales would likely generate large uncertainty about model outputs.

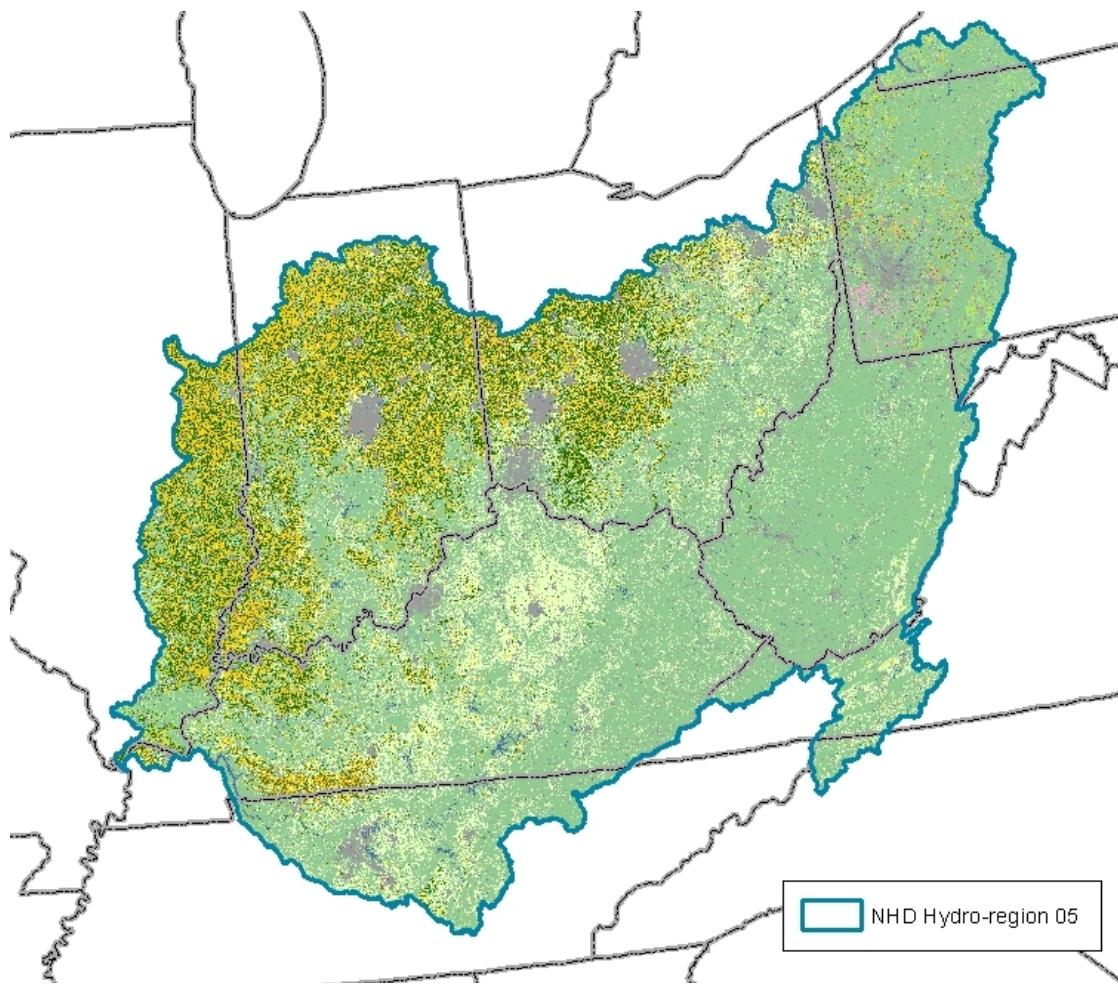


*Figure 1: Conceptual Plot of Level of Model Complexity and Uncertainty in Model Outputs*

Rather than simulating flow routing by field into drainage ways and streams, SAM accumulates pesticide mass and flows at pour points along the stream network (see Sections 2 and 3 for more detail). SAM accounts for spatial heterogeneity in soil, land cover, and hydrologic conditions within each contributing drainage area. In addition, SAM accounts for geographic differences in weather (e.g., precipitation), crop growth and timing, watershed area, and type and flow characteristics of receiving waters.

USEPA OPP is following USEPA's Council for Regulatory Environmental Modeling's (CREM) guidance on model development and evaluation (USEPA, 2009) which was generated in response to an earlier report by the National Research Council on the use of environmental models in regulatory decision-making (NRC, 2007). Key components of the model development guidance are (1) scientific soundness of model routines, (2) characterization of model sensitivity and uncertainty analysis, and (3) comparison of model outputs against measured data, taking into account uncertainty in measured data. These are described in Section 2. In the case of SAM, the measured data consist of pesticide monitoring at sufficient sampling frequency to minimize inherent underestimation biases that often result from less-frequent sampling.

USEPA OPP developed an alpha version of SAM (SAM alpha1.0), using the Ohio River Basin (Figure 2), to evaluate and refine the conceptual model for incorporating more spatial detail in surface water modeling (Section 1), develop and evaluate the adequacy of key modeling components for runoff and pesticide transport at watershed scales (Section 2), automate methods for compiling model inputs from spatial data (Section 3), and determine the data storage and computational requirements for supporting the model on a national scale.



**Figure 2: NHD Hydroregion 5, the Ohio River Basin, with land cover from the Cropland Data Layer. The predominantly corn-soybean agriculture (yellow and dark green colors) occurs in the northern and western portions of the basin; pasture (pale yellowish-green) and forestry (pale green) dominate the rest of the basin. Major urban areas are in gray.**

This alpha version has been the subject of workshops/webinars (October, 2014, and April, 2015) with stakeholders and interested parties to provide an overview of the model, offer a chance to test an early version of SAM, and solicit feedback on key components in the model. Because data storage and computer processing requirements exceed the capacities of most

personal computers, OPP worked with USEPA's Office of Research and Development (ORD) to set up a web application for SAM through USEPA's test version of the übertool web site (web applications for ecological risk assessment)<sup>6</sup>. Data storage and processing are done in a cloud environment and outputs can be displayed or downloaded for further analysis.

This SAP is a continuation of the model development and evaluation process for SAM, building on feedback from the earlier public workshops. The SAP-test version of SAM described in Section 2 is similar to the alpha version except where noted below. The SAP-test version of SAM focuses on hydrology and pesticide runoff routines in a dominantly corn-soybean-small grains setting. It does not yet take into account pesticide loadings from sediment transport or spray drift; nor does it account for pesticide fate in the water body (degradation, sorption to sediment). USEPA OPP plans to add these processes to the model in future iterations. For this SAP consultation, USEPA OPP is asking for panel feedback on the model design, the streamlined pesticide transport calculations, and methods for calculating pesticide concentrations in water.

The alpha version of SAM on the übertool site generates outputs at the HUC-12 (USGS Hydrologic Unit Code<sup>7</sup>) level. This version only accounts for daily runoff and pesticide loadings locally generated from soil-land cover-weather station scenarios within each HUC-12. This version did not account for contributions from upstream HUC-12s. The SAP-test version of SAM replaces the HUC-12 units with National Hydrography Dataset (NHDPlus) catchments for individual reaches. The NHDPlus reaches not only are at a more detailed scale than HUC-12 units, but also provide a more efficient framework for modeling mass movement downstream and accounting for upstream contributions.

The alpha version also does not include two potential model improvements described in this document:

- (1) Incorporating upstream (i.e., full watershed) loadings, accounting for dispersion and other dilution effects generated by surface water transport and residence time differences, described in Section 4; and
- (2) Using empirical data (such as US Department of Agriculture [USDA] Crop Progress Reports) and/or crop growth models to better define the timing and duration of likely pesticide application windows tied to crop stages. This approach is presented in Section 5 of this paper.

USEPA OPP is seeking feedback on these approaches from the SAP before incorporating the algorithms and supporting data into the model.

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<sup>6</sup> The alpha version of SAM is available through the übertool site at <http://qed.epa.gov/ubertool/SAM>. Model testers, including SAP panel members, can access by contacting the SAM development team. As noted above, this version generates outputs by HUC-12 unit and does not account for contributions from upstream HUC-12s. It also does not include to proposed improvements to the model described in Sections 4 and 5.

<sup>7</sup> Hydrologic Units are a hierarchical naming convention developed by USGS to subdivide watersheds into 2-, 4-, 6-, 8-, 10-, and 12-digit codes (HUCs) for spatial coverages. More information is available through the USGS Hydrologic Unit Maps site at <https://water.usgs.gov/GIS/huc.html>.

SAM currently simulates pesticide loadings from runoff for a corn-soybean-small grain agricultural area of the country (Section 2). Model components for pesticide loadings into water through sediment transport or by spray drift are not yet functional. SAM includes pesticide transport downstream for streams, rivers, reservoirs, lakes, and other impounded water bodies, but does not yet account for in-stream degradation or sorption to sediments. SAP feedback on approaches to incorporate these additional processes into the model also will be useful as USEPA OPP expands model development and testing to other agricultural settings across the country.

## 1. Conceptual model for SAM

This section describes the conceptual watershed modeling approach for SAM, contrasting it with OPP's current conceptual model (single soil watershed, fixed geometry, fixed water body), in support of the following charge question to the SAP:

**Q1.** The conceptual watershed model for SAM accounts for spatial and temporal variability in soil, land cover, weather, and crop/management inputs and integrates outputs at watershed pour points by area-weighting.

- a. *Please discuss the strengths and limitations of the conceptual watershed model for representing spatial and temporal variability in pesticide concentrations in water.*
- b. *Please comment on how clearly this conceptual approach is explained. What additional documentation, description, and/or characterization is necessary to ensure clarity and transparency?*

Section 1.1 describes the current conceptual model USEPA OPP uses for surface water exposure assessments; Section 1.2 describes the watershed conceptual model used in SAM and contrasts it with the current approach.

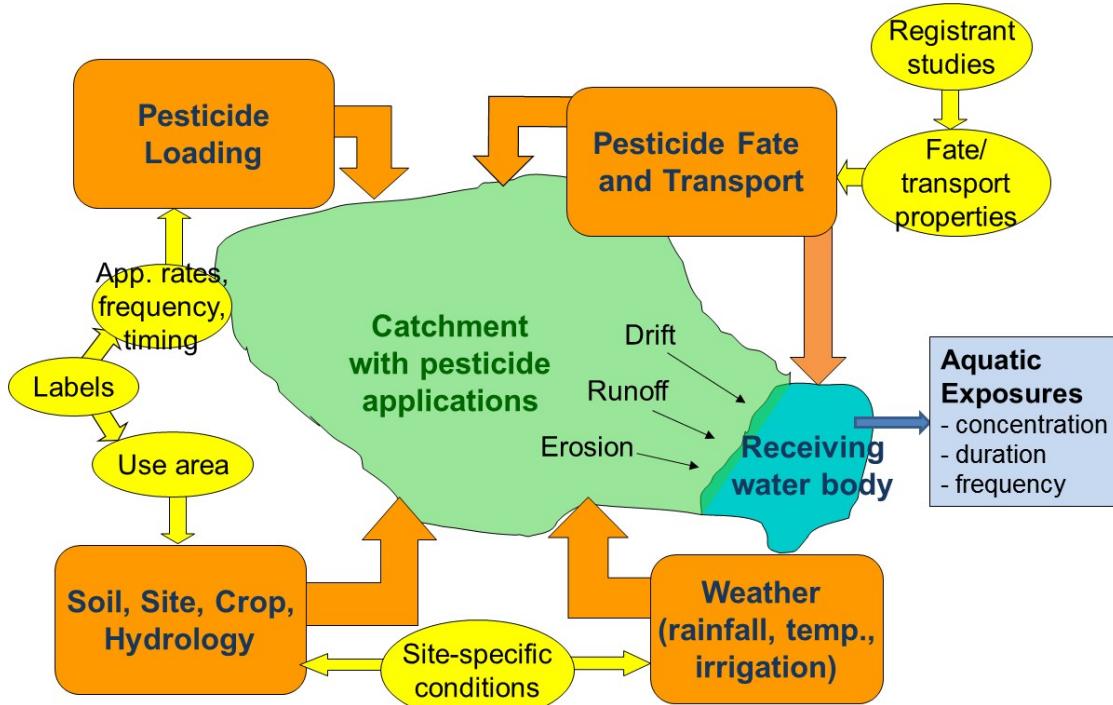
### 1.1 Conceptual Model for Current Surface Water Assessments

In its current surface water exposure assessments, USEPA OPP uses models to estimate pesticide concentrations in water bodies resulting from labeled use of pesticides outdoors. These models provide aquatic estimated environmental concentrations (EECs) that can occur at labeled application rates, using inputs derived from laboratory data that characterize how fast a pesticide breaks down and how and where it moves in the environment. In these models, the amount of pesticide that moves from the field to a nearby water body depends not only on the pesticide application rate and pesticide properties, but also on the site conditions, management practices, and weather (Figure 3).

The Pesticide Root Zone Model (PRZM) simulates pesticide fate and transport processes in the field, tracking the pesticide in the plant canopy, soil, and root zone. This field-scale model estimates daily edge-of-field runoff, sediment, and pesticide loads delivered to a receiving water body. Pesticide fate in the receiving water body is simulated with the Variable Volume Water Model (VVWM), which is based on the Exposure Analysis Modeling System (EXAMS).

PRZM simulates surface runoff using the USDA curve number technique and erosion using the modified Universal Soil Loss Equation (MUSLE). Water movement into and downward through the soil is simulated in a tipping-bucket manner using soil parameters for water retention and saturated water content. The chemical transport component simulates pesticide application on or into the soil or on plant foliage. Dissolved, sorbed, and vapor-phase concentrations of the pesticide in soil are estimated by simultaneously considering the processes of degradation,

sorption, uptake by plants, surface runoff, soil erosion, leaching, volatilization, foliar degradation and washoff.



**Figure 3: Conceptual Model for Current USEPA OPP Pesticide Surface Water Exposure Assessments.**

Modeled field scenarios in PRZM consist of crop management practices, site-specific soil, hydrology, and weather conditions, and pesticide-specific application and dissipation processes. For screening purposes, USEPA OPP uses a combination of site, crop, and pesticide practices that are expected to result in a high-end exposure in the aquatic environment. These conditions are assumed to be uniform across the modeled catchment area: a 10 ha (25 ac) field for ecological exposure and a 173 ha (427 ac) watershed for drinking water<sup>8</sup>. The ecological scenario assumes that the treated crop covers the entire field (drainage area). Because of the larger catchment area in the drinking water scenario, a crop area adjustment is applied to account for the percentage of the watershed that is planted with a specific crop or set of crops<sup>9</sup>.

<sup>8</sup> The watershed area and index reservoir for drinking water assessments are based on a small, vulnerable Midwestern community water system that had elevated levels of corn herbicides in the water supply. The development and use of the index reservoir approach is described in the USEPA OPP Water Models web site at [http://www.epa.gov/oppefed1/models/water/index\\_reservoir\\_dwa.html](http://www.epa.gov/oppefed1/models/water/index_reservoir_dwa.html).

<sup>9</sup> Based on recommendations from earlier FIFRA SAPs, USEPA OPP developed percent crop area adjustments for major crops and crop combinations. A description of the approach for use in drinking water assessments is available on the USEPA OPP Water Models site at [http://www.epa.gov/oppefed1/models/water/Development\\_and\\_Use\\_of\\_Community\\_Water\\_System.pdf](http://www.epa.gov/oppefed1/models/water/Development_and_Use_of_Community_Water_System.pdf).

Current assessments use 30 years (1961-1990) of measured weather (rainfall, temperature) data to cover year-to-year variability in runoff. The model discharges daily edge-of-field loadings of pesticides dissolved in runoff and sorbed to eroded sediment into a modeled water body – a 20,000 m<sup>3</sup> “standard pond” for ecological exposure or a 144,000 m<sup>3</sup> “index reservoir” for drinking water exposure.

VVWM uses the edge-of-field pesticide fluxes and spray drift loadings to estimate the concentration in the water body. The model accounts for pesticide degradation (hydrolysis, biodegradation, and photolysis), partitioning to benthic sediments, and volatilization losses. In most instances, the water bodies are modeled with a constant volume, although the model can vary volumes with weather.

The outputs – 30 years of daily estimated pesticide concentrations – are used to evaluate the probability of exceeding toxicity thresholds of concern in any given year when the pesticide is used according to label directions under vulnerable field conditions over a range of weather conditions that are representative of the use area. These results are summarized to provide 1-in-10-year maximum daily, 4-day, 21-day, 60-day, and annual average concentrations for comparison against ecotoxicological endpoints of concern. Drinking water exposure assessments use the entire simulated time series to assess acute effect endpoints of concern, 1-in-10 year annual average concentrations for chronic endpoints of concern, and overall (30-year) average concentrations for cancer-related endpoints. The full range of daily concentrations is also available for detailed temporal analyses, such as magnitude, duration, and frequency of exposures.

While USEPA OPP describes and characterizes the use of pesticides within this framework for a limited number of crop-specific scenarios, these tiered approaches do not easily distinguish between areas where pesticide concentrations in water may possibly result in risks to human health and/or the environment and areas where potential risks are expected to be negligible.

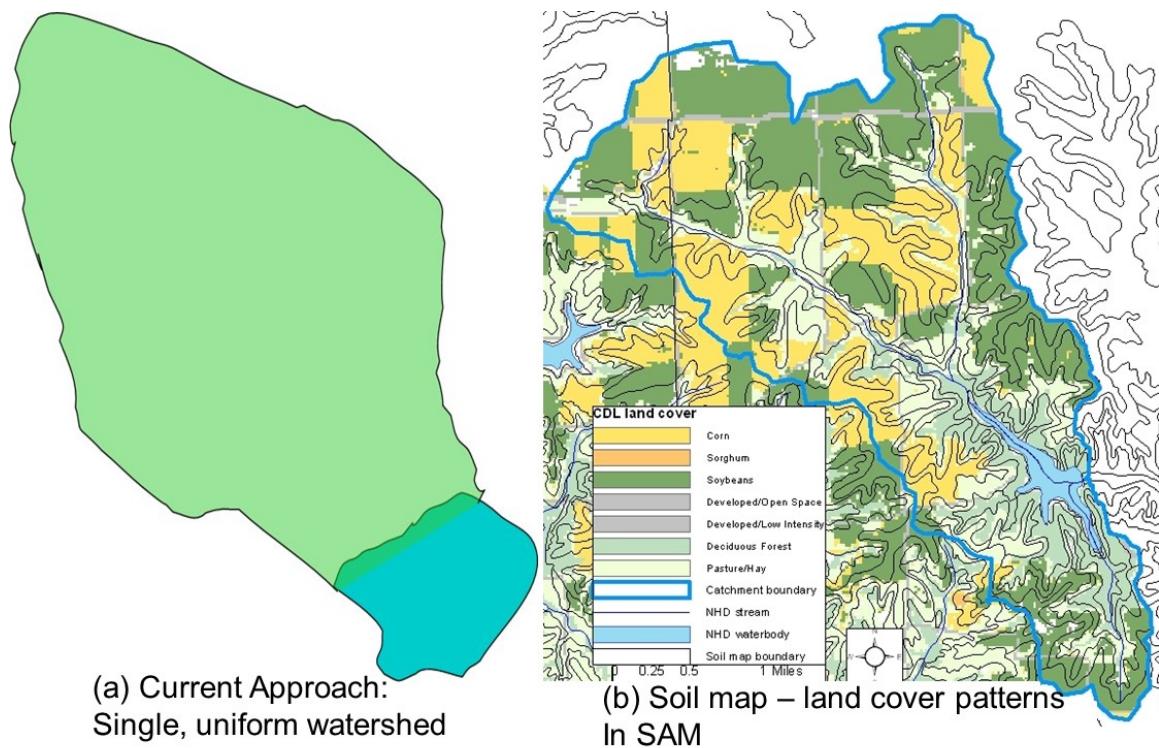
## **1.2 Adding a Spatial Context to Aquatic Exposure Assessments**

SAM adds more spatial detail and context to USEPA OPP’s scenario-based aquatic modeling approach to pesticide exposure estimates. Using mappable data and routines to automate scenario-building and exposure modeling, SAM allows risk assessors to more effectively and efficiently characterize the spatial extent of areas where pesticide concentrations in water may exceed toxicity thresholds.

OPP’s current field-scale aquatic modeling approach assumes uniform soil and landscape properties across an entire drainage area, with runoff, sediment, and pesticide loads routed into a standard, non-or minimally-flowing receiving water body (pond or reservoir). While soil, meteorological, hydrological, and crop-related inputs are representative of the crop geographic

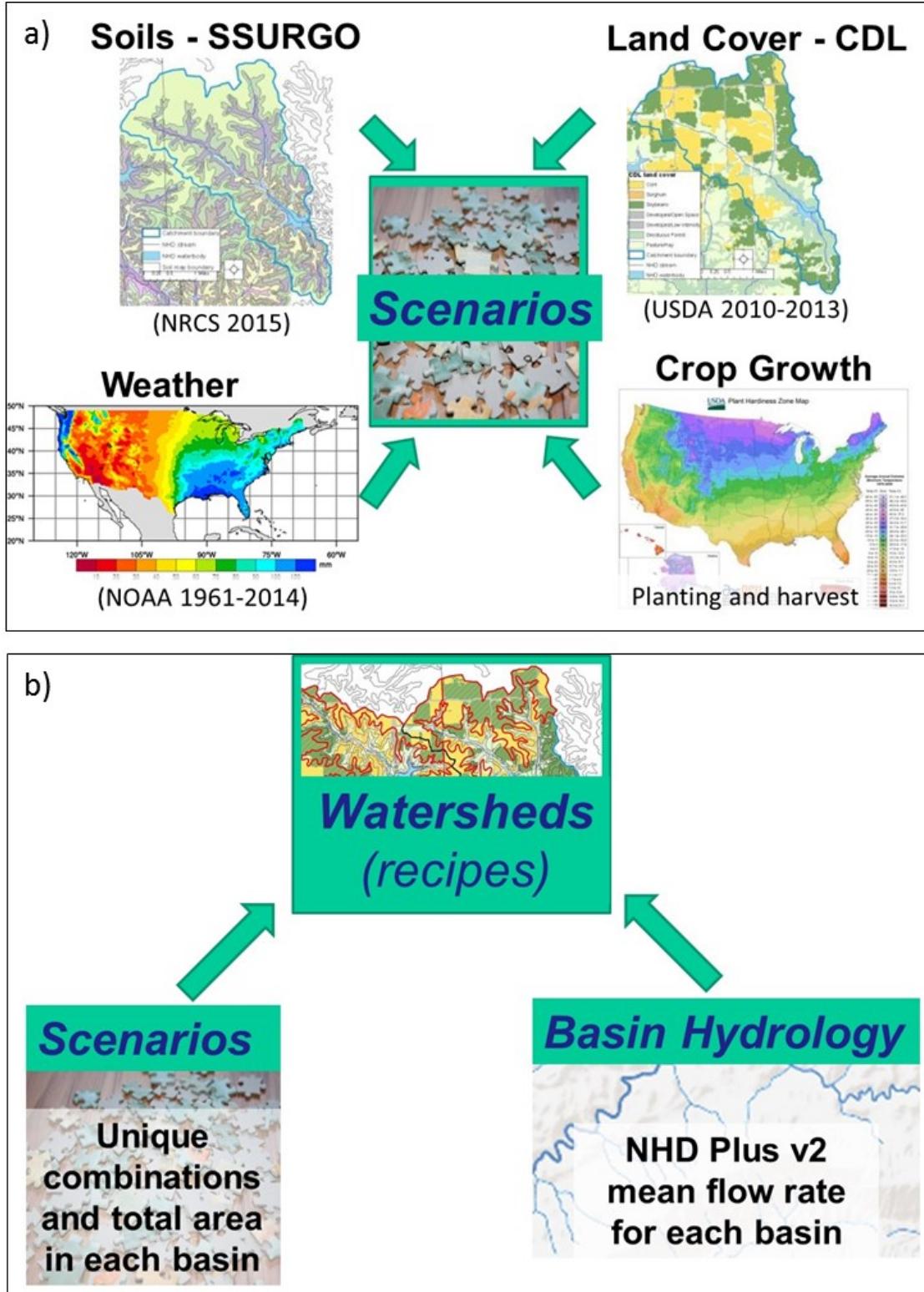
area that is expected to have high-end exposures, watershed and water body dimensions are generic and fixed. SAM incorporates spatial heterogeneity in soil properties, land use/cover, hydrology, meteorology, and crop growth and management practices within specific catchments and across the geographic range of the crop(s) under evaluation.

One key difference in the conceptual model for SAM is that it accounts for a continuum of soil-land cover-weather combinations within each watershed, rather than assuming a single, uniform set of soil properties and crop cover (Figure 4).



**Figure 4: Contrasting Current Single-Soil/Single-Crop Watershed Approach to SAM Approach of Accounting for Combinations of Soil and Land Cover Types.**

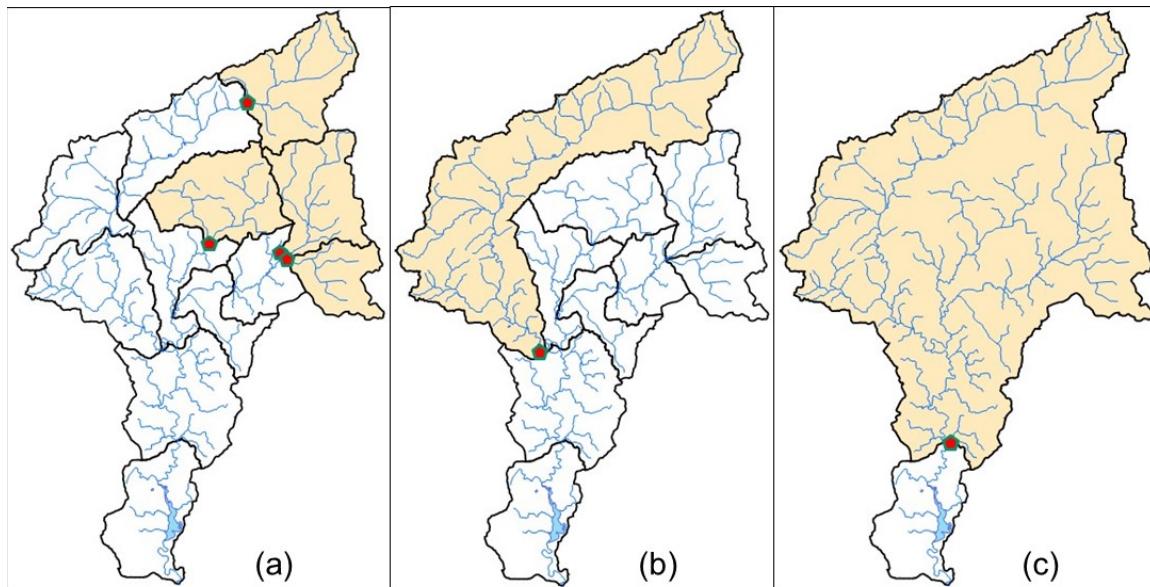
Rather than a single soil-crop-weather station scenario for the entire drainage area, each combination of land cover type, soil map unit, and weather station grid (described in Section 3) is treated as a separate scenario in SAM, similar to pieces in a jigsaw puzzle (Figure 5a). These jigsaw pieces come together as the daily runoff, sediment, and pesticide mass fluxes generated from each soil-land cover-weather grid scenario are weighted by their contributing area within each catchment and summed as inputs to the pour point water body (Figure 5b).



**Figure 5:** SAM scenarios are constructed from soil, land cover, weather, and crop data (a). The unique combinations of scenarios in each watershed are combined with catchment hydrology in recipe files that are used to generate outputs at the pour points (b).

A second difference in the conceptual model is that SAM no longer assumes fixed water body volumes and catchment areas. Instead, SAM incorporates geographic differences in watershed areas, receiving water body volumes, and expected flow and water body residence times. In the alpha test version of the model, daily concentration estimates were generated at the pour points of each HUC-12 unit. Runoff volume and pesticide mass were assumed to enter the water body that was identified at the HUC-12 pour point. Whether stream, river, lake, or reservoir, concentrations in these receiving water bodies were estimated using the “mixing cell” or completely mixed stirred tank reactor (CSTR) approach described in Section 2.

In this approach, only concentration estimates for headwater HUC-12 units, which have no farther-upstream contributing areas [Figure 6(a)], take into account all upstream pesticide and runoff loadings. To more adequately address pour points farther downstream [Figure 6(b) and 6(c)], SAM should account for all upstream loadings. The most straightforward method for doing so is to aggregate runoff and pesticide mass for the entirety of an upstream drainage area in calculating concentrations at the pour point (this approach was taken in the model evaluation in Section 2.4). A more sophisticated method, under examination in Section 4, attempts to address “time of travel” effects (i.e., the influence longitudinal dispersive mixing and differences in travel time) on pesticide concentration dynamics at the pour point.



**Figure 6: Conceptual Illustration of Stream Network (blue) and HUC-12 Units (black).** (a) All Headwater HUC-12s (no upstream outlet). (b) Identifies Upstream Drainage Area From Downstream Pour Point. (c) Further Aggregates Upstream Drainage Areas.

Another difference in the SAM conceptual model relates to the interplay between catchment area and pesticide application dates. The larger the drainage area, the less likely that pesticide treatments will all occur on the same day across the entire area. To address this, SAM allows distribution of applications to occur over user-defined application periods. To better identify

the timing, duration, and distribution of pesticide applications, USEPA OPP is exploring the use of a variety of USDA data on the timing of planting, harvesting, and different crop stages that can provide a framework for identifying the pesticide application period (see Section 5).

Table 1 summarizes differences in the conceptual model approaches between SAM and the current aquatic screening models used by USEPA OPP.

**Table 1 - Comparison of the Current Aquatic Modeling Approach and SAM.**

Model Component/ Process	Current Aquatic Modeling Approach	Spatial Aquatic Model
Catchment area	Drinking Water (DW): Small (173 ha/ 427 ac) midwestern agricultural watershed. Ecological Assessment (Eco): 10 ha (25 ac) agricultural field for eco exposure.	DW: Area varies depending on drainage area feeding the drinking water intake. Eco: Builds from NHDPlus catchments, estimates concentrations by reach.
Catchment soil conditions	Single, runoff-prone (Hydrologic Soil Group C or D) soil type for entire field or watershed. Runoff driven by curve numbers (crop and no crop) that represent the single soil and crop use being modeled.	Multiple soil types identified using USDA Soil Survey Geographic (SSURGO) database map units. Multiple curve numbers based on Hydrologic Soil Group (A, B, C, or D) and land cover combinations.
Pesticide inputs into catchment	Application according to label rates, adjusted for crop area (assumes 100% of field for eco exposure; national or regional maximum percent crop area for drinking water).	Application according to label rates, adjusted for crop area on a local (watershed-specific) basis, using USDA Cropland Data Layers (CDL).
Timing of pesticide applications	Single application date, based on best available USDA information on crop profiles, planting/harvesting dates, and likely application period.	Application window to simulate applications to multiple fields in the watershed; timing of application varies spatially and temporally based on USDA information on crop profiles, planting/ harvesting dates, crop progress data, and/or crop growth models, likely application period.

Model Component/ Process	Current Aquatic Modeling Approach	Spatial Aquatic Model
Pesticide fate in catchment (and amount available for transport)	<p>First-order degradation and linear equilibrium sorption in soil.</p> <p>Multiple compartments with finite difference solution to advection/dispersion equation.</p> <p>Pesticide applied below runoff depth is unavailable (25% typical).</p> <p>Exponentially-declining runoff flow profile in top 2 cm (PRZM5 documentation).</p> <p>26% of runoff flow interacts with soil.</p> <p>Erosion from surface compartment based on MUSS (Carousel et al, 2005).</p> <p>Leaching (tipping bucket) through soil profile.</p>	<p>Same.</p> <p>Single mixing cell with first-order analytical solution.</p> <p>Same.</p> <p>Uniform runoff flow profile in top 2 cm.</p> <p>Same.</p> <p>Not yet implemented.</p> <p>Same.</p>
Weather drivers	<p>30 years of rainfall (1961-1990) from nearest meteorological (MET) station based on location, Major Land Resource Area (MLRA).</p> <p>242 stations unevenly distributed across the US.</p>	<p>Rainfall data from 1948 to the present for 0.25x0.25 degree US grids.</p> <p>27,850 grid points evenly distributed across the US.</p>
Water body	<p>DW: 5.3 ha x 2.7 m deep (13 ac x 9 ft) reservoir (144,320 m<sup>3</sup>).</p> <p>Eco: 1 ha (2.5 ac) x 2 m deep (avg) pond (20,000 m<sup>3</sup>).</p>	<p>Flowing water bodies and reservoirs/lakes of varying size; water body volumes based on NHDPlus version 2 flow and velocity estimates for streams; lake/reservoir volume estimates based on method by Hollister and Milstead (2010), Hollister et al. (2011).</p>
Pesticide inputs to water	<p>Pesticide mass flux in runoff (dissolved) and sediment (sorbed) by rain events.</p> <p>Spray drift mass on application.</p>	<p>Pesticide mass flux in runoff (dissolved) and sediment (sorbed) by rain events.</p> <p>Spray drift methods in development.</p>
Pesticide fate in water	<p>Aerobic aquatic half-life (metabolism, hydrolysis, photolysis); first-order mass transfer between water column and benthos; equilibrium partitioning to sediment; washout from Index Reservoir.</p>	<p>First-order washout from water body; degradation in water (aerobic aquatic metabolism half-life) and sediment layer not currently implemented in test version.</p>
Water flow/ dilution	<p>Pesticide mass added to fixed water volume in Standard Pond or Index Reservoir.</p>	<p>Pesticide mass added to volume of reservoir or flowing water body at the watershed pour point.</p>

Model Component/ Process	Current Aquatic Modeling Approach	Spatial Aquatic Model
	No flow in pond (static); steady flow based on long-term mean simulated runoff in Index Reservoir.	Daily-varying flow through water body, based on NHD Plus v2 monthly mean flow data and modeled event-driven runoff.
	Although not typically considered, some endangered species assessments used downstream dilution from the edge of the use area based on a percent use area adjustment, reducing farm pond concentrations by the use area factor until concentrations are below toxicity thresholds.	Exposure estimates at each downstream pour point reflect the spatial heterogeneity of soil properties, crop areas. Relevant exposure estimates at each point compared to toxicity thresholds. Convolution method added to simulate effects of time of travel.

### 1.2.1 SAM and the other OPP surface water models

SAM algorithms consist largely of recompiled and streamlined hydrology, sediment, and pesticide transport components from PRZM5 (Young and Fry, 2014). SAM reduces model code redundancies and takes advantage of programming and hardware advances that have occurred since PRZM was first developed to speed up the modeling process.

SAM includes a graphical user interface (GUI) that allows for user-defined inputs, including pesticide use (i.e., application rate, frequency, timing, method) and chemical fate parameters. SAM creates unique scenarios based on location-specific information, rather than using the SWCC scenarios, the current standard used for surface water simulations. SAM calculates daily runoff and pesticide yields for specific watersheds and daily pesticide concentrations in receiving water bodies (e.g., flowing, reservoir, pond) that serve as a drinking water supply or as habitat for non-target aquatic organisms.

Results generated using SAM are not directly comparable to those from SWCC because of differences in spatial inputs and underlying assumptions. One important distinction between the models is that, for each scenario, SWCC has a much coarser resolution (intended to cover not-well-defined cropping areas within a MLRA or state), while SAM accounts for full range in soil-crop-weather heterogeneity within specific watersheds.

## 2 SAM Model Components: Core Modeling Components/Approach

In order for SAM to process inputs, model algorithms, and outputs at a national level, USEPA OPP streamlined model routines to focus on the main processes that simulate pesticide movement to water. This SAP-version of SAM focuses on the pesticide runoff routines in a dominantly corn-soybean-small grains setting. This section describes the key model components used for SAM in support of the following questions for the SAP:

**Q2.** Please comment on the model organization and improvements to model code.

- a. SAM is organized into three components (scenario generator, hydrology, and calculator) to reduce redundant calculations, increase model efficiency, and make use of pre-processing for creating standalone scenarios and hydrology (Section 2.1). USEPA OPP found this to be the best approach for handling the large quantity of the spatial and temporal inputs, while preserving the user's ability to run unique simulations every time. ***Please comment on the separation of independent processes (e.g., hydrology, pesticide transport) to maximize computational efficiency and minimize user run-time.***
- b. USEPA OPP has improved the PRZM model code to eliminate inefficiencies and excessive calculations. For example, simplifying the soil surface into a single layer, as described in Section 2.1.1, increased computational time by 10-fold with negligible change in results. ***Please comment on this general approach to improve the model's speed and efficiency without sacrificing accuracy and provide any additional recommendations for improving model efficiency.***

**Q3.** Sections 2.3 and 2.4 describe initial model evaluation steps for SAM to evaluate model uncertainty, sensitivity, and performance in comparison to measured (monitoring) data. Additional model evaluations occur in Sections 4.3 and 5.4.

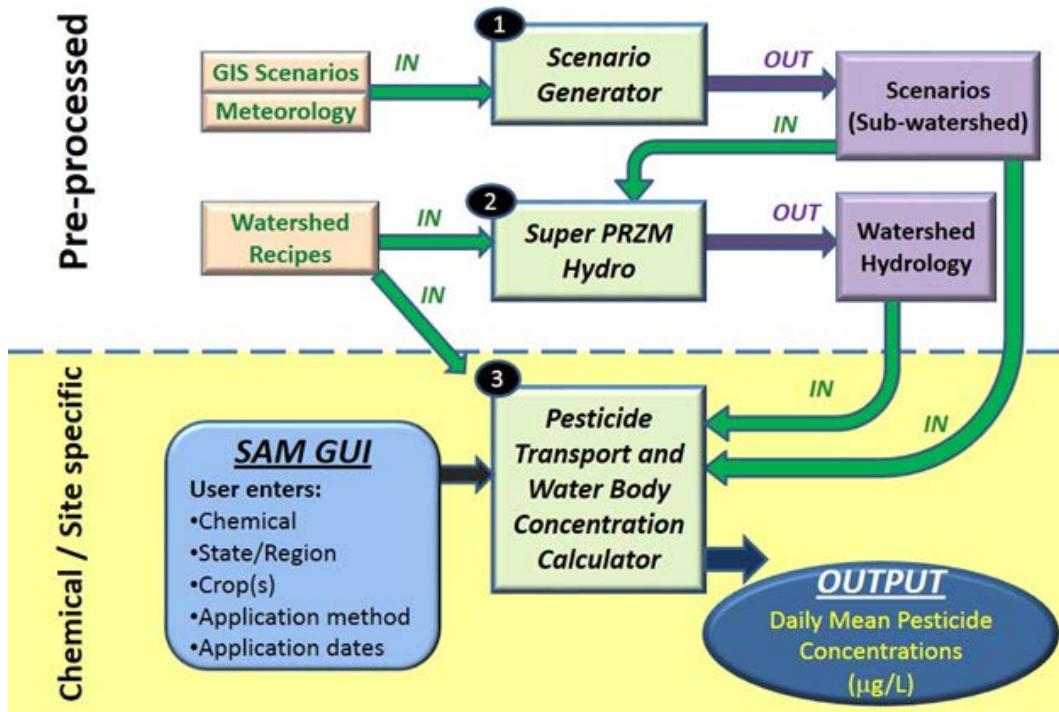
- a. ***What additional sensitivity analyses would the SAP recommend for model evaluation?***
- b. Current model evaluation compared SAM estimates to available atrazine monitoring data collected at daily to weekly intervals. Given the importance of robust, frequently-sampled monitoring data for evaluation, ***what additional monitoring and other types of data are currently available to test and evaluate how well SAM meets EPA objectives of transparent processes and clear, consistent, and reasonable products for risk assessments and risk characterization?***

Section 2.1 describes the modeling approach used in SAM, focusing on the model design, pesticide transport, and calculation of pesticide concentrations in water. Additional model components and details can be found in Appendix 2-A. Section 2.2 references proposed updates to the model that are explored in Sections 4 and 5 and discusses additional model improvements that are under consideration for addressing several limitations of the test version. Section 2.3 provides a brief description of the sensitivity and uncertainty analyses for SAM while Section 2.4 provides initial comparisons of SAM outputs with monitoring data.

## **2.1 Modeling Approach Used in SAM**

For SAM, USEPA OPP has followed the guidance on the development, evaluation, and application of environmental models established by the USEPA Council for Regulatory Environmental Modeling (CREM) (USEPA, 2009). USEPA OPP has applied the model development practices (i.e., problem definition, framework development, and parameterization) and used comprehensive model evaluation techniques (i.e., quality and performance evaluation). Transparent and open communication, including comprehensive documentation, has been provided to stakeholders and decision makers. USEPA OPP has held two public workshops (October 29, 2014 and April 29, 2015) to further engage stakeholders in the development process. Following the first workshop, a public SharePoint website was launched to aid communication with the public on key model approaches. An alpha version of the model was made available to stakeholders for testing and evaluation purposes. The model is also undergoing extensive peer review internally and externally through the SAP, in accordance with USEPA CREM best practices and recommendations.

SAM was built to simulate the impact of pesticide use across heterogeneous land cover areas in US watersheds. SAM aggregates daily runoff and pesticide loads for defined drainage areas, and estimates daily concentrations in receiving water bodies. Under the SAM framework, scenario generation, hydrology, and chemical transport are handled as separate model components to reduce model code redundancies and increase computational speed. This is possible as the movement of pesticide does not influence the movement of water. Soil and crop properties, weather, and hydrology are pre-processed and packaged into unique combinations called “scenarios” (Scenario Generator) (see Section 3 and Appendix 3-A for specific inputs and sources). Total runoff for each watershed (or drainage area) is calculated and stored based on the contributing scenarios and their corresponding areas (Super PRZM Hydro) (Figure 7). Finally, pesticide runoff loads and receiving water body concentrations are estimated using the Pesticide Transport and Water Body Concentration Calculator (“Calculator”). Here the user defines the chemical properties, crop(s), application method, and application dates in a GUI to estimate aquatic exposure concentrations in receiving water bodies.



**Figure 7: Overview of the SAM structure and components: Scenario Generator, Super PRZM Hydro, Pesticide Transport and Water Body Concentration Calculator, and SAM Graphical User Interface (GUI).**

### 2.1.1 SAM Components

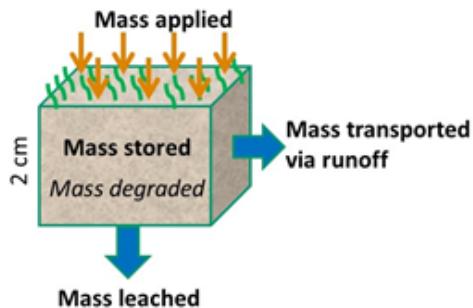
Each SAM component has an important role in the overall framework and progression of simulations (Figure 7). The Scenario Generator organizes the spatial inputs (Section 3) and calculates key input parameters for each scenario. These parameters include the daily runoff, erosion, vertical velocity, and plant growth stages. Each scenario represents a unique soil, crop, and weather combination that exists within a simulated watershed or other drainage area. Appendix 2-A provides further details about the Scenario Generator's calculation methods.

Super PRZM Hydro uses recipes (Section 3.2; Figure 5) to define the scenarios (soil-crop-weather) and associated areas ( $m^2$ ) that make up each watershed (or in the current SAP version, NHDPlus catchment) in a given year. Currently, recipes have been prepared for four recent crop years (2000-2013) using USDA National Agricultural Statistics Service's (NASS) Cropland Data Layer (CDL), but could be expanded as new data is released (Section 3.1.2). Super PRZM Hydro processes each NHDPlus catchment by summing the scenarios' daily runoff, weighted by area, to produce a daily time series of total runoff.

The third component of the model, the Calculator, uses the pre-processed hydrology from Super PRZM Hydro and implements chemical fate and transport routines to estimate pesticide

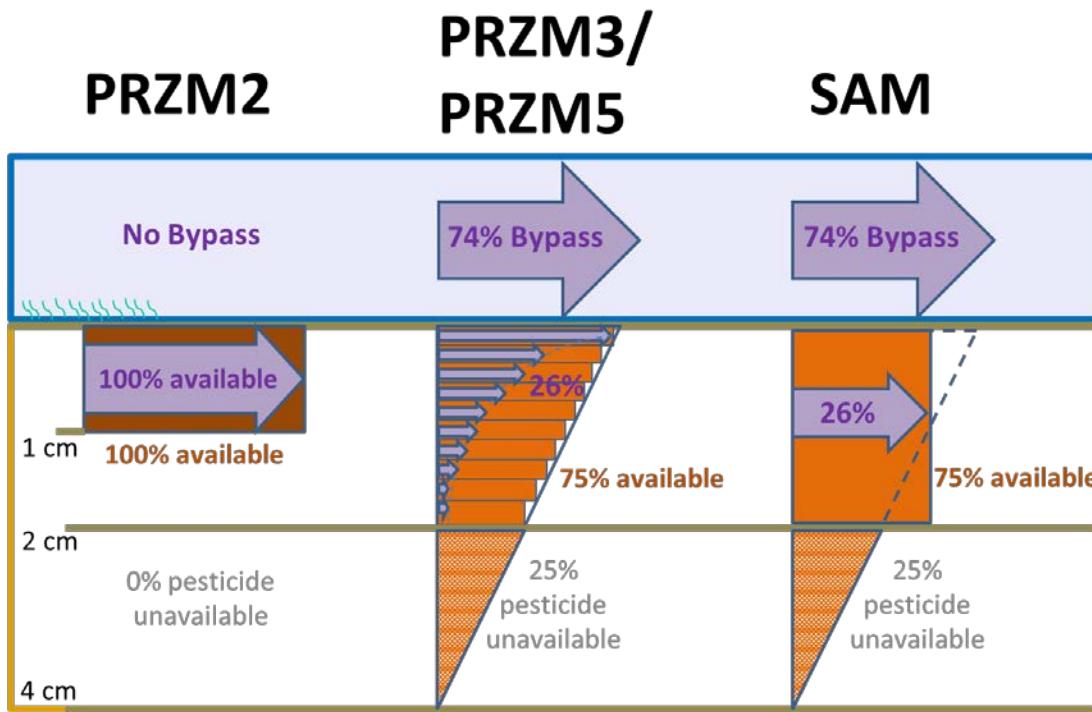
concentrations in the receiving water body associated with each catchment. Consistent with PRZM5, users specify an application rate and application timing, and the applied pesticide mass is divided between crop canopy and soil. In the soil, as in PRZM, only a fraction of the applied pesticide mass (75%) is available for transformation and transport in all simulations. The basis for this conceptualization comes from a limited number of documented PRZM evaluations (Carousel et al., 2005), which showed PRZM overestimated select monitoring locations prior to applying this percentage universally.

Given the available pesticide mass, the SAM Calculator simulates leaching, sorption, degradation, and runoff of pesticide from the field for a single soil compartment in the top 2 cm (Figure 8). This single compartment is modeled as a zone of uniform mixing in the soil down to a specific depth (Ahuja, 1986; Ahuja and Lehman, 1983; Frere et al., 1980; Haith, 1980; Steenhuis and Walter, 1980). In PRZM2, a single soil compartment was similarly used, while PRZM3 (and PRZM5) assumed multiple sub-compartments with a declining amount of mass available with depth (Figure 9). SAM uses a single mixing cell in the surface layer, rather than the 10 sub-compartments in the current PRZM5 because these two methods provide similar results, yet the latter is computationally 10 times slower. USEPA OPP has chosen computational speed (and simplicity) to take precedence over slower, more complex calculations. Appendix 2-A includes additional information on the SAM transport routine conceptualization and solution technique.



**Figure 8: Pesticide mass transport in the Pesticide Transport and Water Body Concentration Calculator simulates leaching, sorption, degradation, and transport via runoff.**

As in PRZM5, runoff only partially flows through the soil. It includes a fraction that interacts with the soil (26% of total runoff flow) and a fraction that does not (74%) (Figure 9). In SAM, the interacting portion of runoff has a uniform flow profile, whereas PRZM3 and PRZM5 use an exponentially declining runoff flow profile (Young and Fry, 2014). USEPA OPP found that estimated concentrations were insensitive to the use of uniform (single compartment) mass and flow distributions compared to non-uniform, multi-compartment approaches (Appendix 2-B). As a result, SAM implements the most efficient and least computationally intensive approach, using uniform, single compartment mass and flow distributions.



**Figure 9: Runoff (in purple) and pesticide (in orange) extraction conceptual models in SAM, with PRZM2 and PRZM3/PRZM5 shown for comparison.**

A closer look at the validation work of Carousel et al. (2005) indicates that the primary reduction in pesticide runoff realized by PRZM3 over PRZM2 was due to reducing the fraction of mass available (0.75) and the fraction of interacting runoff flow (0.26). The product of these is 0.19, which is the same as the reduction in observed concentrations. Thus, the use of multiple compartments and non-uniform extraction by Carousel et al. (2005) had, at most, a non-observable impact.

To calculate the daily mean pesticide concentrations in receiving water bodies, the Calculator uses the daily mass transported by runoff, and receiving (pour point) water body volume and flow rate. For lotic water bodies (e.g., streams, rivers), water body volume is estimated as reach cross-sectional area (derived from NHDPlus version 2) multiplied by a representative length. Using a mixing cell approach for the water body, a representative length of 40 meters is used, based on typical longitudinal dispersivities measured in rivers (Fischer, 1979; Rutherford, 1994). For lentic water bodies (i.e., reservoirs, lakes, ponds) that are part of the drainage network, flows are also obtained from NHDPlus and volumes are preliminary estimates developed by USEPA's Office of Research and Development (ORD) Atlantic Ecology Division based upon surrounding landscape topography. The methods used by USEPA ORD are similar to those documented in Hollister and Milstead (2010) and Hollister et al. (2011).

Flows are allowed to vary daily and are calculated as the sum of monthly-varying base flow and daily-varying runoff. For each tabulated reach, NHDPlus provides overall long-term and monthly mean flow estimates (Section 3.1.5). Monthly mean base flows are estimated as the difference between monthly mean flows (as reported by NHDPlus) and the long-term mean runoff (derived from the daily runoff generated by Super PRZM Hydro). Simulated daily runoff values are then added back to the monthly mean base flows, generating a daily hydrograph at each modeled location for the duration of the simulation. These hydrographs account for peaks and lulls in daily flow not captured in the monthly variability alone.

In the alpha version of SAM, receiving water body concentrations were calculated for each HUC-12 unit based on volumes and flow rates for the immediate (local) HUC-12. For the SAP-test version, similar concentration calculations were done for each NHDPlus catchment based on the volumes and flow rates for the immediate water body or reach. However, since these estimates did not account for the contributions from upstream catchments, recipes files were modified to include the areas of all upstream NHDPlus catchments contributing to a single water body into one recipe. Concentrations were then recalculated using the updated recipes. Section 5 describes an additional approach to further refine calculated concentrations by temporally re-distributing daily pesticide loads from upstream NHDPlus catchments within a drainage area, based on their in-stream travel time to the water body.

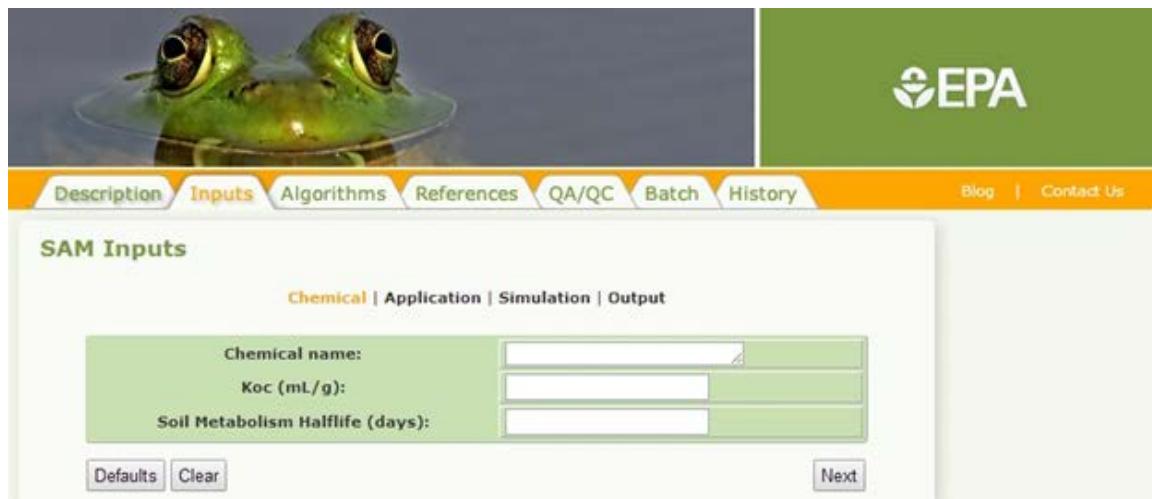
Within each receiving water body or reach, first-order dissipation is assumed for a single compartment due solely to washout, as described in Appendix 2-A. A benthic sediment layer is not currently included in the model, and sorbed pesticide transport by eroded sediment is currently under consideration, but depends on the availability of relevant monitoring datasets for validation (Section 2.4).

### **2.1.2 Alpha Version of SAM (*über*tool Site)**

The alpha version of SAM on the übertool site calculates concentrations for each HUC-12 unit based on volumes and flow rates for the immediate (local) HUC-12. As noted above, such estimates do not account for contributions from upstream HUC-12 units and the results could be misleading. Adjustments will be made to this model based on feedback from the SAP.

To run the alpha version of the SAM, the übertool SAM GUI can be accessed at  
<http://qed.epa.gov/ubertool/sam>

The SAM GUI is hosted as part the USEPA übertool project ([www.qed.epa.gov/ubertool](http://www.qed.epa.gov/ubertool)). It allows a user to run SAM simulations after specifying chemical and application details (Figure 10). The Calculator runs each time a new simulation is launched, reading in the user-defined inputs and accessing all relevant pre-processed scenarios and hydrology for the particular region/crops being simulated.



**Figure 10: SAM Graphical User Interface with four input tabs: Chemical, Application, Simulation, and Output.**

In the GUI, the Chemical tab requires the chemical name, organic carbon partitioning coefficient ( $K_{oc}$ ), and soil metabolism half-life (in days). The Application tab asks the user to specify the crop(s), application rate, application method, and other application refinements. The Simulation tab allows for the user to select the region (Ohio River Basin in the test version), simulation type (Ecological in the test version), and simulation start and end dates. The Output tab allows for selection of output tables, plots, and geospatial maps.

## 2.2 Proposed Updates and Additional Improvements under Consideration

Based on model evaluations discussed in Section 2.4, USEPA OPP has proposed updates and refinements to the test version of SAM for SAP consideration: re-distributing daily pesticide loads from individual catchments based on their travel time to receiving water bodies in larger drainage networks (Section 4) and defining application windows (Section 5).

Additional improvements to the model are under consideration to address several limitations of the test version. This section describes additions that USEPA OPP is evaluating for future versions of SAM. As part of the peer review process, USEPA OPP welcomes recommendations and feedback on these and other model improvements. Recommendations will be considered based on their scientific merit, ease of incorporation into the model, and the availability of intensive monitoring data for validation.

### 2.2.1 Erosion and Sediment Routines

SAM currently uses a modified version of the Universal Soil Loss Equation (USLE), MUSS, to simulate soil erosion (Carousel et al, 2005). MUSS has been used in USEPA OPP's Surface Water Concentration Calculator (SWCC) for calculating erosion at the field level, as well as in previous

PRZM versions. The MUSS soil erosion routine, however, may not be scalable to a watershed model like SAM. At the watershed level, SAM can estimate erosion loss events for individual scenarios and then use an area-weighted sum of those losses for a given watershed. It may be difficult to track erosion and sediment yield between or across basins though, since those processes are not well understood and have not been modeled rigorously at the national scale in the past.

This area of improvement is important for determining sediment loadings that will affect soluble and sorbed pesticide concentration estimates in any modeled watershed. From the literature, the USLE usually performs well at simulating erosion loss due to rainfall at the field level (Wischmeier and Smith, 1978). However, less is known about modeling erosion and sediment yields at watershed scale. Recent literature also suggests that a more recent revised version of USLE (RUSLE) may overpredict erosion in certain instances (Brooks et.al. 2014).

Some factors affecting sediment delivery at a watershed-scale include texture, distance from the main channel, channel density, field slope, length, land use/cover, and rainfall /runoff (Ouynang and Bartholic, 1997). Field measurements and observations would be necessary to validate watershed-level erosion and sorbed pesticide concentration estimates generated by SAM.

USEPA OPP could consider chemicals with a higher affinity to sorb to soil or sediment and be transported to water by erosion. However, up to this point, the test version of the SAM has focused on evaluating the runoff transport algorithms using chemicals that are not highly sorbing, given the availability of monitoring data (Section 2.4). USEPA OPP is looking for similarly-robust water-column and sediment monitoring data for highly-sorbed chemicals to evaluate how well the SAM erosion and sediment routines perform in estimating pesticide concentrations in water.

## **2.2.2 Spray Drift**

The current test version of SAM does not account for the fraction of pesticides that may reach water bodies by spray drift. USEPA OPP's current aquatic exposure assessment approach uses the AgDRIFT model to generate screening-level estimates of the fraction of pesticide applications that reach a water body from an adjacent treated field.<sup>10</sup> The AgDRIFT model provides estimated deposition for pesticides applied by aerial, ground, and airblast equipment using both mechanistic algorithms and field data.

USEPA OPP is considering methods to estimate spray drift at the watershed scale, taking into account that not all fields will contribute drift equally (both in terms of distance from the water body and prevailing wind direction). USEPA OPP is also open to considering other scientifically-defensible options for estimating spray drift at a watershed level.

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<sup>10</sup> More information on AgDRIFT can be found on USEPA OPP's Water Models website at <http://www.epa.gov/oppefed1/models/water/>

### **2.2.3 Irrigation**

Irrigation is built into the SAM Scenario Generator (Appendix 2-A), although the routine is not turned on in the alpha version. Additional inputs from the user are needed for the irrigation routine, including an irrigation depth and an available water fraction, below which irrigation is required. USEPA OPP plans to make these additional user inputs available in upcoming versions.

### **2.2.4 Ponds and other small non-flowing water bodies**

While numerous ponds and other small non-flowing (lentic) water bodies are identified in the NHDPlus Waterbody spatial data set, many of these do not have well-defined catchment areas or connections to flowlines. This makes it difficult for USEPA OPP to estimate concentrations in these disconnected water bodies. One option may be to use pesticide concentration estimates for the NHDPlus catchment as a surrogate for ponds and small water bodies within the catchment. However, monitoring data to evaluate estimates for small water bodies are, for the most part, lacking.

### **2.2.5 Other agricultural crops**

Some agricultural crops such as vegetables and orchards may present challenges in processing the necessary land cover information because of a lack of training and evaluation data needed in the error analysis for USDA NASS's Cropland Data Layer. USEPA plans to develop test approaches using a variety of land cover data sources in areas of the country that have a wider diversity of crops and land cover types.

### **2.2.6 Non-agricultural uses**

The test version presently focuses on evaluating pesticide applications for agricultural purposes. Non-agricultural uses may be considered in the future, but may be limited by the availability of monitoring datasets for validation.

## **2.3 Uncertainty and Sensitivity Analyses**

Key elements of environmental model evaluation are sensitivity and uncertainty analyses and comparisons of model outputs to measured data (USEPA, 2009). Sections 2.3.1 and 2.3.2 provide a brief summary of uncertainty and sensitivity analyses that have informed the development of SAM. Section 2.4 provides initial comparisons between SAM outputs (estimated concentrations) and measured data (pesticide monitoring).

### **2.3.1 Uncertainty Analysis**

Uncertainty analysis considers the effects of lack of knowledge or potential errors of model inputs (USEPA, 2009). The following is a quick summary of the major inputs that contribute to uncertainty in model outputs and how USEPA OPP is addressing those uncertainties.

- **Pesticide environmental fate properties:** OPP relies on registrant-submitted studies to reflect the rates and modes by which a pesticide degrades, and the degree to which a pesticide sorbs to soil or sediment. The accuracy of model inputs will depend on the quality of these studies, which will be pesticide-specific. Guidance for model inputs focuses on central tendencies of measured pesticide properties, and confidence limits as appropriate to ensure a degree of conservatism (USEPA OPP, 2009b).
- **Pesticide application:** This is one of the important drivers in pesticide exposure. All other conditions being equal, the mass of pesticide reaching water bodies is proportional to the mass of pesticide applied, which is itself a function of area treated. By assuming maximum label application rates and 100% crop treated, USEPA OPP can set an upper bound on potential exposure. In refinements, proprietary or USDA NASS survey data, if available, can be used to estimate less-than-maximum application rates, from “typical” or median rates to upper percentiles of reported rates. This introduces additional uncertainties related to the sample size of the survey and to the geographic scope represented by the sampling.
- **Weather:** The amount, intensity, timing and frequency of rainfall have a major impact on pesticide transport to water. Because precipitation varies over time (as well as by location), OPP runs multiple years of historical weather data to reflect this variability. OPP’s currently-used regulatory models rely on a few hundred weather stations to reflect variations across the country, and run simulations driven by 30 years of data (from the years 1961-1990). SAM will employ many more weather data points at 0.25-degree grids across the country to obtain finer spatial resolution, with the flexibility to cover time periods from 1948 to the present. Further evaluations of the weather data can be found in Appendix 3-C.
- **Soil properties:** Most soil properties vary within a range that has been defined for each soil map unit. Depending on the property, the map unit may provide a non-overlapping bound with adjacent map units (for instance, soil map units are often separated by distinct slope classes). The range in other properties, such as bulk density and water capacity, may overlap among soil map units. The soil property inputs to SAM use a representative value that is generally a central tendency (mean or median) from the reported range in properties for the particular soil type. While a single representative quantity doesn’t represent the range in properties, it is expected to generally be value-neutral in terms of impact on concentration estimates. Appendix 3-A includes a characterization of the relative impact of each input parameter on model outputs.
- **Land cover:** Land cover is used as a surrogate for pesticide use by defining the extent of the land cover type being treated. The USDA Cropland Data Layer (CDL) provides the most detailed spatial resolution for various crops and crop groups. Key areas of uncertainty include (a) the relative accuracy of the CDL in identifying actual crops, which

is covered in detail in their accuracy assessments<sup>11</sup>, (b) generic land cover classes (for example, orchards and vineyards, vegetables and ground fruit) used for crops that, individually, have poor accuracy in CDL, and (c) year-to-year variation in crop cover. The first two points are described elsewhere (Appendix 3-B). To address year-to-year variation in land cover, USEPA OPP currently plans to use the most recent 5 years of national CDL coverage, with model simulations covering the variations in land cover patterns over the 5 year period for each watershed (or other drainage area). However, the number of years of coverage can be expanded, provided that the national coverage continues to be collected in the future.

- **Crop and Management Practices:** Crop planting, growth, and harvesting times are important parameters in terms of their impact on the timing of pesticide applications. These vary across the country based on general climate differences, and vary from year to year with annual differences in weather. The test version of SAM uses USDA Usual Planting and Harvesting Dates publications (USDA NASS, 2006, 2007, 2010) to define the planting and harvesting windows in a given location. Pesticide applications are currently spread across the most active window. Other approaches to better define application windows are considered in Section 5.

### 2.3.2 Sensitivity Analysis

Sensitivity analysis evaluates the effect of changes in input values or assumptions (including boundaries) on model outputs (USEPA, 2009). The general factors that affect the transport of pesticides from the field(s) of application to water bodies in SAM are the amount of pesticide applied, persistence and mobility of the pesticide, timing and intensity of rainfall (particularly in relation to the time of pesticide application), and vulnerability of the application area to pesticide loss via surface runoff (determined in the model primarily by the curve number).

In the late 1990's the FIFRA Environmental Modeling Validation Task Force (FEMVTF) compared edge-of-field outputs from PRZM against measured data and conducted a sensitivity analysis of input parameters (Jones and Russell, 2001; Jones and Mangels, 2002). The results helped identify inputs and ranges for which the PRZM model was most sensitive.

FEMVTF found that the following input parameters were important for runoff outputs:

- Rainfall during the key period when the pesticide is on the field/crop
- Runoff curve number (CN)
- Pesticide half-life
- Pesticide sorption coefficient, Koc
- Soil organic carbon fraction

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<sup>11</sup> The description of NASS's accuracy assessment is available at <http://www.nass.usda.gov/research/Cropland/Method/cropland.pdf>. Metadata that include error analysis are available for download at <http://www.nass.usda.gov/research/Cropland/metadata/meta.htm>.

- Available water in the soil surface horizon, derived from field capacity, bulk density
- Bulk density of soil in the surface horizon
- Total pesticide applied

For fixed pesticide properties, the sensitivity of runoff loading to model inputs is as follows:

Weather (rainfall) >> Curve Number >> all other inputs

While OPP expects to see similar results for SAM because similar runoff and pesticide fate/transport algorithms are used, some inputs that are dominant at a field scale, such as those based on soil properties, may be less so at watershed scales that integrate the contributions of multiple soils and crops. Other factors, such as the relative proportions of various components in a watershed (captured in the recipe files), are expected to affect pesticide concentrations. Watershed-scale properties that have been shown to affect pesticide concentrations in water include the acreage in crop(s) upon which the pesticide can be used, pesticide use intensity within the watershed, proportion of runoff-prone soils (reflected by properties such as hydrologic soil groups (HSG) C and/or D, soils with a drainage-restrictive layer, surface runoff potential), amount of rainfall during or shortly after the pesticide application period, broad management conditions such as area in artificial drainage, and hydrologic indicators of runoff (USEPA OPP, 2009a; Stone and Gilliom, 2012; Stone et al, 2013).

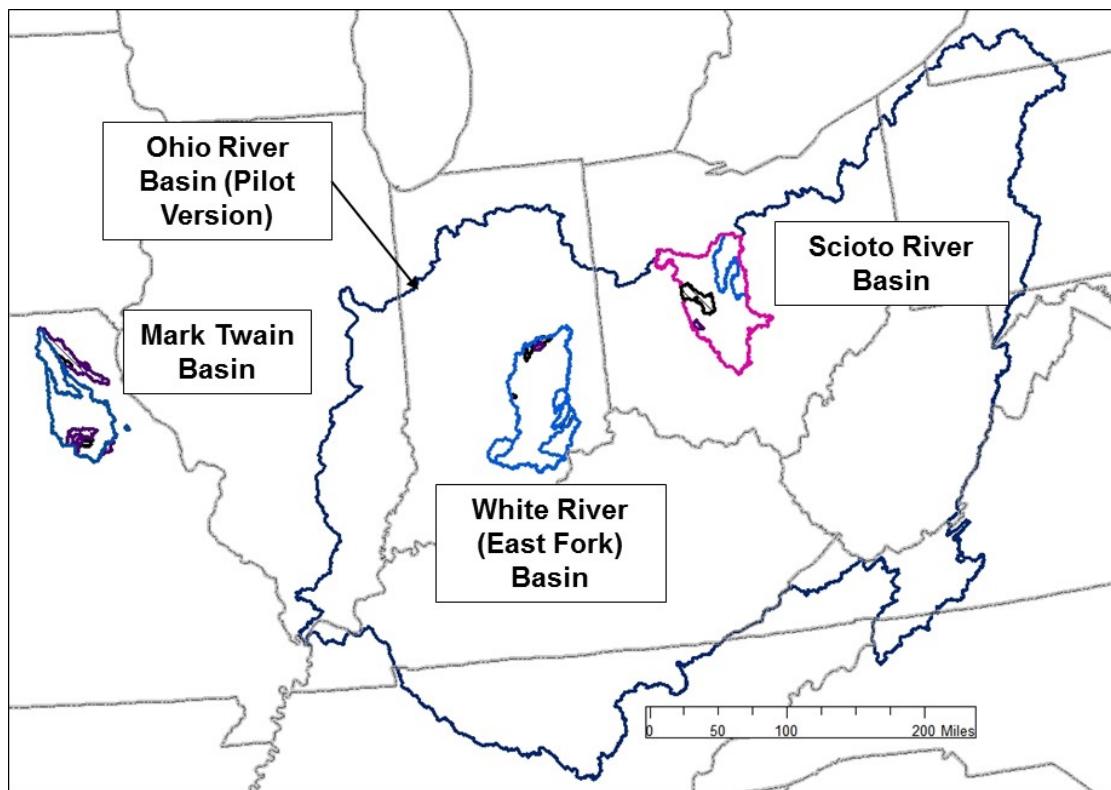
## **2.4 Comparison of Model Outputs with Measured Data (Monitoring Data)**

Evaluation of models should consider the uncertainty in both model outputs and the measured data used for comparison (USEPA, 2009). To be useful in evaluating how accurately SAM estimates pesticide concentrations in water, monitoring data need to be collected sufficiently frequently to capture day-to-day, seasonal, and yearly variations in pesticide concentrations in water (USEPA OPP, 2011). The extent to which monitoring data adequately reflect short-term variability in pesticide concentrations in water depends on how frequently samples are collected, and whether the sampling was targeted to pesticide use areas and times of the year in which pesticides have been applied. As the interval between sampling events increases, the likelihood of capturing short-duration or single-day peaks in pesticide concentrations decreases, particularly in fast flowing waters. Even weekly sampling will often provide a biased (underestimating) perspective on pesticide concentrations in water as variations in pesticide concentrations over time may be defined on daily or sub-daily time scales. Sampling bias has been discussed in recent FIFRA Scientific Advisory Panel meetings on atrazine (USEPA OPP, 2010a, 2010b, 2011, 2012). To evaluate the potential uncertainty in sampling frequency for predicting actual concentrations, USEPA OPP (2011) simulated 4-, 7-, 14-, and 28-day sampling intervals on monitoring datasets that had daily- to near-daily sampling intervals. Median annual peak estimates ranged from 75-78% of the true annual peaks for a 4-day interval, 36-70% for a 7-day interval, and 25-54% for a 14-day interval (USEPA OPP, 2011).

#### **2.4.1 Atrazine Monitoring Datasets Used for Comparison**

For the initial evaluation of SAM here and in Sections 4 and 5, USEPA OPP used two monitoring studies for atrazine conducted in the corn-growing regions of the US between 2003 and 2014. Syngenta Crop Protection's Atrazine Ecological Exposure Monitoring (AEEMP) of headwater streams in areas expected to be vulnerable to atrazine runoff is one of the few pesticide monitoring studies that include daily sampling for pesticide concentrations in water at some sites (USEPA OPP, 2009a). A second set of atrazine monitoring data – Syngenta's Atrazine Monitoring Program for Drinking Water (AMP) – included weekly sampling for atrazine during the likely use season (USEPA OPP, 2011, 2012). These two data sets, which covered a range of watershed sizes and water body types (headwater streams to larger streams and rivers, reservoirs and other lentic waters), focused on areas where atrazine is widely used. Details on these studies, as well as the data themselves, can be obtained through USEPA OPP's Atrazine Information page (<http://www.epa.gov/opprrd1/reregistration/atrazine/>).

USEPA OPP focused on three test basin areas – the Scioto River (OH) basin and the White River/East Fork (IN) basin within the greater Ohio River basin and the Mark Twain basin in northeastern Missouri (Figure 11). These three basins were selected because they contain multiple monitoring sites, predominantly for atrazine, with multiple years of sampling and sampling frequencies that range from weekly to daily. Appendix 2-C contains more information, including monitoring data for each test basin.



**Figure 11: Location of Test Basins for Further Model Development and Evaluation.**

## **2.4.2 Future Comparisons with Other Pesticides**

Ultimately, SAM needs to reliably estimate concentrations for pesticides that have a wide range of properties, including those with a higher potential to sorb to soil and sediments and those with shorter or longer half-lives than atrazine. Initial model evaluations used atrazine because of the ready availability of robust monitoring data. However, USEPA OPP plans to expand the model evaluation to include additional pesticides and other areas of the country. For monitoring data with less frequent sampling intervals, USEPA OPP will use methods considered in USEPA OPP (2011 and 2012) to characterize the uncertainty in concentration estimates based on less frequent sampling.

In an effort to obtain monitoring data with more frequent sampling intervals for a wide range of pesticides, USEPA's OPP and Office of Water (OW) are collaborating with USGS's NAWQA Program to sample and analyze daily surface water samples from selected regions of the United States for pesticides. The multi-year effort is an outgrowth of initial collaboration that leveraged USEPA OW's National Aquatic Resource Survey (NARS) National Rivers and Streams Assessment (NRSA) program to assess stream quality. In 2013 NRSA evaluated the condition of the Nation's rivers and streams with an emphasis on ecological condition at over 1000 sites selected using statistical survey methods. As part of the overall effort, USGS NAWQA and USEPA OPP collaborated on a focused sampling effort at a subset of 100 sites across a region embedded within the national NRSA effort. The initial region selected was the Midwest "corn belt" region with the goals to characterize water-quality stressors, such as pesticide contaminants, nutrients, and suspended sediment, and to determine the effects of these stressors on ecological communities in the streams. Each of the 100 USGS sites included weekly surface water samples across a four month window and were analyzed for 230+ pesticides and degradates.

Additionally, USGS and USEPA OPP selected 7 of the 100 sites for daily analysis. USEPA's analytical laboratory at Ft Meade, MD, analyzed the daily samples. After quality assurance checks are completed, the expanded set of pesticide will be used not only for evaluating SAM but also for a more robust analysis of sampling bias across chemical types (e.g., organophosphate pesticides) and modes of action (e.g., insecticides, fungicides).

USEPA OPP and USGS NAWQA have since expanded this monitoring effort into other regions of the country including the Southeastern US and Pacific Northwest. Both of these data sets have been collected and are undergoing final QA of the analytical results. Planning is underway for additional sampling in the Northeastern US in 2016 and within irrigated portions of California in 2017. Once sampling is completed, USGS and USEPA OPP will have a robust data set spanning a range of geographies, land use types, climatic and hydrologic conditions that will allow for a robust analysis of this high quality data.

### **2.4.3 Criteria for Model Evaluation**

SAM is an uncalibrated model and USEPA OPP does not expect that SAM estimates of pesticide concentrations to exactly match the patterns of pesticide concentrations in measured data. Instead, evaluations focus on how well the magnitude and ranges in estimated concentrations compare to measured concentrations within years and across the span of sampling periods. The following criteria were used to compare estimated annual maximum concentrations to reported monitoring data, taking into account potential bias errors from sampling frequency:

- Minimal model underestimates compared to monitoring (Type II errors), with no estimated annual maximum concentrations that are more than an order of magnitude (10X) less than measured data;
- Most SAM estimates of peak concentrations should fall within the range of 1 to 5X greater than corresponding measured maximum concentrations;
- Minimal overestimates by factors of 10 or greater; model estimates that are within 5-10X greater than measured concentrations should be considered in the context of potential underestimations in measured maximums due to sampling frequency.

Where model estimates do not correspond well with measured data, USEPA OPP will be looking for systematic trends that may help explain the differences and lead to model upgrades that result in improved accuracies in estimated concentrations.

### **2.4.4 Initial Comparisons with Atrazine Monitoring Data**

Available monitoring data from these programs covered 2003 through 2014. For an initial test comparison, USEPA OPP simulated daily atrazine concentrations from 2000 through 2014, using the following conditions:

Chemical	Atrazine
Half-life in soil	123 days
Sorption coefficient (Koc)	100
Years Simulated	2000-2014
Application Rate	1.69 kg/ha (MO), 1.32 kg/ha (OH), 1.47 kg/ha (IN), based on average application rates over 2004-09 in the AEEMP study sites reported by Syngenta (USEPA OPP, 2009a)
Application Window Determination	Begin 14 days before emergence (from USDA Typical Planting/Harvest Dates; consistent across years); pesticide application divided across 50-day window using uniform distribution (based on average length of planting period)
CDL Crop Years Used for Recipes	2010-2013 (4-year rotation repeated across the simulation period)

Test Basins, MO (Mark Twain Basin, northeastern MO)	AEEMP sites MO-01 (comid 4989415) <sup>a</sup> , MO-01c (4988183), MO-01d (4988241), MO-02 (5042358), MO-4a (4989385), MO-04b (4989739), MO-05 (5042400), MO-05b (5039952), MO-08 (2508563)  AMP sites MO-16 (4867529), MO-17-river (5641174), MO-17-reservoir (5641630), MO-19 (4869843), MO-21 (4867727)
Test Basins, IN (East Fork of White River Basin, central IN)	AEEMP sites IN-10 (18459870)  AMP sites IN-04 (18454511), IN-06 (18450057), IN-07 (18445592), IN-08 (18445664), IN-13 (18451035)
Test Basins, OH (Scioto River Basin, central OH)	AEMP sites OH-04 (3483775)  AMP sites OH-10 (5214753), OH-11 (5213585)  Heidelberg Univ. NCWQR Scioto River station (3486865)
Pesticide, Runoff Processing	Daily flux outputs accumulated at the pour point for each test basin; no adjustments for time of travel.

<sup>a</sup> For modeling purposes, each test basin is also identified by the NHDplus comid that is associated with the monitoring site/pour point location.

Appendix 2-D includes the daily concentrations, pesticide mass losses, runoff fluxes, and flows generated by SAM, along with yearly summaries and comparisons to monitoring data for each test basin. Table 2 summarizes the comparison of estimated yearly maximum concentrations for the individual sampling stations within each test basin. Sampling bias errors in the measured (monitored) data are not considered in this evaluation. Particularly for daily concentrations, those sites with sampling intervals of 4-7 days or more are more likely to underestimate maximum concentrations.

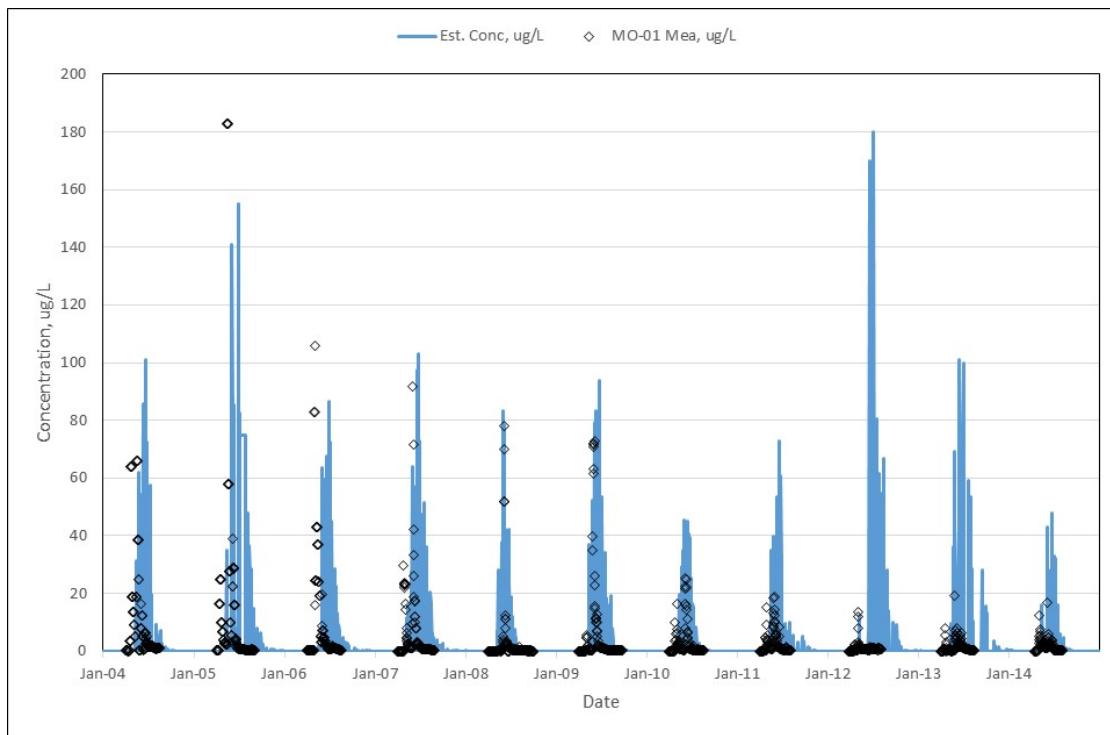
**Table 2: Summary of Comparisons of SAM Estimated Annual Maximum Concentrations with Monitoring Data for Test Basins in MO, OH, and IN.**

Monitor-ing Site	Range in Annual Maximum Concentrations (ug/L)		Number and % of site years underestimating measured annual maximums by a factor of			Number and % of site years overestimating measured annual maximums by a factor of		
	Measured	Modeled	>10X	5-10X	1-5X	1-5X	5-10X	>10X
MO-01 AEEMP	14-183 (11 yr)	64-183	0	0	3	7	0	1
MO-02 AEEMP	9-155 (11 yr)	64-183	0	0	1	8	1	1
MO-04a AEEMP	41-145 (6 yr)	28-159	0	0	4	2	0	0
MO-04b AEEMP	24-43 (3 yr)	22-96	0	0	2	1	0	0

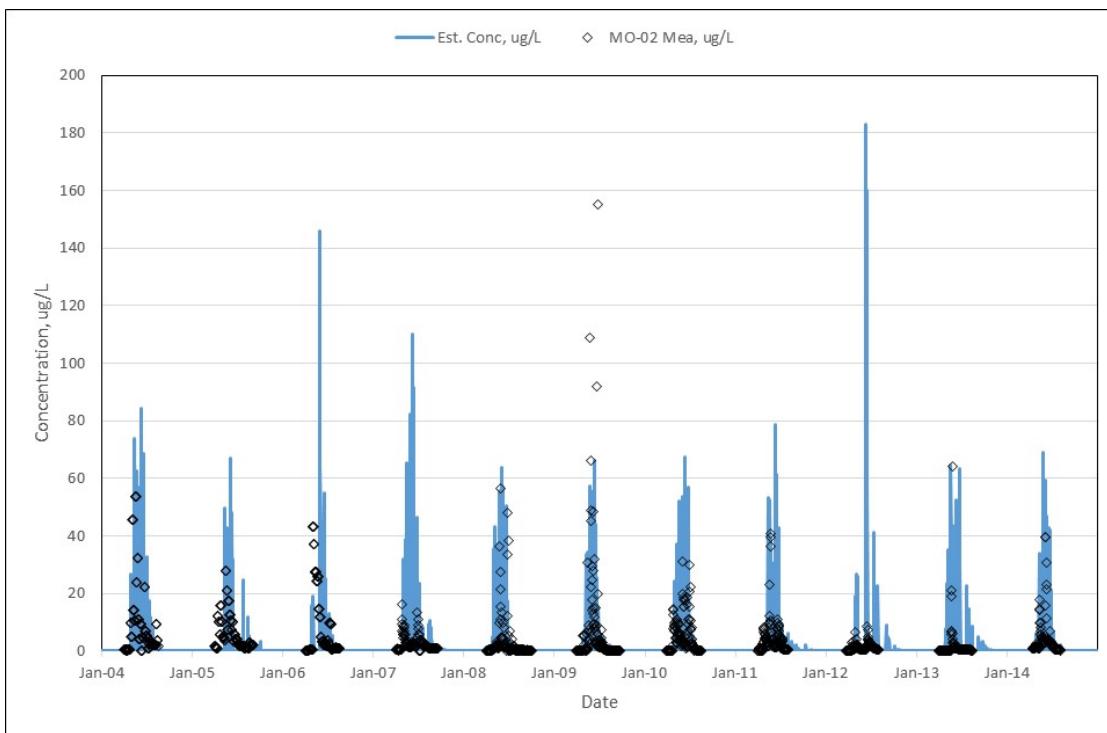
Monitoring Site	Range in Annual Maximum Concentrations (ug/L)		Number and % of site years underestimating measured annual maximums by a factor of			Number and % of site years overestimating measured annual maximums by a factor of		
	Measured	Modeled	>10X	5-10X	1-5X	1-5X	5-10X	>10X
MO-05 AEEMP	14-84 (6 yr)	61-193	0	0	0	4	1	1
MO-05b AEEMP	22-112 (5 yr)	49-139	0	0	1	4	1	0
MO-08 AEEMP	41-70 (5 yr)	53-179	0	0	2	3	0	0
All MO AEEMP			0 (0%)	0 (0%)	14 (22%)	31 (48%)	17 (26%)	3 (5%)
MO-16 res. AMP	0.5-5 (6 yr)	49-183	0	0	0	0	0	6
MO-17 river AMP	8-13 (6 yr)	17-54	0	0	0	6	0	0
MO-17 res. AMP	2-7 (6 yr)	16-94	0	0	0	1	1	4
MO-19 res. AMP	1-11 (6 yr)	46-136	0	0	0	1	1	4
MO-21 res. AMP	2-7 (4 yr)	36-147	0	0	0	0	1	3
All MO AMP			0 (0%)	0 (0%)	0 (0%)	8 (29%)	3 (11%)	17 (61%)
OH-04 AEEMP	12-16 (2 yr)	33-67	0	0	0	1	1	0
OH-10 river AMP	6-30 (9 yr)	27-63	0	0	0	7	2	0
OH-11 res AMP	0.5-8 (5 yr)	20-45	0	0	0	2	2	1
NCWQR Scioto R	3-15 (5 yr)	23-55	0	0	0	3	1	1
All OH			0 (0%)	0 (0%)	0 (0%)	13 (62%)	6 (29%)	2 (9%)
IN-10 AEEMP	12-16 (2 yr)	44-159	0	0	0	1	1	0
IN-04 river AMP	1-3 (9 yr)	41-154	0	0	0	0	0	9
IN-06 river AMP	3-26 (5 yr)	49-161	0	0	0	1	3	1
IN-07 river AMP	5-28 (9 yr)	39-91	0	0	0	4	4	1
IN-08 river AMP	6-21 (6 yr)	39-91	0	0	0	3	3	0
IN-13 river	2-20 (7 yr)	21-114	0	0	0	5	1	1
All IN			0 (0%)	0 (0%)	0 (0%)	14 (37%)	12 (32%)	12 (32%)

The model best met the evaluation criteria (Section 2.4.3) with the MO AEEMP monitoring sites. For these sites, the concentration patterns produced by SAM generally tracked the

patterns in measured concentrations (Figures 12 and 13). While annual maximum SAM estimates didn't always match maximum annual measured concentrations within a given year, the correspondence was generally reasonable, and the overall range in estimated annual-maximum concentrations overlapped the corresponding range in measured concentrations.



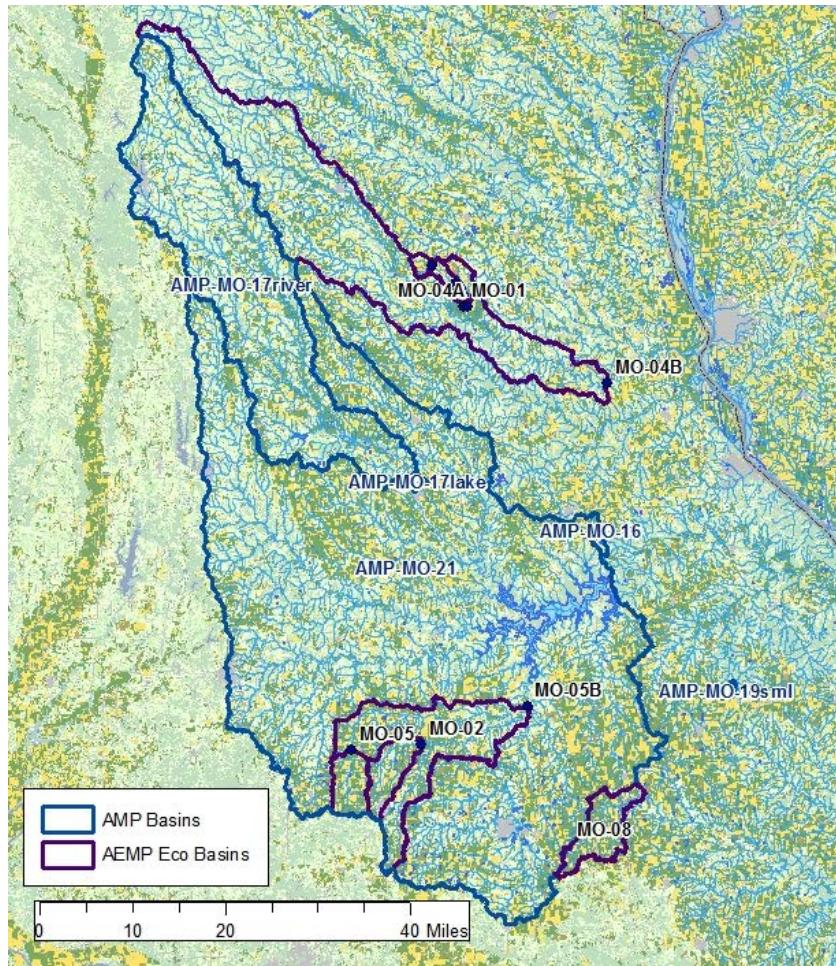
**Figure 12: Comparison of Estimated Concentrations of Atrazine from SAM with Measured Concentrations from the AEEMP MO-01 Site (NHD comid 4989415).**



**Figure 13: Comparison of Estimated Concentrations of Atrazine from SAM with Measured Concentrations from the AEEMP MO-02 Site (NHD comid 5042380).**

SAM estimates consistently exceeded monitored concentrations at the 5 AMP sites in MO, often by more than 10X (61% of site years). Estimated concentrations for the reservoir sites in Table 2 reflect the effective influent concentrations into the reservoirs rather than concentrations in the reservoir itself. SAM is designed to generate estimates for both lotic (flowing waters such as streams and rivers) and lentic (lakes, reservoirs, other impounded waters) waters. However, given the need to account for time of travel differences described below, USEPA OPP shifted the water volume processing for lentic waters to follow the convolution process described in Section 4.

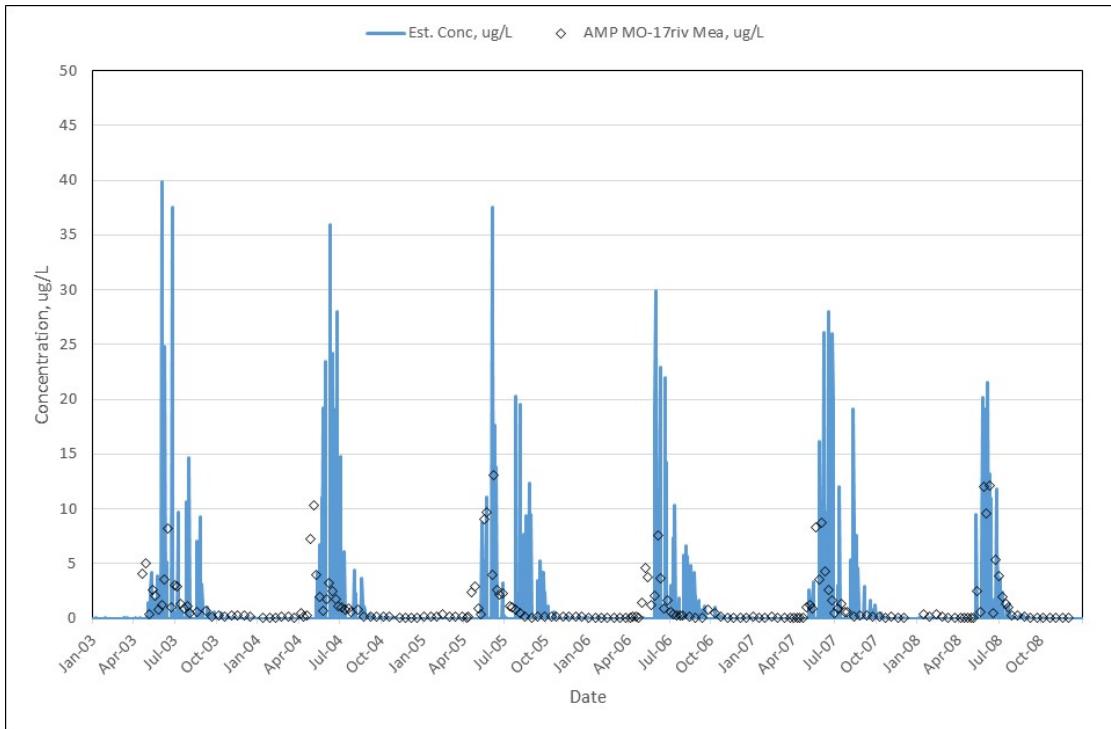
While SAM results also exceeded monitored concentrations at the IN and OH sites, the estimated annual maxima were within an order of magnitude for the majority of site years (Table 2). As discussed below, further examination of the model-monitoring comparisons and the monitoring sites and associated water body types and drainage areas (Figure 14) provides insights regarding the estimation errors.



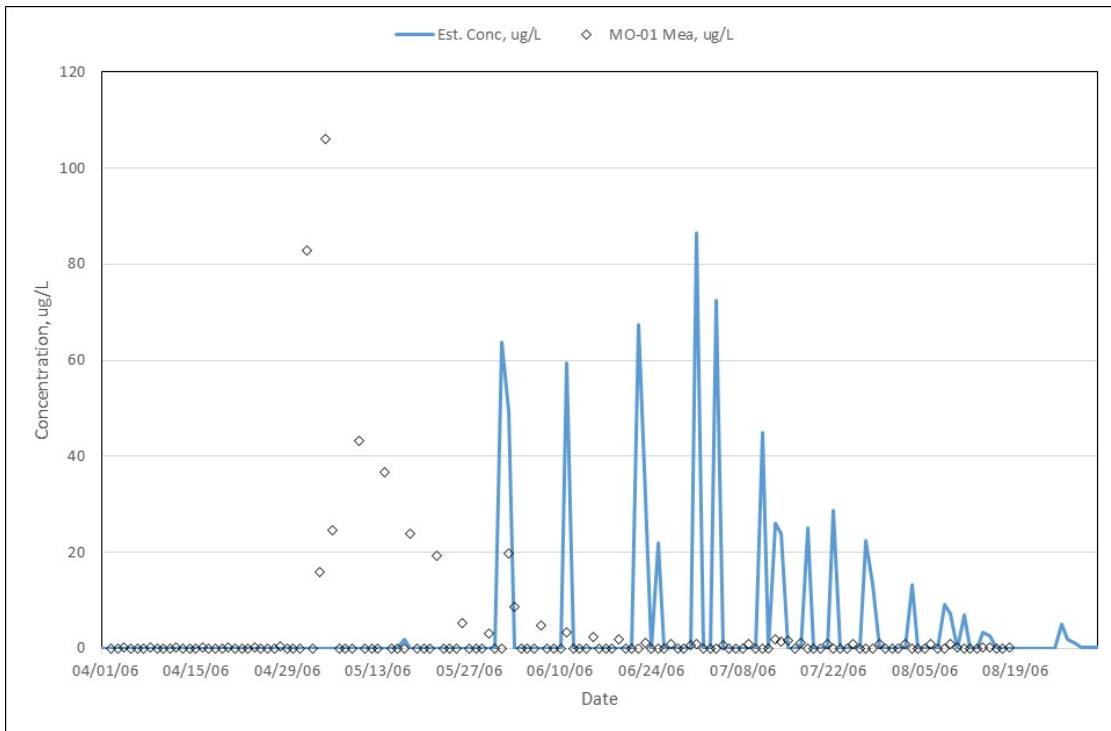
**Figure 14: Locations of the AEEMP and AMP Monitoring Sites within the Mark Twain Basin in Northeastern MO. The Underlying Land Cover Map Shows Corn (yellow) and Soybeans (dark green).**

These initial comparisons identified areas where model adjustments may improve concentration estimates:

- Results for larger watersheds, such as MO-17 river (Figure 15), overestimate concentrations to a greater degree (Appendix 2-D), suggesting potential for improvement by accounting for travel time related dispersive effects in larger watersheds.
- In some years, the timing of estimated concentrations from SAM does not coincide with that seen in monitoring data (Figure 16). The timing of pesticide runoff loading to water reflects timing of both applications and rain events. In cases when plantings (and related pre-emergent pesticide applications) begin earlier than usual due to an early warm spring, or later than usual due to a cold spring, the altered timing of pesticide applications would lead to different temporal concentration profiles in the water body.



**Figure 15: Comparison of Estimated Concentrations of Atrazine from SAM with Measured Concentrations from the AMP MO-17 Site (NHD comid 5641174).**



**Figure 16: Estimated Concentrations of Atrazine from SAM Occur Later than Measured Concentrations from the AEEMP MO-01 Site (comid 4989415) in 2006.**

Section 4 presents an approach USEPA OPP is exploring to address the influence of upstream lentic waters, and travel time related dispersive effects; section 5 presents approaches USEPA is exploring to address year-to-year variations in the timing of pesticide applications.

### 3 SAM Data Inputs

This section describes the national data sets for soil, land cover, weather, crop characteristics and management practices, and hydrology, and how these diverse data sets are organized as soil-land cover-weather combinations (scenarios) for inputs to the model and to reflect the spatial diversity in conditions. USEPA OPP is requesting the SAP to respond to the following questions related to data inputs:

- Q4.** To substantially lessen the number of scenarios and improve computational speed of the model, USEPA OPP evaluated the option of grouping soil map units into classes based on factors that have the greatest impact on pesticide loss due to runoff and erosion (USDA water quality index, described in Section 3.3). A comparison of runoff volume, pesticide mass, and pesticide concentration outputs showed little difference between the two approaches. ***Please comment on any implications for using soil grouping classes for watershed-scale modeling.***
- Q6.** In order to generate the soil-land cover-weather station scenarios needed for modeling, USEPA OPP took spatial data at different scales and re-gridded them to the same scale for aggregation (Section 3.2). Based on comparative testing of the model (Sections 2.4, 4.3, and 5.4), this appears to be a feasible approach. ***Please comment on the implications for aggregating spatial inputs across varying scales.***

The SAM model described in Section 2 uses scenarios that are created by intersecting soil map units from USDA's Soil Survey Geographic database (Section 3.1.1), general land cover/crop groups of the Cropland Data Layer (Section 3.1.2), and weather station grids generated from NOAA data (Section 3.1.3). Each of the spatial datasets described in Section 3.1 represents what USEPA OPP has determined to be the best nationally-available data for SAM. These data (and corresponding model frameworks) were chosen so that, as newer and/or improved datasets become available, they can be used in place of existing datasets.

As described in Section 3.2, USEPA OPP conceptually “stacks” the spatial data layers on top of each other, and then creates scenarios identified by the unique combinations of soil identification, weather station grid identification, and crop group value. An input table generated from this intersection of datasets provides model inputs for each scenario. These inputs are used by the Scenario Generator and Super PRZM Hydro components of SAM (Section 2.1).

To process model outputs for NHDPlus catchments or other drainage areas (such as HUC-12s), SAM employs “recipe” files that contain lists of scenarios and their corresponding areas within each catchment or drainage area being modeled (described in Section 3.2). SAM takes daily runoff and pesticide load values and aggregates them at the catchment pour point, based on the area represented by each scenario in a recipe.

Detailed documentation on input data sources and compilation are available in Appendices 3-A through 3-F. Section 3.3 contrasts the differences in model inputs and outputs between scenarios developed using individual soil map units and soil groupings based on USDA water quality index criteria (Lal and McKinney, 2012).

### 3.1 Data Inputs Used in SAM

USEPA OPP compiled spatial data for a twelve-state region (Figure 17) that encompasses the Ohio River Basin used in the initial model development and the three test basins (Figure 11), which were used for further model development and testing. Ultimately, USEPA OPP intends to expand the data compilation to a national scale. The scenarios used for SAM are derived from the spatial intersection of soil map units (Section 3.1.1), land cover classes (Section 3.1.2), and weather grids (Section 3.1.3). Other data inputs are spatially associated with these scenario components. The National Hydrography Database Plus version 2 (NHD+) provides catchment areas (both on NHD+ reach and HUC12/watershed boundary scales) and flow data used in the water body calculator, as described in Section 2.1.



**Figure 17: NHD Hydroregion 5, the Ohio River Basin, and Monitoring Site Locations.**

### **3.1.1 Soil-Related Inputs from SSURGO**

Soil-related inputs are available through the USDA's Natural Resources Conservation Service (NRCS) Soil Survey Geographic (SSURGO) database. In the standard aquatic exposure modeling approach currently used for regulatory decision making, USEPA OPP employs data for a single, runoff-prone (typically hydrologic group C or D) soil associated with a particular crop, corresponding to a soil-crop combination that occurs in the major crop-growing area. By contrast, in SAM OPP is using the entire soil coverage, with data including each soil map unit on which crops are grown.

USEPA obtained the gridded version of SSURGO (gSSURGO) for soil map unit boundaries and associated parameters from the USDA Geospatial Data Gateway<sup>12</sup>. The pixel resolution for the gridded product is ten (10 x 10, or 100 m<sup>2</sup>) meters.

SSURGO spatial data layers depict the extent of the soil map unit on the landscape. The spatial data include a map unit key (MUKEY) that links map units to soil data attributes.

Modifications to the gSSURGO tabular data extracts included:

1. converting units to those used in the SAM model,
2. calculating Universal Soil Loss Equation (USLE) slope/length (LS) values
3. processing soil horizon data to match SAM horizons, including generation of depth-weighted averages
4. replacing missing values, if needed, as described below
5. aggregating soil properties as described in Section 3.3

SSURGO map units can have one to three major components and a number of minor components. The SSURGO data provide a range and representative percentage of each component in each map unit. The presence of multiple components in a map unit reflects both the degree to which differing soils can be distinguished in the field and the scale of the map. For SAM, USEPA OPP generally selected the major component consisting of the greatest percentage of the map unit. However, if the major component did not include all of the soil-derived data required for model inputs, then USEPA OPP selected the highest-percentage component that did include a complete set of these values. In instances when one or more major components made up an equal percentage of the map unit, USEPA OPP selected components according to hydrologic soil group in order from more to less prone to runoff: D > C > B > A.

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<sup>12</sup> Available at <https://gdg.sc.egov.usda.gov/>. The 2015 Gridded Soil Survey Geographic (gSSURGO) database, derived from a December 1, 2014, snapshot of the Soil Data Mart database, was released on February 23, 2015 (FY2015 Soil Survey Geographic Database or SSURGO source).

The SSURGO database includes non-soil map units such as quarries, pits, mines, etc., that do not contain data. For this version of SAM, such non-soil map units were not included in scenario input datasets or in watershed recipe files. USEPA OPP plans to develop systematic rules for distinguishing non-soil units that might contribute runoff to surface waters (such as unidentified urban/ developed map units) from units that are less likely to contribute runoff (such as quarries and pits).

### **3.1.2 Crop/Land Cover from the Cropland Data Layer (CDL)**

USDA NASS's Cropland Data Layer (CDL) provides detailed spatial distributions of numerous crops using satellite imagery<sup>13</sup>. The CDL offers cropland coverage for the 48 contiguous states from 2008 to the present. This provides USEPA OPP with the opportunity to use multiple years of CDL data to determine cropping patterns and to capture year-to-year variations in crop practices. Because 2008-09 CDL data are provided at 56-m pixel size while subsequent data are available at 30-m (30x30, or 900 m<sup>2</sup>) pixel resolution, USEPA OPP began with the 2010 CDL data; this SAP version of SAM uses CDL data for four years, through 2013. Additional years of land cover can be added as they become available. To generate scenario combinations for SAM (see Section 3.2), USEPA OPP intersected SSURGO soil map units with each year of CDL coverage separately. This resulted in four sets of watershed recipes, one for each year of CDL.

While the CDL identifies 111 agricultural land classes and 133 total land classes, not all of these land classes are equally reliable. Accuracy assessments documented by USDA NASS on a state-by-state basis show that the CDL is relatively accurate (90% or greater) for major commodity crops, such as corn, soybeans, wheat, and cotton, which are grown over extensive contiguous areas, and for which the USDA has sufficient independent data for training and quality assurance analysis<sup>14</sup>. However, a high frequency of error for a number of crops suggests that the CDL may not be suitable for representing minor crops such as individual vegetables or orchards.

As an alternative, USEPA OPP is exploring ways to group some of these minor crops together. Viable crop groupings should account for agricultural similarities, likely rotations, and the ability of the CDL to differentiate among crop signals from remotely sensed imagery. Ideally, the crop groups would be sufficient to distinguish major commodity crops (such as corn, soybeans, wheat, and cotton), as well as reasonably distinct crop groupings (such as vegetables, orchards, vineyards, grain crops, row crops, and total cultivated crops). They should also be sufficient to identify the general agricultural and non-agricultural land classes used for deriving curve numbers based on USDA NRCS (2008b) guidance: fallow, row crop, small grain, close-seeded

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<sup>13</sup> National CDL coverage for 2008-2014 is available for download from the USDA NASS site at <http://www.nass.usda.gov/research/Cropland/SARS1a.htm>.

<sup>14</sup> The description of NASS's accuracy assessment is available at <http://www.nass.usda.gov/research/Cropland/Method/cropland.pdf>. Metadata that include error analysis are available for download at <http://www.nass.usda.gov/research/Cropland/metadata/meta.htm>.

legume or rotation meadow, pasture/grassland/range, orchard [woods-grass], woods, brush/weed/grass, meadow, various developed/ residential intensities.

The current land class groupings are described in Appendix 3-B. The general land cover class groupings that are relevant to the Ohio River Basin/test basins are described below.

**Corn:** Includes corn and those double-cropped classes (corn with wheat, soybeans, or other grains) with corn in the rotation.

**Soybeans:** Includes soybeans and those double-cropped classes (soybeans with corn, cotton, wheat, or other grains) with soybeans in the rotation.

**Wheat:** Includes durum, spring, and winter wheat classes, along with those double-cropped classes (wheat with corn, cotton, soybeans, other grains, or vegetables) with wheat in the rotation.

**Vegetable and ground fruit:** This pulls together individual all of the vegetable crops, which have low accuracy rates in CDL. It also includes ground fruit which, while using different cultivation patterns, aren't well distinguished from surrounding vegetable (or other) land classes.

**Orchards and vineyards:** This includes all nut and fruit trees, citrus crops, and grape vineyards. Crops in this group have a relatively high error rate. A number of orchard areas are often misidentified as pasture, grassland or pasture (presumably the grass lanes between tree rows contribute more to the optical signal than do the trees), shrubland, or forest.

**Other grains:** This includes all small grain crops other than wheat.

**Pasture/hay/forage:** This includes specific hay crops, such as alfalfa, clover, and vetch, and general pasture, hay, and forage classes. It also includes the grassland class, which may include pasture land in some parts of the country.

**Forest:** This merges deciduous, evergreen, and mixed forest classes, along with more generic forest classes.

**Grassland** and **Shrubland** classes remain separate because they fall into different land cover types for curve number determination.

**Developed** categories (open; low, medium, and high intensity) were kept separate because the intensity differences can be used to estimate turf area and relative impervious surface area and curve number determination also depends on intensity of development.

**Wetlands:** Herbaceous and wetlands were kept as separate groups because of differences in curve number determinations.

### 3.1.3 Weather Data

Currently, USEPA OPP's aquatic exposure models use SAMSON (Solar and Meteorological Surface Observation Network) weather station data, publically available from NOAA's National Climatic Data Center (NCDC). SAMSON provides daily precipitation, pan evaporation, solar

radiation, temperature, and wind speed required for aquatic exposure models, for 237 National Weather Service (NWS) locations, spanning the years 1961 to 1990. The SAMSON dataset was originally developed by NOAA's NCDC and USEPA's National Exposure Research Laboratory (NREL), but is no longer maintained and will not be updated in the future.

SAM uses publically available gridded meteorological datasets that provide a source of updated daily weather data at uniform spatial resolution across the country, for a wide variety of meteorological variables. The attributes of gridded datasets, characterized by continuous and uniform spatial densities, are thought to be optimal for the spatial computational approach to pesticide fate and transport modeling in SAM. The gridded meteorological dataset used to evaluate SAM's performance was developed from the following sources maintained by NOAA: Unified Gauge-Based Analysis of Daily Precipitation from the Climate Prediction Center (CPC) (NOAA ESRL, 2014) and Reanalysis Data from the National Centers for Environmental Prediction (NCEP). Both datasets provide national gridded weather analyses available between 1948 and the present day (Kalnay et al., 1996; NCEP/NCAR, 2014). Together, these two sources provide all the weather inputs needed for SAM.

The NCEP/NCAR and CPC analyses are actively maintained by NOAA, and continue to be extended to the present day, as of this writing. As a result, the compiled dataset can be easily expanded as needed with the most recent NCEP/NCAR and CPC daily values as they become available.

SAM requires precipitation, temperature, wind speed, solar radiation, and potential evapotranspiration. Table 3 lists the variables within each dataset from NOAA used in deriving the SAM computational weather gridded dataset.

**Table 3: Weather variables from NOAA NCEP/NCAR Reanalysis and NOAA CPC Unified Rain Gauge Analysis.**

NOAA NCEP/NCAR Reanalysis (global)	NOAA CPC Unified Rain Gauge Analysis (US)
Air temperature at 2m <sup>a</sup> Maximum air temperature at 2m <sup>a</sup> Minimum air temperature at 2m <sup>a</sup> Zonal wind speed at 10 m <sup>a</sup> Meridional wind speed at 10 m <sup>a</sup> Downward solar radiation flux at surface <sup>a</sup> Downward solar radiation flux at nominal top of atmosphere (NTAT) <sup>b</sup>	Daily Total Precipitation <sup>c</sup>

<sup>a</sup> Available: <http://www.esrl.noaa.gov/psd/data/gridded/data.ncep.reanalysis.surfaceflux.html>  
NCEP/NCAR Reanalysis 1 data provided by NOAA/OAR/ESRL PSD, Boulder, Colorado, USA

<sup>b</sup> Available: [http://www.esrl.noaa.gov/psd/data/gridded/data.ncep.reanalysis.other\\_flux.html](http://www.esrl.noaa.gov/psd/data/gridded/data.ncep.reanalysis.other_flux.html)  
NCEP/NCAR Reanalysis 1 data provided by NOAA/OAR/ESRL PSD, Boulder, Colorado, USA

<sup>c</sup> Available: <http://www.esrl.noaa.gov/psd/data/gridded/data.unified.daily.conus.html> (1984 – 2006);  
<http://www.esrl.noaa.gov/psd/data/gridded/data.unified.daily.conus.rt.html> (2007 – 2014)  
CPC US Unified Precipitation data provided by NOAA/OAR/ESRL PSD, Boulder, Colorado, USA

The NCEP Reanalysis data are available at  $2.5 \times 2.5$  degree grid resolution; the CPC data are at  $0.25 \times 0.25$  degree US grid resolution. To combine the CPC precipitation data with the NCEP Reanalysis meteorological fields for use in SAM, the SAM computational weather gridded dataset was produced by re-gridding the coarser-scale NCEP data to the finer grid resolution of the CPC precipitation ( $0.25^\circ \times 0.25^\circ$ ). Daily potential evapotranspiration (not offered explicitly by the NOAA gridded datasets) was derived using NOAA NCEP/NCAR Reanalysis daily mean temperature, daily minimum and maximum temperatures, and downward solar radiation at the nominal top of the atmosphere. A more detailed methodology for the development of the processing of the NOAA meteorological parameters and the development of the final computation weather grid for SAM is provided in Appendix 3-C. This compiled dataset was used as input to the pre-processed scenarios for the example simulations discussed in this document. An evaluation and comparison of this fine-scale meteorological computation gridded dataset for SAM to the existing SAMSON dataset shows similar magnitudes and meteorological trends. This evaluation is provided in Appendix 3-C.

### **3.1.4 Crop Data Collection and Processing**

As noted in Section 2.3 and Appendix 3-A, key crop-related inputs needed for SAM are planting and harvesting dates (both to provide a reference point for pesticide applications and to simulate canopy cover), maximum canopy cover and crop intercept (for rainfall and pesticide applications), depth of the active rooting zone (to define the zone of water extraction from soil), and crop-specific USLE inputs.

USEPA OPP made use of available USDA publications to obtain key agricultural crop stage dates – active planting and harvesting dates for field crops (USDA NASS, 2010) and vegetables (USDA NASS, 2007) and blooming and harvesting dates for fruits and tree nuts (USDA NASS, 2006). These date ranges represent variations in time over individual states. USEPA OPP explored using the USDA Plant Hardiness Zone (PHZ) Map<sup>15</sup> to split up the range in planting, harvesting, and blooming dates in geographic subdivisions within each state.

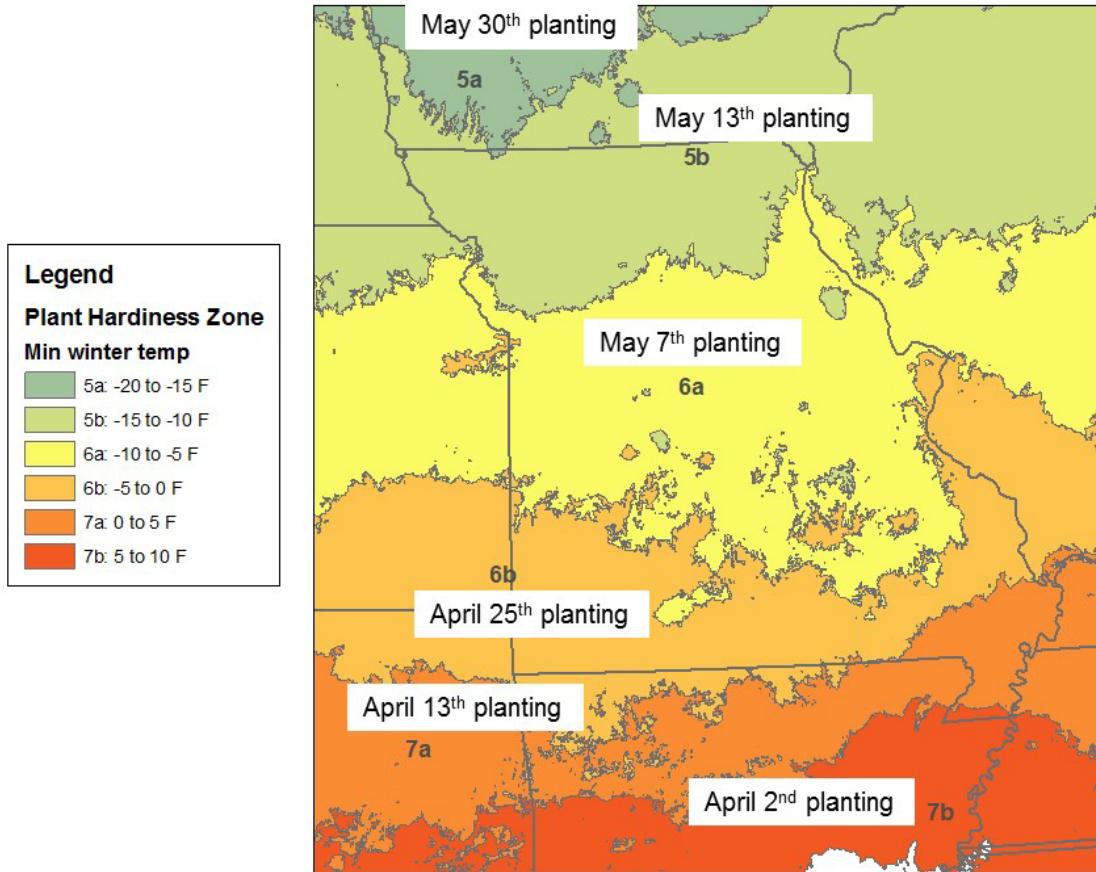
Figure 18 illustrates the approach used to divide the beginning of the corn planting range for a single state (in this case, MO) by the plant hardiness zones (PHZ) within that state. The beginning of the range in planting dates was assigned to the warmest PHZ; the initial planting date was then adjusted to progressively later dates through increasingly colder PHZs. A similar proportioning was done for the end dates in the plant range, as well as for harvest dates. Appendix 3-D summarizes the date ranges for the dominant agricultural crops found in the pilot project study region.

The PHZ map is simply used to proportion the ranges in crop milestone dates within states, as reported in the USDA publications. Since these publications do not provide year-to-year data,

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<sup>15</sup> The 2012 USDA Plant Hardiness Zone (PHZ) Map is available at <http://planthardiness.ars.usda.gov/PHZMWeb/>

USEPA OPP is exploring alternative methods for capturing both spatial and temporal variations in crop planting and harvesting dates, and other stages (see Section 5).



**Figure 18: Illustration of the Method Used to Proportion the Beginning of the Corn Planting Date for MO Across Plant Hardiness Zones.**

Additional crop-related inputs related to canopy cover, rainfall interception, active rooting depth, and USLE factors (Appendix 3-A) have been collected from a variety of sources, including the PRZM Manual (Carousel et al, 2005), existing USEPA OPP standard crop scenarios<sup>16</sup>, and USDA Crop Profiles<sup>17</sup>. Appendix 3-D also includes data compiled for the major crops in the pilot project, published planting and harvesting dates, and crop class relations between CDL and NASS crop date publications. Such data will be updated as additional data sources are found.

<sup>16</sup> The individual crop scenarios are imbedded in the SWCC currently used by USEPA OPP. Data and documentation for the scenarios have been archived in [http://www.epa.gov/oppefed1/models/water/water\\_models\\_archive.htm](http://www.epa.gov/oppefed1/models/water/water_models_archive.htm) and can be downloaded from links under the “PRZM/EXAMS SHELL – Superseded” section.

<sup>17</sup> Crop profiles, with descriptions of crop production and pesticide management practices, can be found in links provided by the National Integrated Pest Management (IPM) Centers: <http://www.ipmcenters.org/cropprofiles/>

### 3.1.5 National Hydrography Dataset (NHDPlus, Version 2.0)

The National Hydrography Dataset is a national spatial data set widely used as a framework for mapping and analyzing hydrologic information. The NHDPlus<sup>18</sup> is a USEPA data product that provides value-added information to a “snapshot” (taken April 2010) of the NHD, including stream catchment delineations and stream flow-related information. As noted in Section 2.1, USEPA OPP used the NHDplus for river/stream networks, water bodies, watershed boundaries (HUC12 and reach catchments), and the hydrology data associated with these features. The NHDplus provides the best available data, at a national scale, on stream networks, flow data and flow direction, and associated drainage areas for use in modeling.

Pesticide concentration calculations for rapidly-flowing (lotic) water bodies require estimates of cross-sectional area orthogonal to the direction of flow, to enable calculation of the volume of the pour point mixing cell (Section 2). NHDPlus Version 2 provides monthly mean streamflow and velocity estimates for each reach that can be used to generate such values with the following equation:

$$Area_x = \frac{FLOW}{VELOCITY} = \text{mean cross-sectional area for the reach}$$

For use in SAM, USEPA OPP employed flow and velocity estimates generated by the Enhanced Unit Runoff Method (EROM, see McKay et al, 2012, for information):

Mean flow = Q0001E, which represents the best estimate of streamflow, reported in ft<sup>3</sup>/s (cfs)

Mean velocity = V001E, which represents the best estimate of velocity, reported in ft/s

The mean cross-sectional area, converting from ft<sup>2</sup> to m<sup>2</sup>, is calculated as:

$$A_x = \left( \frac{Q0001E, \text{ ft}^3/\text{s}}{V0001E, \text{ f/s}} \right) x \left( \frac{\text{m}^2}{10.7639 \text{ ft}^2} \right) = \text{mean cross-sectional area (m}^2\text{) for the reach}$$

The relevant flow and velocity data were collected by identifying the most-downstream (highest hydrologic sequence) NHDplus reach to intersect the boundary of the watershed or HUC-12 of interest. Reach mixing cell volume was calculated as the product of reach cross-sectional area and a representative mixing length.

For lentic receiving waters (e.g., lakes, reservoirs), USEPA OPP used preliminary volume estimates developed by USEPA ORD’s Atlantic Ecology Division. Although the dataset, which provides estimates of lake depth and volume has not been finalized or publically released, the methods used to calculate the estimates are similar to those documented in Hollister and Milstead (2010), and Hollister et al. (2011).

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<sup>18</sup> Version 2 of NHDplus is available for download at [http://www.horizon-systems.com/nhdplus/NHDPlusV2\\_home.php](http://www.horizon-systems.com/nhdplus/NHDPlusV2_home.php).

## **3.2 Creating Scenarios, Input Data, and Watershed Recipes**

Scenarios used for modeling were created by intersecting soil map units, general land cover/crop groups of the CDL, and weather station grids (Figure 6). The resulting scenarios are identified by unique combinations of soil identification, weather station grid identification, and crop group value.

### **3.2.1 Creating Scenarios**

Scenarios were created from the intersection of SSURGO soil map units or groupings, weather station grids, and general crop groups of the CDL, based on a reclassification of the CDL classes into general land cover classes.

The data sources that define the spatial extent of a scenario are published in varying spatial resolutions. The weather data has a pixel size of 0.25 X 0.25 degree (or approximately 15 km<sup>2</sup>), the CDL has a pixel resolution of 30 m (30x30, or 900 m<sup>2</sup>), and the gridded SSURGO is at 10 m resolution (10x10, or 100 m<sup>2</sup>). The variation in pixel resolution creates the potential for generating unrealistic scenarios, for example a corn pixel that crosses over a shoreline to overlap with open water. The extent of such unrealistic scenarios is expected to be relatively small, likely < %1 of watershed area. Where identified, these were omitted from recipes.

Differing spatial resolutions will likely impact modeling results, although quantifying the impact of this effect may be difficult, and has not yet been attempted.

For the current effort, all spatial data layers were resampled to 10 meter resolution raster images for ease of processing. USEPA OPP used ESRI's Spatial Analyst toolbox to generate a list of individual scenarios from unique combinations of the three component raster layers. ESRI's "Combine" tool was used to generate sets of unique combinations of soil, weather and crop, with a unique key field created to identify each such combination. A new raster layer was thus created and classified to represent the combined (scenario) data. All of the remaining SAM inputs for running each scenario are obtained using information linked to one or more of the three underlying identifiers.

Scenario input data, described in Appendix 3-A, were gathered into a matrix using a spreadsheet template (listing all of the required model inputs in the correct order) using Python scripts. The scenario IDs, along with soil, weather grid, and general land cover class identifiers, were added to the template for reference.

All of the soil data (in Appendix 3-A) are linked to the scenarios through the MUKEY (soil map unit identifier). For the soil grouping classes (see Section 3.3), the input values represent the mean for all of the individual soil map units that fall into each soil class.

One of the major drivers in SAM (Section 2.3.2) is the curve number, values of which are based on major hydrologic soil group and land cover class (see Appendix 3-E). Curve numbers for both cropped and fallow conditions were assigned to each scenario using a script written in Python based on the tables in Appendix 3-E.

Crop-related inputs (rainfall intercept, maximum canopy cover, USLE C factors, and maximum active rooting depth) were joined to the scenarios by general land cover class.

Plant, bloom, and harvest dates in the crop input database were linked to the scenarios by a State-Plant Hardiness Zone-CDL group field. To create the link in the scenario matrix, OPP assigned a state and USDA Plant Hardiness Zone (PHZ) to each of the weather station grids using a spatial join in ArcGIS, linked this to each scenario using the weather station ID, and then created an equivalent state-PHZ-CDL group field based on the general crop cover for the scenario. Plant, bloom, and harvest dates were then able to be joined by the common State-Plant Hardiness Zone-CDL group field.

### **3.2.2 Generating Watershed Recipe Files**

Watershed recipe files consist of a list of scenarios that fall within each watershed or drainage area, along with the area associated with each scenario. The summed area of the individual scenarios is thus equal to the watershed area. Recipe files have been generated for HUC-12s (used in the alpha model on the übertool site), NHDPlus catchments, and monitoring site watersheds. USEPA OPP plans to use recipes for each individual NHDPlus catchment to estimate runoff volume and pesticide mass loadings contributed by each catchment across the contiguous “lower 48” states. NHDPlus catchments are the finest-resolution surface drainage area dataset available nationally, and represent the drainage area for a single stream reach segment or waterbody at the resolution of the NHD dataset. The contributions from each catchment are aggregated to represent whole watersheds, and may be manipulated mathematically using a process described in Section 4 to allow for a fuller accounting of watershed hydrology and the influences of constituent travel time (from field edge to pour point) heterogeneity on temporal concentration dynamics.

The recipe files for each HUC12, NHD+ catchment, and select monitoring basins were generated using a python script and the combination soil-land cover-weather grid raster layer described earlier. Using the raster layer’s attribute table, unique combinations were translated into scenario IDs based on soil, weather and CDL identification keys. Area estimates were derived for pixel counts included in the combination layer. Each drainage area or watershed has separate recipe files that reflect each of the years of CDL coverage.

## **3.3 Soil Grouping Classes Based on USDA Soil Water Quality Index Groupings**

Because the potential number of individual soil map unit-crop group-weather station combinations would run in the tens of millions, USEPA OPP explored the feasibility of grouping soil map units into classes based on factors that have the greatest impact on pesticide loss due to runoff and erosion, similar to approaches used by the European Union (Schneider et al, 2007). A reduction in the number of scenarios that would need to be stored and processed would have an impact on the amount of storage space that would be required for SAM on a

national scale and on the amount of computer processing time that would be needed for running national-scale risk assessments on a routine basis.

USEPA OPP evaluated grouping individual soil map units into classes based on a USDA NRCS Water Quality Index (WQI) for runoff from agricultural fields (Lal and McKinney, 2012). The WQI used the following grouping classes to derive a WQI for each soil:

- Runoff potential based on **Hydrologic Soil Group (HSG)**: A, B, C, D
- **Slope gradient**: <2%, 2-5%, 5-10%, 10-15%, >15%
- Soil erodibility potential based on **K factor**: <0.10, 0.11-0.20, 0.21-0.32, 0.33-0.43, 0.44-0.64
- **Soil Organic Matter (SOM) content** (surface layer): <0.5%, 0.5-2%, 2-4%, 4-6%, 6-8%, >8%

These grouping class combinations result in a potential of 600 soil group classes:

$$4 \text{ HSG} \times 5 \text{ slope classes} \times 5 \text{ soil erodibility classes} \times 6 \text{ SOM classes}$$

For a given pesticide, the amount that may move from a field to off-field surface water is affected by the vulnerability of the soil to runoff (represented by the curve number in the model) and/or erosion (reflected by the K factor, slope, and associated USLE parameters) and how much pesticide is retained by the soil (reflected largely by the SOM content of the surface layer). Because the grouping classes preserve the hydrologic soil group classification, the curve number for the resulting soil group scenarios will not change. Variations in SOM (represented as soil organic carbon content in the model inputs) are limited to 2% OM (or 1.16% OC) increments.

Variations in slope as a function of slope gradient classes may be limited because soil map units are split out in slope classes that are similar to the class breaks above; the biggest change will be for steeper slopes (>15%). However, agriculture is generally limited on such steeper slopes. Variations in sediment transport are limited by the range in K factor values for each class. Other USLE input parameters, such as the slope/length, or LS, factor, and associated crop and management practice factors, would vary within the limits of the slope-K factor classes.

The soil map units in the pilot project area (Ohio River basin) were classified into HSG-slope-erodibility-SOM classes. Appendix 3-F provides a cross-reference between the individual soil map units (MUKEY) and the new soil classes derived from the WQI groupings (SoilClass1).

These soil group classes were combined with the CDL land cover classes and weather station grids to create unique soil-land cover-weather station scenarios for the pilot project area.

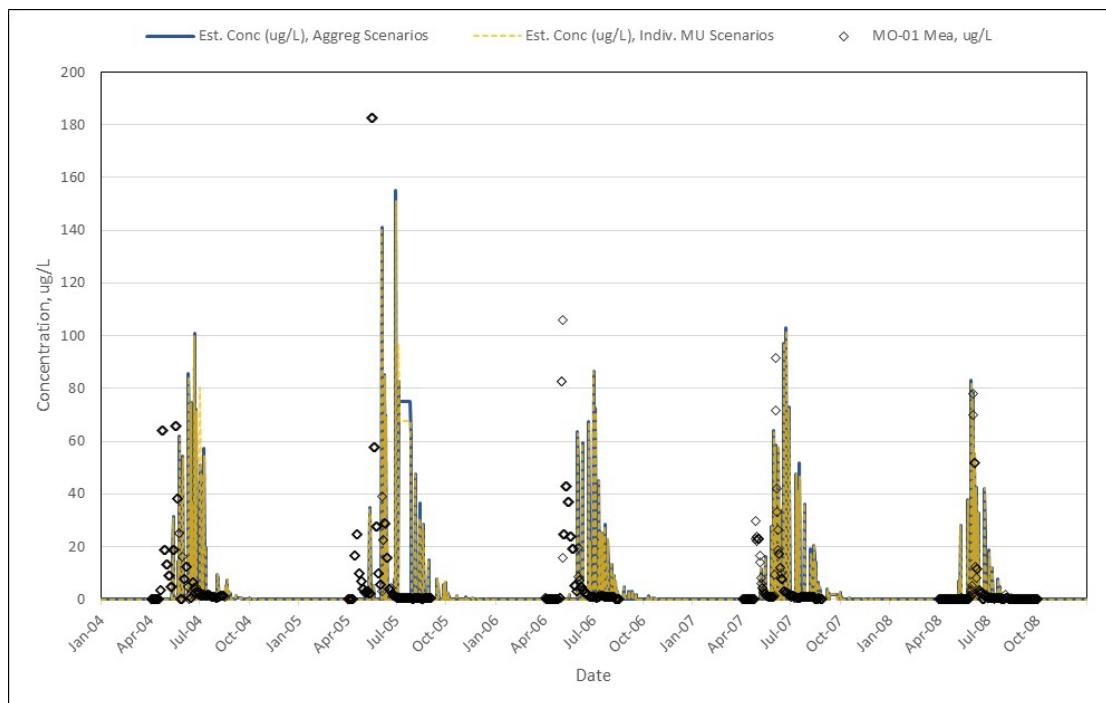
USEPA OPP generated scenarios based on individual soil map units (individual MU scenarios) and on the resulting aggregation of soils into the water quality criteria (aggregated soil scenarios) for the test basins used for this evaluation. Test evaluations covered 15 years of weather data (2000-2014).

USEPA OPP compared the annual total runoff volume, pesticide mass runoff loss, and maximum annual concentrations over the 15 years of simulations in each test basin (Appendix 3-F).

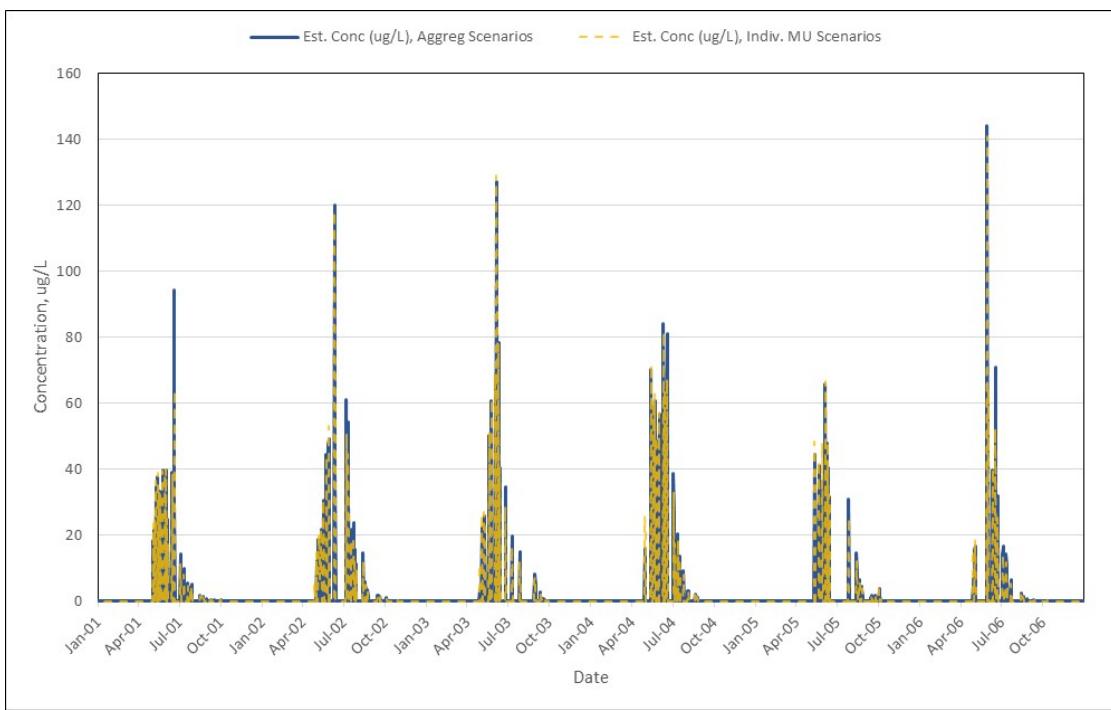
Total annual runoff in all of the test basins was within 1% of that generated based on non-grouped soil units. This suggests that the differences between scenarios based on individual soil map units and those based on soil groupings had negligible impact on the curve number that drives runoff. This was expected since soil aggregation preserved the Hydrologic Soil Group designation, which is one of the key components in curve number determination.

The total annual pesticide mass lost was within 2% of that generated based on non-grouped soil units for all of the test basins. This suggests that soil grouping had minimal impact on pesticide mass lost over the duration of the application period. However, some variations may occur with individual events, which would be reflected in pesticide concentrations. Estimated annual maximum concentrations were within 5% of each other in 11 of the 15 basins and within 10% in 11 of the 12 basins. The MO-02 site showed the greatest difference in estimated maximum concentrations, with estimates generated using scenarios based on aggregated soil groupings more than 10% greater than estimates from individual map units in 3 of 15 model years.

Visual comparison of plots of estimated concentration distributions over time (Figure 19) for the two scenario approaches (individual map units and aggregated soil groups) shows nearly identical patterns, for most test basin sites and years. Figure 20 shows the difference between the results using the two methods, for the years with greatest variability. Even for these sites, the majority of estimated peak concentrations are in close agreement.



**Figure 19: Comparison of Estimated Atrazine Concentrations Using Individual Soil Map Unit (blue) or Aggregated Soil Group (yellow dash) Scenarios for MO-01 (NHD comid 4989415).**



**Figure 20: Comparison of Estimated Atrazine Concentrations Using Individual Soil Map Unit (blue) or Aggregated Soil Group (yellow dash) Scenarios for MO-02.**

## 4 Accounting for Time of Travel and Downstream Accumulations

In initial SAM evaluations (Section 2.4), USEPA OPP noted that SAM outputs overestimated pesticide concentrations in comparison to measured (monitoring) data for the sampling sites that draw from larger watersheds, indicating the need to account for differences in time of travel for pesticide mass across larger watersheds. This section provides a description of USEPA OPP's proposed approach for addressing time of travel differences using convolution, in support of the following charge questions to the SAP:

- Q6.** As described in Sections 4.1 and 4.2, USEPA OPP has evaluated an approach for representing concentrations at the pour points of drainage networks that involves aggregating upstream drainage areas into integer-day stream travel-time zones, and the use of mathematical convolution to represent in-stream dispersive spreading of both influent runoff volumes and pesticide masses. *Please comment on the use of this approach, and on any modifications or alternative approaches that USEPA OPP might consider for accomplishing the same ends.*
- Q7.** USEPA OPP has not yet investigated possible adaptations of the approach referred to in Question 6 to simulate reactive and/or sorbing chemicals. Please comment on the potential for modifying this approach to simulate such chemicals.
- Given the risk assessment purpose of SAM, *please comment on the applicability of the described approach in dual-compartment (aqueous and benthos) systems for representing chemical decay and sorption during transport in surface waters across a range of spatial scales.*
  - Please recommend any watershed-scale monitoring datasets that may be suitable for use in evaluating estimated concentrations of pesticides that sorb non-negligibly to sediment, and any possible sources of data for representing the benthic sediment layer in surface waters throughout the country.*

Section 4.1 provides more depth to the approach for accumulating runoff volumes and pesticide mass loadings by watershed using a simple watershed recipes described in Section 2.1. It also notes where the model greatly overestimates pesticide concentrations in comparison to measured concentrations. Section 4.2 describes the proposed approach to address this issue. Section 4.3 provides initial comparisons between the proposed model improvement, the current approach, and monitoring data.

### 4.1 “Instantaneous” Approach Used in the Initial Version of SAM

As described in Section 2.1, SAM generates daily time series of area-normalized runoff (water) volume and runoff-entrained pesticide mass transported from the land to the water for each “scenario” (i.e., soil/land cover class/weather combination). Recipe files specify the land areas

of the scenarios that together comprise each hydrologic unit or drainage area (e.g., HUC-12, NHDPlus catchment, or monitoring basin). SAM uses these recipe files to weight the simulated hydrologic and pesticide mass time series by each scenario's contributing area, then sums the results to produce net time series representing total runoff water and pesticide loading contributed by the drainage area.

At a particular pour point, pesticide load is assumed to enter the receiving water body instantaneously at the beginning of the time step. Receiving water bodies are of two basic types: lotic (streams, rivers) and lentic (lakes, reservoirs). Because these are the simplest possible representations, both types are assumed to be completely mixed and in steady flow during the time step. First-order wash-out thus occurs, and mean concentration  $\bar{C}$  during the time step (in the absence of decay or sorption) is given by:

$$\bar{C} = \frac{M}{Q} (1 - e^{-Q/V})$$

or

$$\bar{C} = \frac{M}{Q} (1 - e^{-1/\tau})$$

where  $M$  is influent pesticide mass,  $V$  is water volume of the water body,  $Q$  is the volume of water that passes through the water body during one time step (*i.e.*, daily flow volume), and  $\tau$  is hydraulic mean residence time. It can be shown that when  $\tau \ll 1$  day,  $\bar{C} \approx \frac{M}{Q}$ , and that when  $\tau \gg 1$  day,  $\bar{C} \approx \frac{M}{V}$ .

Although lentic water body volumes were not used in the model comparisons in Section 2.4, SAM can estimate pesticide concentrations in lakes, reservoirs, and other lentic waters using water body volume estimates derived by USEPA ORD's Atlantic Ecology Division. The methods are similar to those documented in Hollister and Milstead (2010) and Hollister et al. (2011).

SAM derives lotic water body pour point volumes from tabulated NHDPlus reach monthly mean flows and velocities, and daily runoff volumes generated by PRZM Hydro. Daily flow is divided by velocity to produce daily-varying reach cross-sectional area, which together with representative mixing cell length specifies a daily-varying reach water volume ( $V$ ).

Representative mixing cell length is assumed to be 40 m, which is based on typical longitudinal dispersivities (the rationale being that this is a length below which it would not be hypothetically possible to simulate advection-dispersion using a finite-difference approach, and thus in effect the ultimate spatial limit of resolution for representing Fickian longitudinal dispersion) measured in rivers (Fischer, 1979; Rutherford, 1994).

The alpha version of SAM processes watershed-water body pairs one at a time, as if they existed in isolation from each other. In doing so, certain mixing processes are inevitably ignored that may be relevant to the accuracy of concentration calculation, including longitudinal

dispersive effects (peak spreading and flattening) and differential arrival times at the pour point, of solute pulses that originate from different upstream travel distances/times (peak de-synchronization).

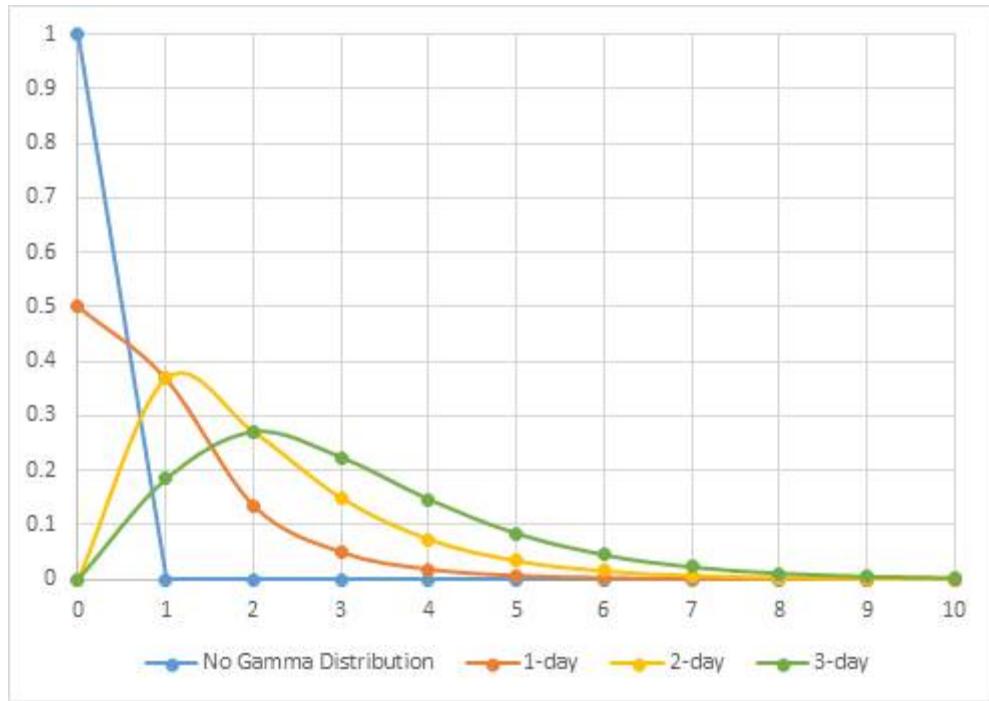
In its initial “alpha” implementation, SAM treats each HUC-12/water body pair as if they constituted essentially a headwater system: hydrologic and pollutant loads originating from upstream of the HUC12 are simply ignored. A more thorough approach considers hydrologic and pesticide loadings originating from throughout the entirety of a pour point location’s catchment. This approach is expected in general to generate higher-accuracy estimates and, indeed as documented in Section 2.4, appears to reasonably represent peak atrazine concentrations in example comparisons against monitoring data. However even this more thorough approach entails conceptual weaknesses that may tend to systematically distort results at some kinds of locations. In addition to previously-mentioned dispersive and peak de-synchronization effects, errors are likely to be introduced by the fact that SAM only accounts for the hydraulic properties of the water body at the pour point. Consider for example the calculation of concentrations in a stream at a point a short distance downstream from where the stream receives effluent from a reservoir possessing a large hydraulic residence time. In reality, mixing within the reservoir will have a profound influence on the temporal concentration dynamics in the reservoir’s effluent (dampening, or decreasing, but lengthening the duration of influent peaks), and this effect will continue to be evident for some distance downstream. However, even in a more-thorough implementation such as described above, and as documented in Section 2.4, SAM does not account for such effects. The proposed update described below represents an initial effort to enhance the sophistication of SAM in order to remedy such deficiencies.

## **4.2 Proposed Update to Account for Time of Travel Dispersion**

USEPA OPP developed a conceptual modification of SAM – a convolution approach – to address limitations in the model to account for time of travel dispersion. A preliminary evaluation of results was made using a subset of the test basins described in Section 2.4.

In a mathematical context, a convolution is a function derived by integrating two separate functions such that one function changes the shape of the other. In the case of the SAM time-of-travel convolution routine, the chemograph (pesticide mass in runoff over time) and hydrograph (runoff over time) generated as output are convolved with a gamma distribution, a two-parameter probability distribution that closely fits the movement of water and solutes through drainage networks. The parameters of the gamma distribution are altered based on the time of travel between the source reach and the watershed pour point to generate an impulse response function (IRF) that is used in the convolution. Longer travel times result in the lengthening and flattening of peaks in the hydrograph and chemograph. Figure 21 displays IRFs

for 1, 2, and 3 day travel times, compared with a null IDF in which the gamma distribution is not applied.



**Figure 21: Graph Illustrating Impulse Response Functions (IRF) for Different Travel Times.**

For a hydrologic transport system with assumed linear, statistically stationary properties, convolution can be used to calculate the water body's effluent concentration  $C_o$  at a given time point  $t$ , as a weighted sum of its influent concentrations ( $C_i$ ) at all previous time points. The influent concentration weightings are given by the water body's time-invariant IRF,  $G(t)$ , which describes the effluent response to a unit pulse input:

$$C_o(t) = \int_0^{\infty} G(\theta) C_i(t - \theta) d\theta$$

For a non-reactive constituent, the IRF is the same as the water body's residence time distribution. The essence of this proposed update is to employ mathematical convolution using gamma-distributed IRFs to redistribute, over time, daily SAM-generated pulses of both pesticide mass and runoff volume, prior to the ultimate calculation of pour point concentrations.

Convolution is intended to ultimately approximate the net influences of upstream hydrology on downstream concentration. The approach is similar to one proposed by Carleton (2015), with a few differences. As in the alpha version of SAM, water bodies (or pour points) are processed one at a time, and the model can thus hypothetically be applied at even the highest currently available level of spatial resolution: the NHDPlus reach/catchment.

The methodology is as follows: SAM processes recipes representing all upstream drainage areas, generating loading time series for each scenario. Any scenarios whose contributions pass through a lentic system on the way to the pour point first have their pesticide load time series' convolved with an IRF consisting of a gamma probability density function that has a "shape" factor equal to 1 (representing a completely-mixed tank) and a "scale" factor equal to the water body's residence time in days. If more than one lentic system lies along a given flow path, convolutions are performed sequentially for each. Next, scenarios located in contributing NHDPlus catchments are grouped into nominal integer-day total travel times (based upon tabulated reach length and mean flow velocity attributes) to the pour point (lentic systems are assumed to contribute no travel time), and summed into total load time series (the summation includes any already-convolved time series for catchments with lentic waters in their flow path). For travel times <1 day, these time series are delivered to the pour point water body unmodified. For travel times >1 day, the load time series are convolved against gamma-distributed IRFs that essentially represent a tanks-in-series style of mixing, with one "tank" per nominal day. This is essentially equivalent to assuming that inert tracer would wash out of a "dayshed" (see Carleton, 2015) in an exponential fashion. The shape factor thus corresponds with the travel time in integer days, and the scale factor is always 1. These convolutions are applied both to pesticide masses and to runoff water volumes, and in this manner both hydrographs and chemographs are ultimately simulated.

With this approach, estimated water body volume  $V$  in essentially all lotic water bodies (reaches) is expected to be  $\ll Q$ , thus  $\tau \ll 1$ , and for all intents and purposes the approximation  $\bar{C} = \frac{M}{Q}$  can be employed to calculate daily pour point concentration. At first glance analogous logic would seem to imply that concentrations in lentic water bodies with large residence times could be adequately approximated using  $\bar{C} = \frac{M}{V}$ . However upon further consideration it becomes clear that a more-proper expression for concentration in lentic water bodies is  $\bar{C} = \frac{M}{Q}$ , where  $Q$  is effluent flow rate. The reason for this has to do with the fact that, for purposes of calculation, convolutions that represent the influence of lentic water bodies are applied to influent mass time series rather than influent concentration time series. Effluent concentration, which for a completely-mixed water body is identical to concentration in the water body, is thus essentially convolved mass divided by effluent reach daily flow volume, rather than by water body volume. The dilution effect created by a relatively large lentic volume is accounted for by the water body's IRF in the convolution itself. In contrast with the process described previously for lotic pour point water bodies, concentration calculations for lentic water bodies employs overall mean daily flow values (for "artificial" NHD reaches that represent lake/reservoir outlets) as "Q", rather than daily-varying (baseflow plus runoff) flow values. This process is expected to generate more reasonable concentration estimates particularly for lentic water bodies with large residence times, in which concentrations necessarily change relatively slowly.

Note that IRFs in this conceptual modification are not required to correspond to gamma-distributed or tanks-in-series mixing as described above. The approach employing convolution is general, and sufficiently flexible to permit essentially any form of IRF, including theoretically or empirically-based functions (indeed other forms of IRFs may be required for simulating chemical sorption and/or decay – see Carleton, 2015). The approach described above was selected for the purpose of initial exploration, and not necessarily because it generates the most-accurate possible representation of dispersion and other mixing/dilution effects. During in-stream transport, atrazine was simulated in the examples described below as if it were an inert tracer, i.e., neither chemical sorption nor decay were considered.

### 4.3 Initial Results and Comparisons with Monitoring Data

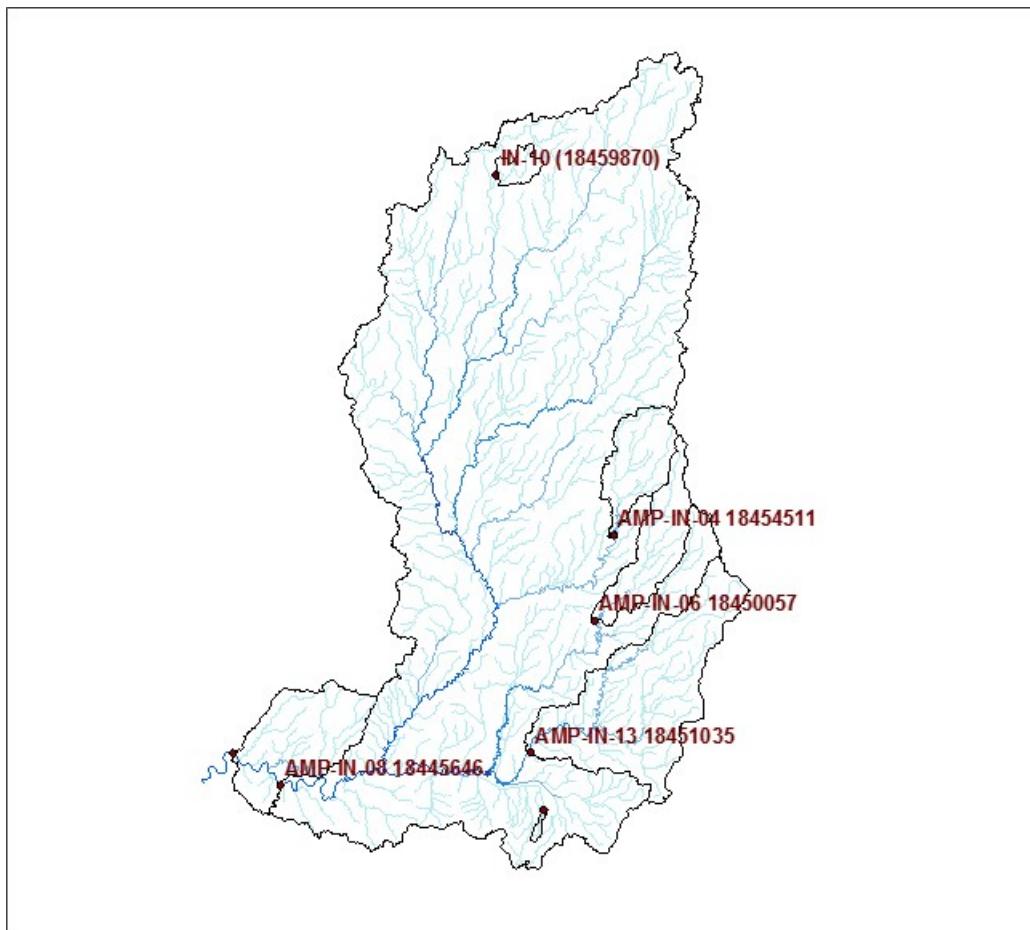
Simulations of atrazine transport in test watersheds in two states (Mark Twain Lake in Missouri and White River in Indiana, described in Section 2.4), have been generated using the “SAM-convolved” test model described above. The maps of the watersheds in Figures 22 and 26 show pour point locations for which extensive monitoring data sets exist, along with their corresponding NHDPlus “comid” attribute, and delineated catchments that drain to these locations. Comparisons between “SAM-convolved” results, original (SAP version) SAM results for the basins that do not account for travel distances, and monitored water column concentration data are shown for some of these locations in subsequent figures. Note that the “SAM” results shown in these figures correspond with the “more-thorough” implementation described above, accounting for loadings from the entire drainage areas to pour points.

Table 4 provides a cross-reference between the monitoring study identifications and the NHDPlus comid attribute used in the figures and graphs that follow. More information on the monitoring sites, along with monitoring data, can be found in Appendix 2-C.

**Table 4: Cross-reference between Monitoring Study Site IDs and SAM Catchment IDs**

Test Basin	Site ID (Study)	NHD comid	Drainage Area (km2)	Monitoring Sampling Interval
Mark Twain Basin (MO)	MO-01 (AEEMP)	4989415	30.1	1-4 da
	MO-01C (AEEMP)	4988183	11.5	1-4 da
	MO-01D (AEEMP)	4988241	23.0	1-4 da
	MO-04A (AEEMP)	4989385	21.8	1-4 da
	MO-04B (AEEMP)	4989739	1004.4	1-4 da
	MO-02 (AEEMP)	5042380	72.9	1-4 da
	MO-05 (AEEMP)	5042400	65.5	1-4 da
	MO-05b (AEEMP)	5039952	472.2	1-4 da
	MO-17 river (AMP)	5641174	1192.5	7 da
	MO-17 (reservoir) (AMP)	5641630	6.0	7 da
	MO-21 (reservoir) (AMP)	4867727	6093.1	7 da

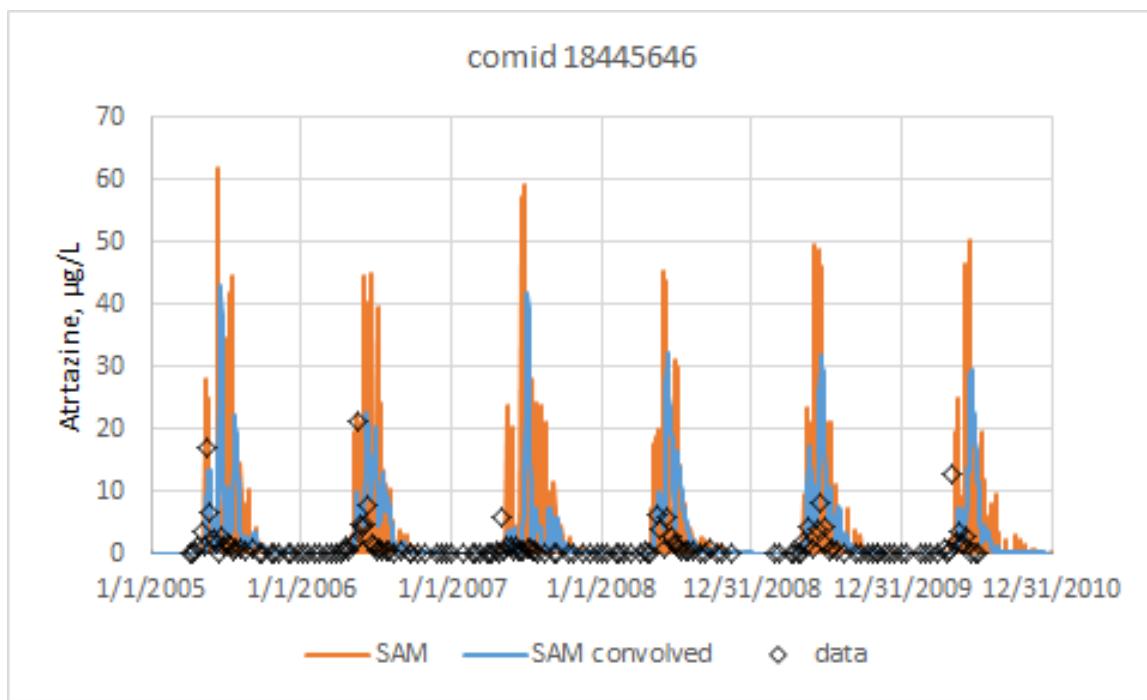
Test Basin	Site ID (Study)	NHD comid	Drainage Area (km2)	Monitoring Sampling Interval
White River (East Fork) Basin (IN)	IN-10 (AEEMP)	18459870	52.3	4 da
	IN-04 (river) (AMP)	18454511	252.2	7 da
	IN-06 (river) (AMP)	18450057	282.9	7 da
	IN-07 (river) (AMP)	18445592	10467.0	7 da
	IN-08 (river) (AMP)	18445664	10013.7	7 da
	IN-13 (river) (AMP)	18451035	924.0	7 da



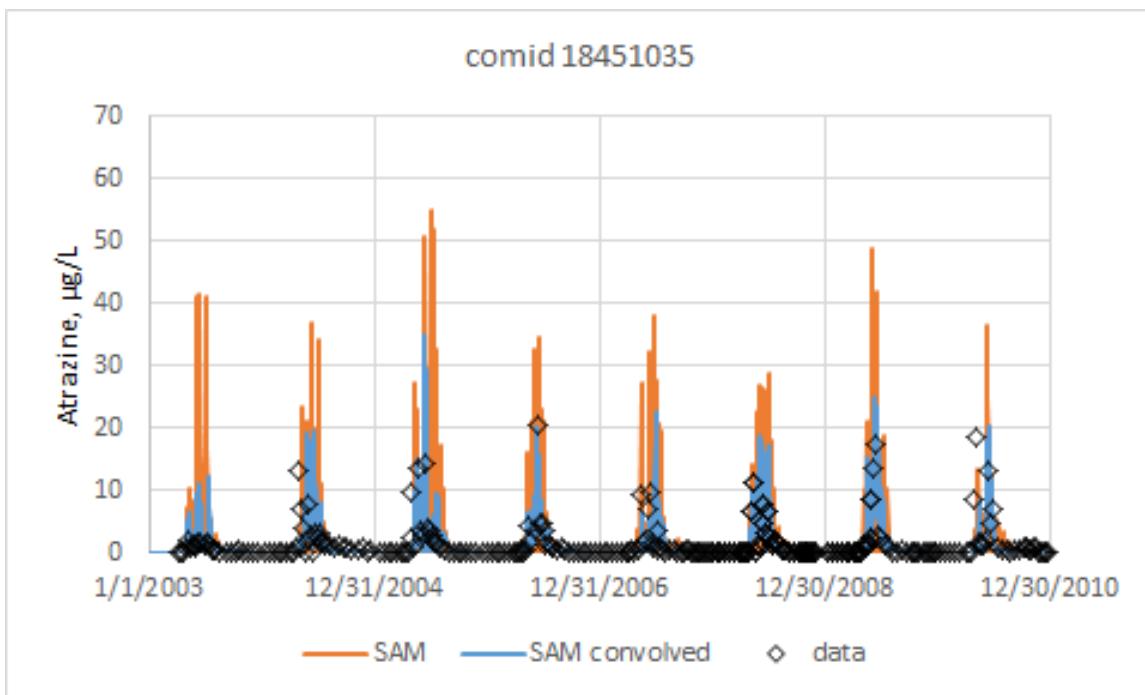
**Figure 22: East branch of White River watershed, Indiana, Showing Test Basins and Monitoring Site Locations.**

In the White River (East Branch) watershed examples in Figures 23-25, the “SAM-convolved” model usually appears to do a somewhat better job than SAM alone at matching observed atrazine concentrations, in terms of both maximum values and temporal dynamics. SAM-

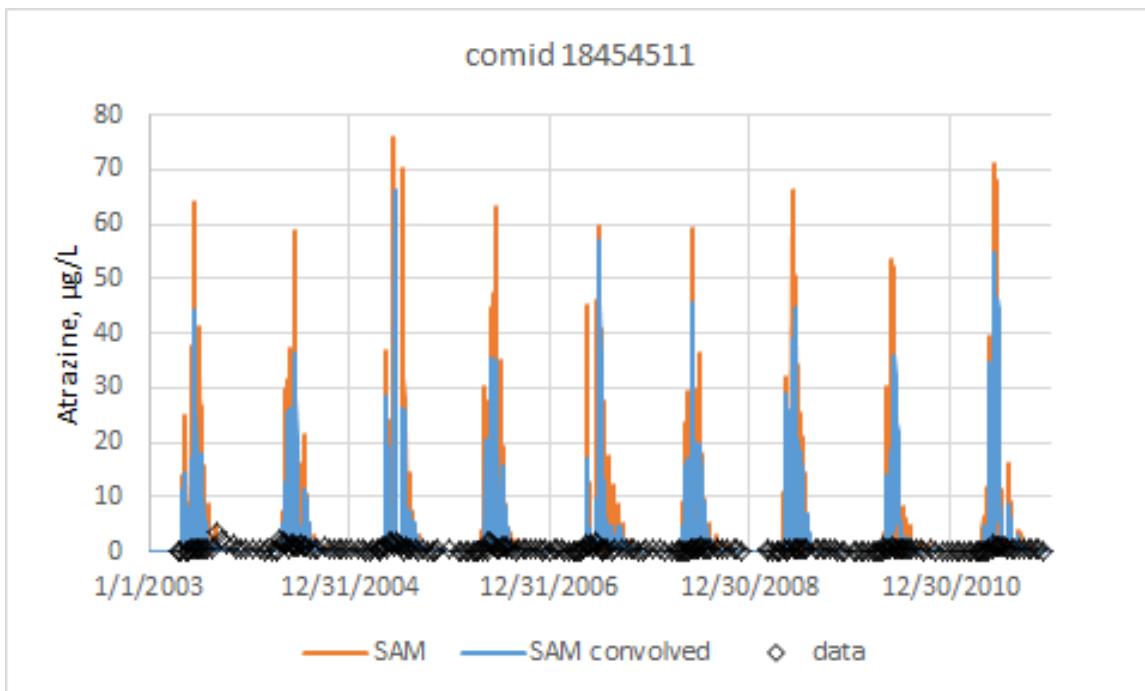
convolved estimates of maximum concentrations drop by roughly 30-50% as compared with SAM estimates for the IN-08 (comid 18445646) site, near the lower end of the White River basin (Figure 23), bringing them generally within 2-5X of monitored concentrations. SAM-convolved estimates for IN-13 (18451035) are generally within 1-2X of monitored concentrations (Figure 24). On the other hand, while SAM-convolved estimates of concentration peaks at IN-04 (18454511) are less than those generated by SAM without convolution, they are nonetheless more than 5X to 10X greater than maximum monitored concentrations (Figure 25). These monitoring samples were collected weekly and are therefore unlikely to reflect true maximum daily concentrations in these water bodies (USEPA OPP, 2010a, 2010b, 2011, 2012). If sampling bias factors (see Section 2.4) were applied to adjust the monitoring data for these comparisons (USEPA OPP, 2011), the SAM model estimates presumably would be more similar to the results.



**Figure 23: Comparison of SAM Outputs with Convolution Approach (Blue) with Original SAM Output (Orange) and Monitoring Data for Basin 18445646 (Site IN-08 river)**

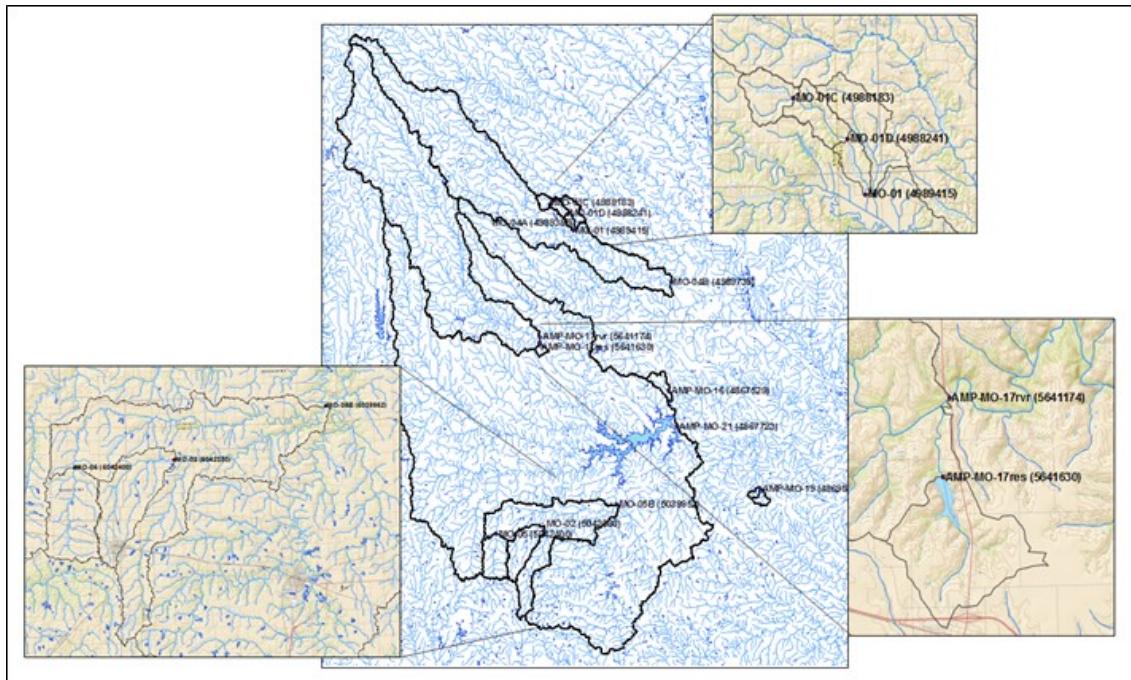


**Figure 24: Comparison of SAM Outputs with Convolution Approach (Blue) with Original SAM Output (Orange) and Monitoring Data for Basin 18451035 (Site IN-13)**



**Figure 25: Comparison of SAM Outputs with Convolution Approach (Blue) with Original SAM Output (Orange) and Monitoring Data for Basin 18454511 (Site IN-04)**

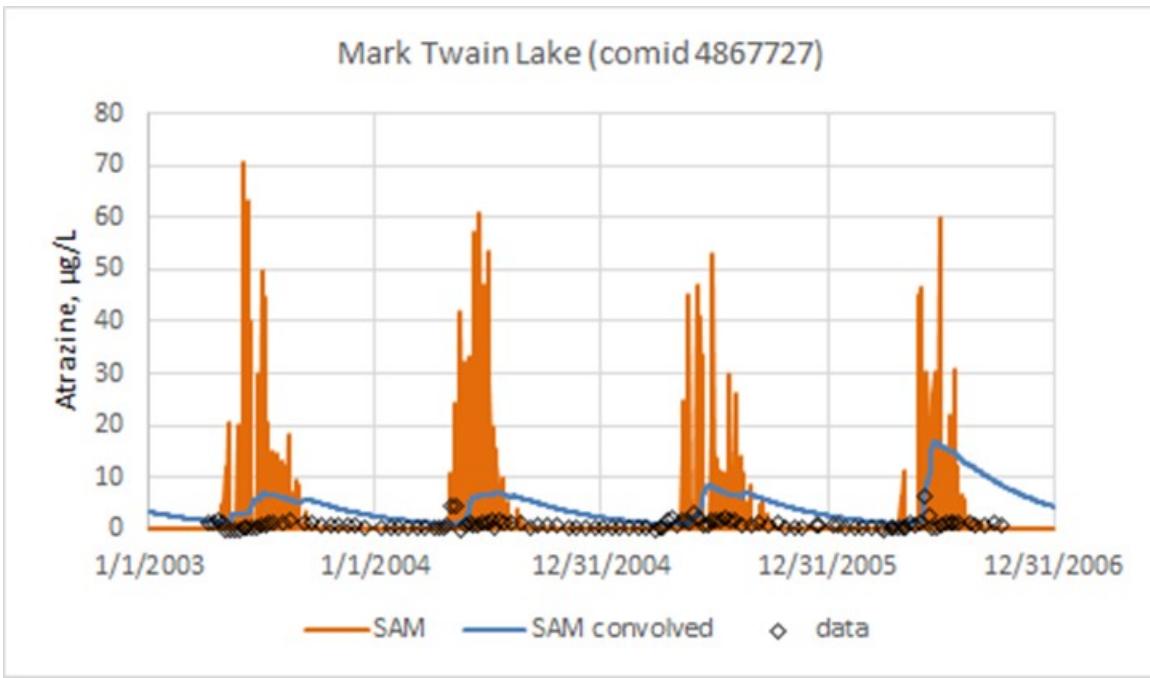
For the monitoring sites around Mark Twain Lake (figure 26), comparisons shown in Figures 27-31, SAM-convolved estimates again appear to better match observed atrazine concentrations than do SAM estimates, in terms of maximum values and temporal dynamics.



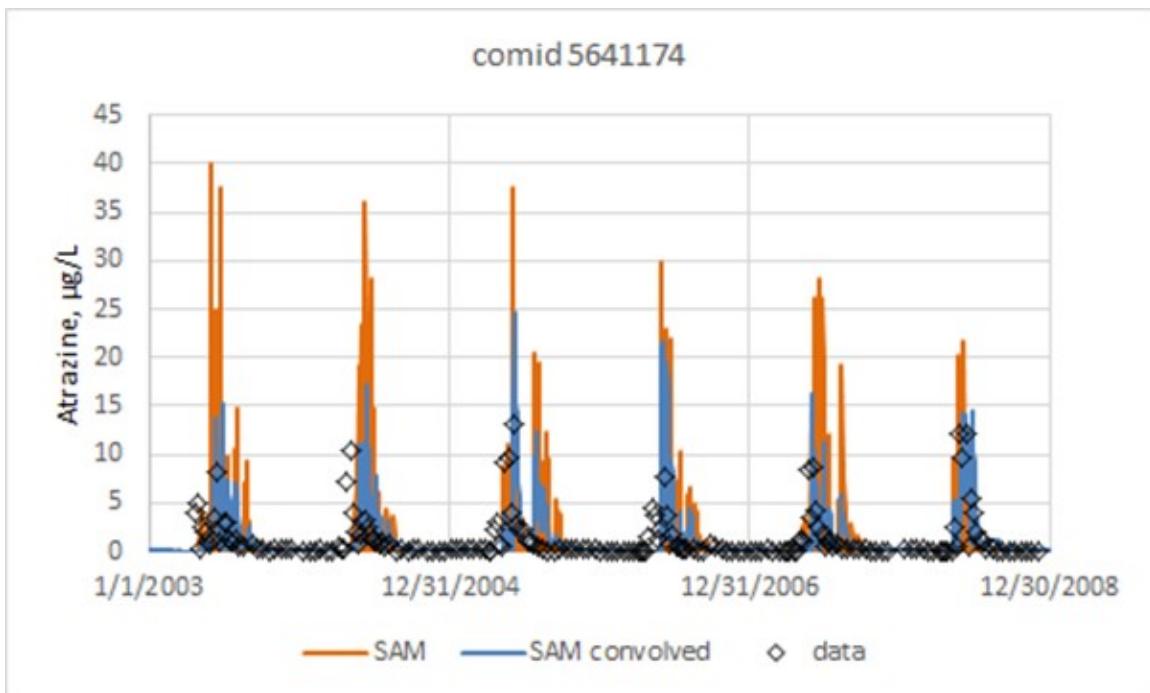
**Figure 26: Mark Twain Lake Watershed, Missouri, Showing Test Basins and Monitoring Site Locations.**

Figure 27 shows SAM-convolved and SAM results compared with monitored concentrations in a large residence time (estimated at 126 days) lentic water body, the Mark Twain Lake reservoir. Maximum SAM-convolved estimates exceed measured concentrations, though not by nearly as much (i.e., <10X) as do unmodified SAM estimates. Convolution dampens and broadens influent pesticide pulses to more accurately reflect temporal trends within the lake, lessening maximum concentrations but also increasing concentrations during later times of the year, when significant exposure might not otherwise be expected to occur.

Figure 28 shows monitored concentrations from a site located on the Salt River within the Mark Twain basin (compare with Figure 15 in section 2.4.4). The SAM-convolved peak concentrations are less than those generated by SAM alone, but are nonetheless within the range of 1 to 5X greater than monitored peak concentrations for all six years of monitoring.

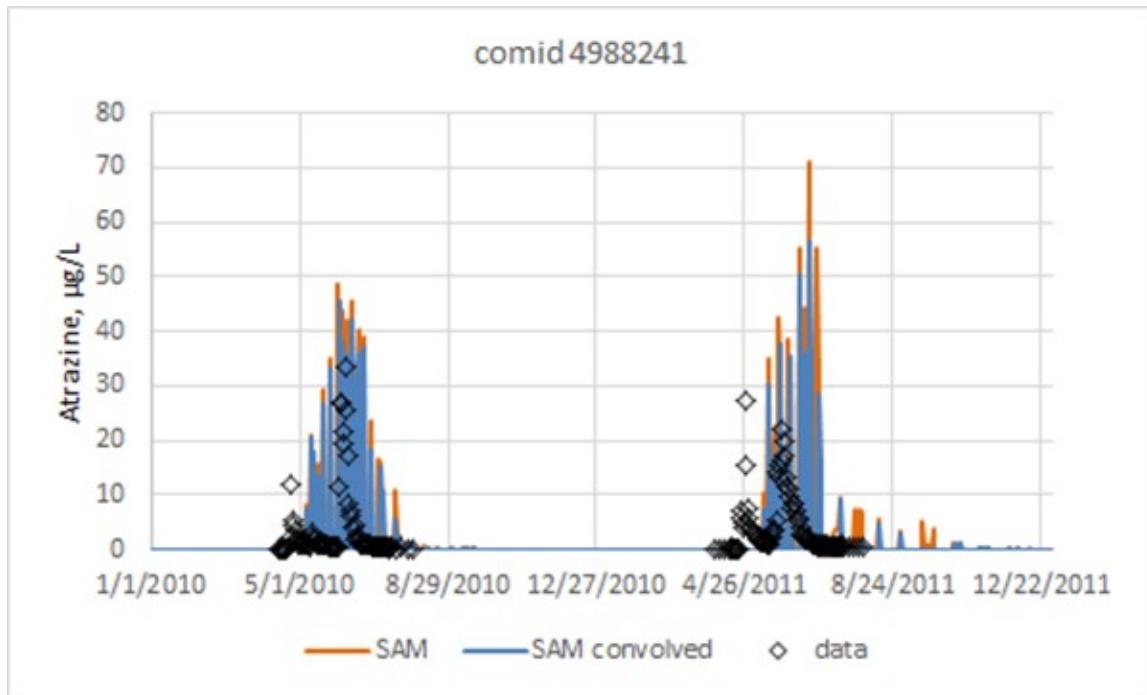


**Figure 27: Comparison of SAM Outputs with Convolution Approach (Blue) with Original SAM Output (Orange) and Monitoring Data for Basin 4867727 (Site 21 reservoir)**

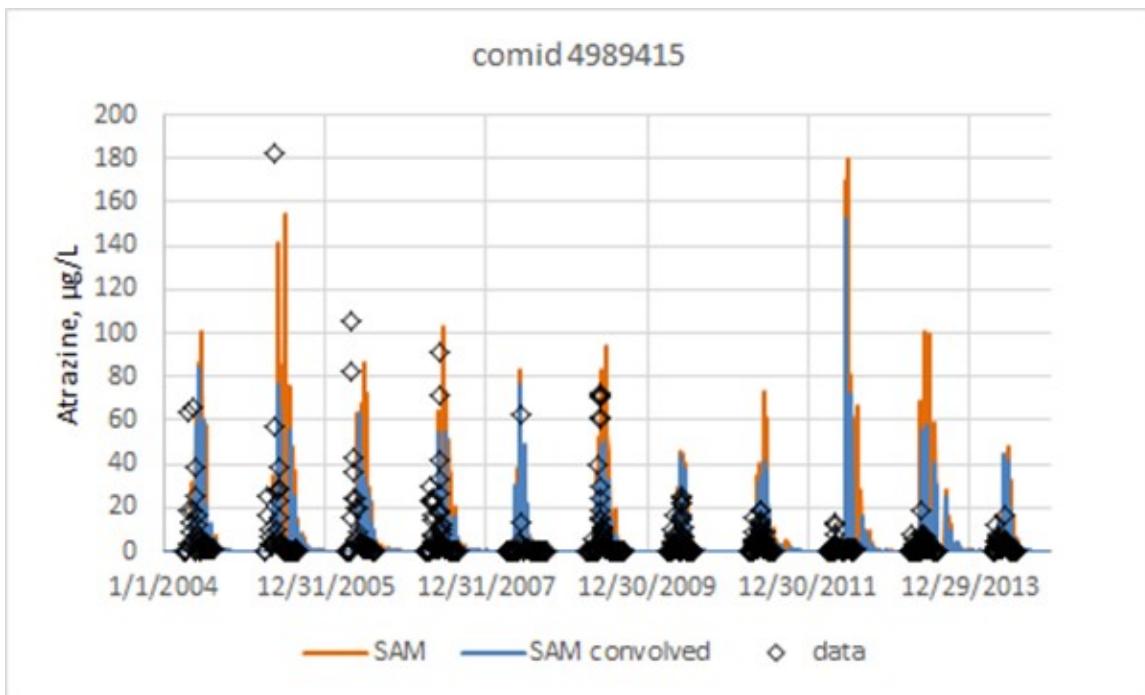


**Figure 28: Comparison of SAM Outputs with Convolution Approach (Blue) with Original SAM Output (Orange) and Monitoring Data for Basin 5651174 (Site MO-17 river)**

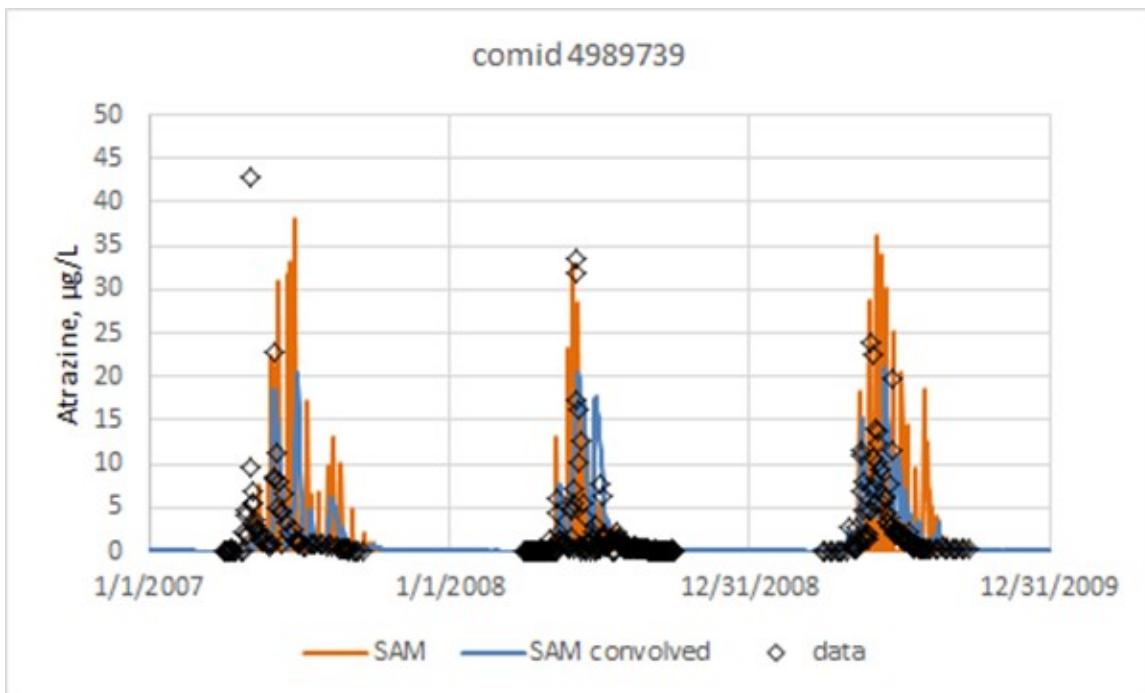
Figures 29 to 31 illustrate model-data comparisons for a series of nested monitoring sites located just north of the Mark Twain Lake basin. MO-01D (4988241) is located upstream from MO-01 (4989415), which in turn is located upstream from MO-04B (4989739). This series provides a good test area to evaluate the effect of the convolution approach as we simulate pesticide mass moving from upper headwaters to increasingly downstream locations.



**Figure 29: Comparison of SAM Outputs with Convolution Approach (Blue) with Original SAM Output (Orange) and Monitoring Data for Basin 4988241 (Site MO-01D)**



**Figure 30: Comparison of SAM Outputs with Convolution Approach (Blue) with Original SAM Output (Orange) and Monitoring Data for Basin 4989415 (Site MO-01)**



**Figure 31: Comparison of SAM Outputs with Convolution Approach (Blue) with Original SAM Output (Orange) and Monitoring Data for Basin 4989739 (Site MO-04B)**

## **5 Defining the Likely Pesticide Application Window based on Crops and Weather**

Not only is the pesticide application date a sensitive parameter in USEPA OPP's aquatic models (Jones and Russell, 2001; Jones and Mangels, 2002), the timing of the application, particularly in relation to rainfall events, impacts both timing and magnitude of the resulting pesticide concentrations in water (USEPA OPP, 2009a, 2011, 2012). For some types of pesticides (particularly herbicides), the timing of applications are often linked to crop milestones such as planting, crop growth stages, and harvest. The timing of these milestones vary spatially and temporally with weather.

In its current aquatic exposure models, USEPA OPP compares pesticide label recommendations with available resources such as USDA crop profiles, published planting and harvest dates, and likely timing of pest pressures to identify a likely application period for the pesticide being assessed. For SAM, the user will still have the option of using these resources. The alpha version of SAM used USDA reports on usual planting and harvest dates (USDA NASS, 2006, 2007, and 2010) and the Plant Hardiness Zone (PHZ) map to stratify planting and harvesting dates within states (Section 3.1.4). This provided a context for varying crop dates spatially and can be used to similarly vary pesticide application windows. However, this approach does not account for yearly variations as a result of differences in weather.

For those pesticides for which the likely application window can be linked to specific crop growth stages or milestones, USEPA OPP is exploring methods to better vary planting, harvest, and specific crop- growth stages spatially as well as temporally. Promising options include using empirical data such as USDA Crop Progress reports, where available, or crop growth (phenology) models where data are incomplete. The preferred approach is to use empirical data when possible. However, due to the complexities of a national scale model, empirical data is not always available across the conterminous US for a single crop, much less for many minor crops that may be of interest. A preliminary evaluations of these approaches using corn is presented in support of the following charge questions to the SAP:

**Q8.** Pesticide applications often depend on planting dates, crop growth, and harvest dates, which vary with weather. To improve upon the initial approach of stratifying planting and harvesting dates within states by using a Plant Hardiness Zone map (Section 3.1.4), USEPA OPP tested the potential for using empirical data (USDA weekly crop progress reports) and, where such data are incomplete, crop growth models (Sections 5.2 and 5.3).

- a. *Please comment on the use of crop planting dates and growth stages to provide reference points for pesticide application windows. How applicable is this approach for predicting the application window for all types of conventional pesticides (e.g., herbicides, growth regulators, fungicides, insecticides, etc.). For pesticide or pest types for which this approach may not work, what alternative methods are available?***

- b. As noted in Section 5.2, empirical crop progress data are not available for all crops, all areas, or all years. ***Please recommend any additional data sources that could provide useful information on spatial and temporal (year-to-year) variability in crop planting, growth, and harvesting dates for use in modeling.***
- c. Where empirical data are missing, USEPA OPP explored the possibility of using crop growth/phenology models such as growing degree days (GDD) to fill in missing data. ***Please comment on the number of crops with available GDD models and availability of alternative models/data for other crops or crop groupings.***

**Q9.** The test version of SAM provides the user with options for defining the extent of the pesticide application window and the distribution of pesticide applications across that window (e.g., uniform distribution, triangular distribution). Crop progress reports or, in their absence, crop growth models, offer an option for defining the application window and shape of the distribution (Section 5.1). ***Please comment on the use of empirical data or models to define the distribution of pesticide applications within an application window.***

Section 5.1 provides a context for using crop growth data as a framework for determining likely windows for applying pesticides. As noted, this approach may be more viable for some types of pesticides, such as herbicides) than for others (such as insecticides and fungicides). Section 5.2 explores the potential for using empirical data such as USDA weekly crop progress reports, to provide the spatial and temporal context to crop growth stages, while Section 5.3 looks at a possible crop growth model to fill in where empirical data are missing. Section 5.4 shows results of preliminary model comparisons with available monitoring data for atrazine.

## 5.1 Context for Using Crop Milestones to Estimate Pesticide Application Windows

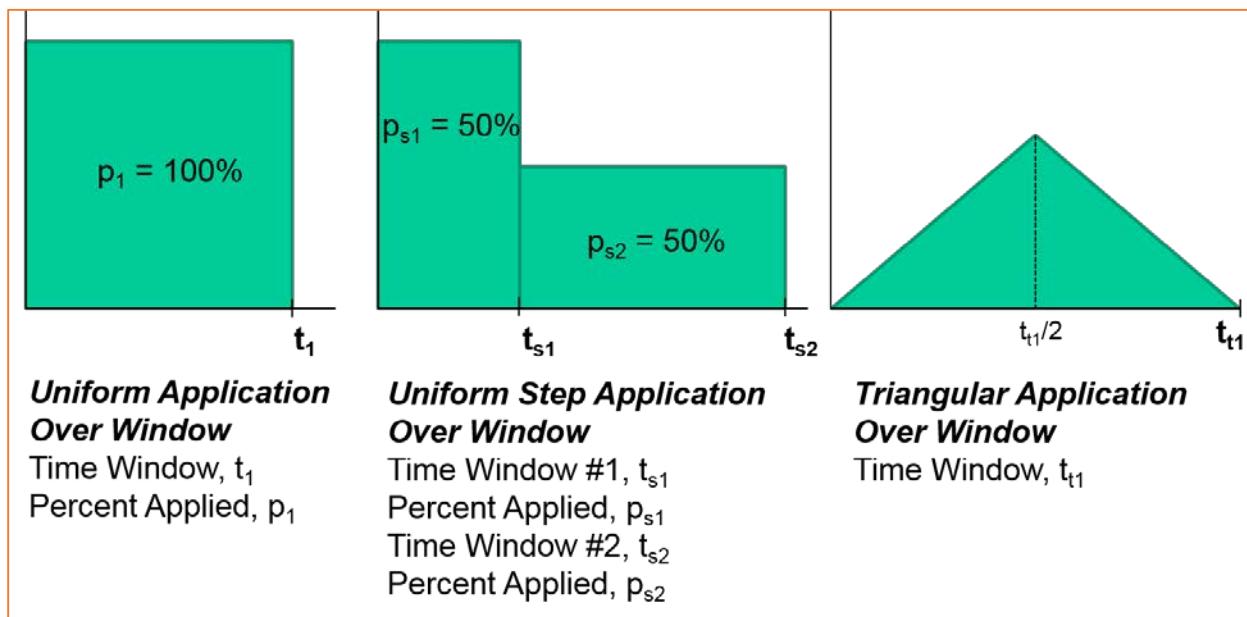
Pursuant to the Federal Insecticide, Fungicide, Rodenticide Act (FIFRA), pesticide product labels must provide information about the target pest (e.g., weeds, insects, fungi, etc.), active ingredient, application rates, application timing, and other production application information. USEPA OPP uses this information, in combination with toxicity data, to assess ecological and drinking water exposure risks from these pesticides. Depending on the type of pesticide (e.g., herbicide, insecticide, fungicide) and the target pest, the pesticide application may coincide with a specific crop milestone (planting, harvest) or phenological (growth) stage (e.g., emergence, bloom, maturity) (Loux et al., 2015). Where such coincidence occurs, USEPA OPP may be able to link application periods to crop stages and vary both spatially and temporally using empirical or model data.

### 5.1.1 Defining Pesticide Application Windows

In USEPA OPP's current aquatic exposure assessments, which use national or regional scenarios for various crops, the risk assessor currently selects a single pesticide application date to represent the label's application timing. While a single date may be reasonable for representing

small watersheds such as those associated with the farm pond used in ecological assessments and the index reservoir used for drinking water, a range in application dates is more likely to reflect actual practice in larger watershed areas, with more farms within the drainage area.

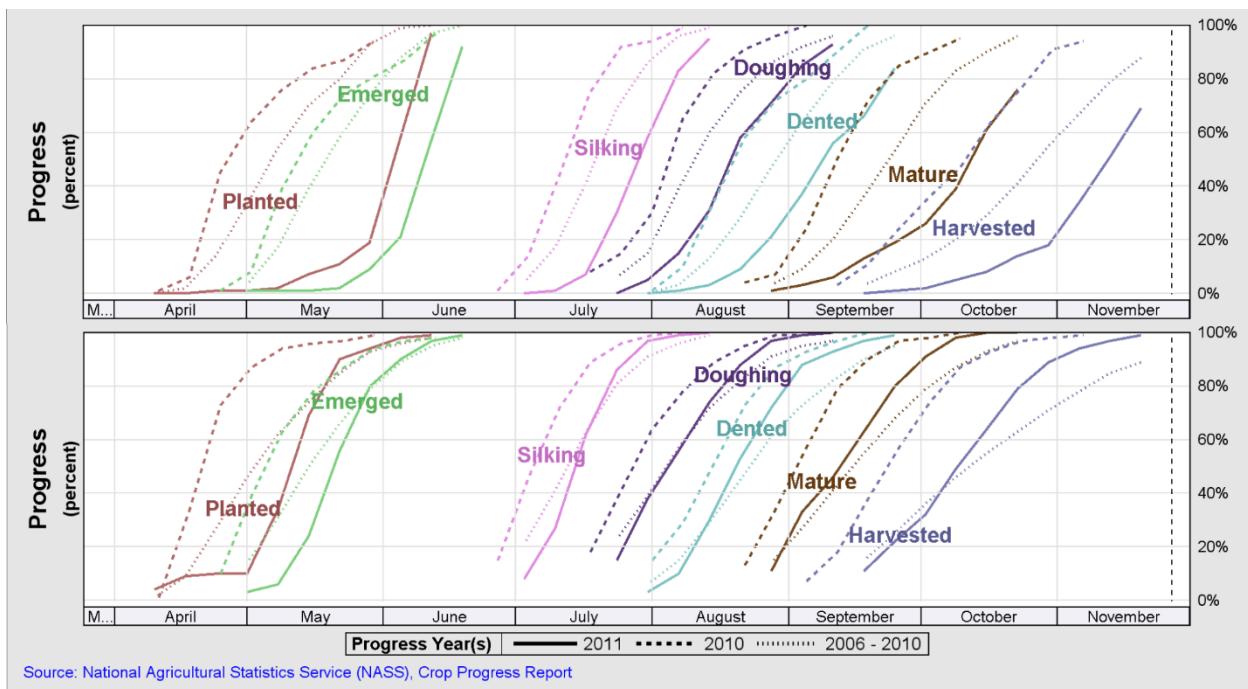
For SAM, the user has the option to simulate pesticide applications over a range of dates or to input multiple dates. The alpha version of SAM includes three options the model user can select for distributing pesticide applications (Figure 32). These application windows are defined relative to crop emergence, maturity or harvest so that actual dates will vary spatially with plant milestones (Sections 1.1 and 3.1.4). In the alpha version of the model, the linkage for application dates relative to crop milestones is used solely to provide a framework for varying application dates spatially (e.g., ensuring that a pesticide application on a post-emergent pest does not occur on the same date in Tennessee as it would in northern Indiana).



**Figure 32: Illustration of the three methods to distribution pesticide application timing in SAM.**

These distributions are mathematical options for proportioning a pesticide application over a user-defined time period. The user determines the timing, duration and shape of the distribution of the application. However, where the pesticide application is linked to one or more crop planting or growth stages, information on the timing and duration of crop milestones may be useful in providing spatial and temporal contexts for defining the timing, duration, and potential distribution of the pesticide application. To illustrate, consider the weekly Crop Progress Report (CPR) data from USDA NASS for corn in Illinois and Ohio (Figure 33)<sup>19</sup>.

<sup>19</sup> CPR weekly survey data are available at state and sub-state levels via the USDA NASS Quick Stats web-site: <http://quickstats.nass.usda.gov/>



**Figure 33: Comparison of CPR milestones for corn among Ohio (top) and Illinois (bottom).**

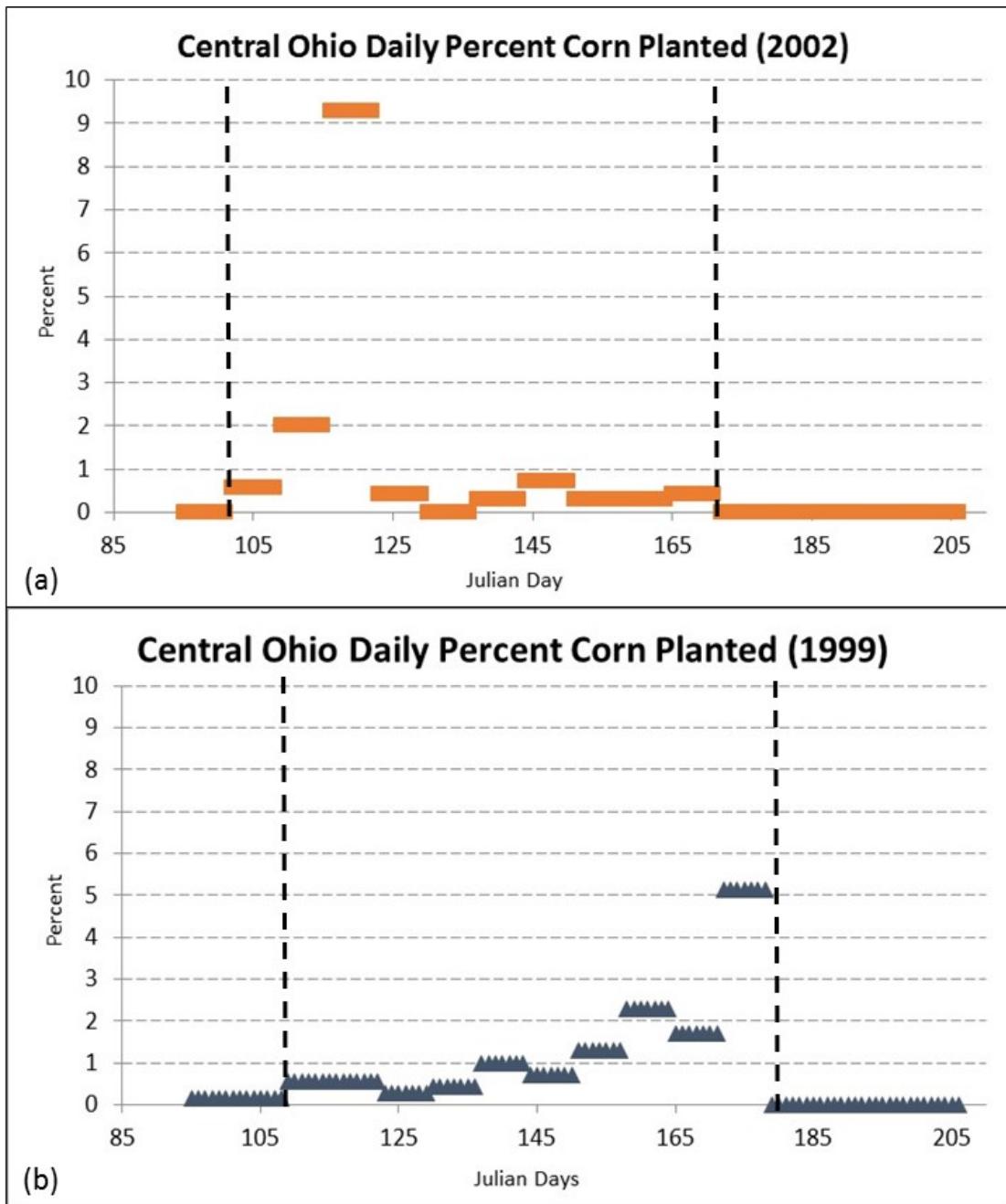
The solid lines in each graph in Figure 33 represent the cumulative percent progress for corn development for 2011. These crop stages are represented: planted, emerged, silking, doughing, dented, mature and harvest. Temporal (year-to-year) variability is evident in the dashed lines that represent previous year and previous 5-year averages for the progress of each stage of corn production.

Spatial variability is evident among these states not only in the timing of the crop stages but also the shape of cumulative progress. For example, while the planting window was broad for both states (*i.e.* April to early June), corn planting intensified earlier in the planting window in Indiana than in Ohio. In Ohio, most of the corn planting occurred nearly two months later than the previous five-year average, likely due to heavy rainfall in Ohio during that time.

For the preliminary evaluation discussed in this section USEPA OPP focused on using the timing of the crop stages, as reported by CPR data, to vary the timing of the pesticide application. However, the CPR data could also be used to define the distribution of the application across the likely window. For instance, the timing and shape of the distribution for a pesticide that is applied around pre-plant or pre-emergence would likely be similar to the planted lines in Figure 33. Applications associated with later crop stages would likely follow those patterns. This is the subject of charge question 9.

Figure 34 illustrates year-to-year variability in percent corn planted in central Ohio, using the NASS reported weekly corn planted data (interpolated to derived daily percent corn planted). In 2002, a warm dry spring resulted in early planting of corn, while in 1999, a cooler wet spring shifted most planting later in the season. When such data are available, USDA NASS crop

progress data could be used to better define the timing and shape of the distribution for pre-plant or pre-emergence pesticide applications.



**Figure 34:** Daily percent corn planted in Central Ohio for 2002 (a) and 1999 (b), with the planting window (dashed lines).

USEPA OPP proposes the following steps to derive appropriate spatially and temporally distributed pesticide application windows, where appropriate:

- 1) Determine pesticide types, modes of action, and crops for which pesticide applications are most likely to correlate to crop milestones/growth stages;
- 2) Define links between pesticide product labeling and target pest(s) and crop milestones/phenological (growth) stages for each crop type, where appropriate;
- 3) Determine the availability and spatial/temporal scale of empirical data for crop growth stages;
- 4) Where necessary, identify and evaluate available crop growth models that could be used to fill in where empirical data are missing;
- 5) Evaluate resulting model estimations; and,
- 6) Update models as needed.

In the charge questions, USEPA OPP is asking the panel for comments on the extent to which such an approach might be applicable and for recommendations on improving the approach. For preliminary explorations, USEPA OPP evaluated empirical data (Section 5.2) and a simple crop growth model (Section 5.3) for corn. Section 5.4 summarizes results of a comparison of the approaches for atrazine using monitoring test basins for evaluation.

## **5.2 Using Empirical Data to Define Crop Milestones: USDA Crop Progress Reports**

USEPA OPP first searched USDA NASS products for empirical data to better characterize the spatial and temporal variability in crop milestones (such as planting and harvest) and growth stages. USDA NASS publishes census and survey agricultural statistics at national, state, county and other geographical levels for major commodity crops that characterize where the crops are grown, and when production activities occur (USDA NASS, 2010).

In the Crop Progress Report (CPR) survey data, USDA NASS collects and tabulates state or crop-reporting district level survey data of agricultural crop development, beginning in the spring of each year. CPR data are surveyed weekly on broad array of crops, with information presented for four groups: Field Crops, Vegetables, Fruit and Tree Nuts, and Horticulture, as previously discussed.

CPR data are used to develop Usual Planting & Harvesting Dates for Field Crops (USDA NASS, 2010); Fruits and Tree Nuts: Blooming, Harvesting, Marketing Dates (USDA NASS, 2006); and Usual Planting and Harvesting Dates for Fresh Market and Processing Vegetables (USDA NASS, 2007). These data were previously used by USEPA OPP to select the average planting and harvest dates entered into the appropriate pesticide exposure models. The CPR weekly survey data are available through the USDA NASS Quick Stats site (<http://quickstats.nass.usda.gov/>). This dataset provides weekly progress on planting, crop phenological stages, and harvest, and can be used to identify and characterize the spatial and temporal distribution of crop stages during the growing season.

The NASS CPR data accounts for year-to-year variations in crop development dates due to weather and other factors, and has been used by others (Sadler et al, 2014; Baffaut et al, 2015). However, CPR data has some limitations:

- 1) Resolution varies (i.e., crop reporting districts to state-level);
- 2) Data are not available for all crops, especially vegetable crops;
- 3) Data are not available for all crops in all states; and
- 4) Some crops have limited historical data sets.

### **5.2.1 Availability of Empirical Data by Crop Groups**

To determine the extent to which empirical data may be available for use in SAM, USEPA OPP inventoried the availability of USDA NASS data (CPR and CDL) for field crops (Table 5). The USDA National Agricultural Statistics Service (NASS) has also organized agricultural commodities into crop groups. These groups have been used for organizing agricultural census and survey data, and include:

- 1) Field crops;
- 2) Fruit and Tree Nuts;
- 3) Vegetables; and
- 4) Horticultural products.

Crop groups listed on the pesticide labels are based on commodity end use for the purpose of establishing crop residue tolerances. These are described the Federal Register under 40 CFR 180.41<sup>20</sup>. The groups are organized by representative crops and related crop subgroups, and some commodities are separated into groups by product end-use. Although these crop groups have been used to establish residue tolerances, registrants often submit pesticide labels linked to all, or a portion of, crops within a crop group.

Because crop groups identified on the label (based on 40 CFR 180.41) may not directly coincide with USDA NASS commodity field crop groups, USEPA OPP generated a crosswalk table for field crops (Table 5). The crosswalk identifies how crops are organized among the various agencies' data sets, and reveals potential data gaps.

A crop group crosswalk for Fruit and Tree Nuts, Vegetables and Horticultural crops will be generated in subsequent phases of the SAM development project.

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<sup>20</sup> Section 40 of the Code of Federal Regulations (Protection of Environment) is available digitally at [http://www.ecfr.gov/cgi-bin/text-idx?tpl=/ecfrbrowse/Title40/40tab\\_02.tpl](http://www.ecfr.gov/cgi-bin/text-idx?tpl=/ecfrbrowse/Title40/40tab_02.tpl). The crop group tables are available at [http://www.ecfr.gov/cgi-bin/text-idx?SID=e725d2005679847d163190d5196aaaad&mc=true&node=se40.24.180\\_141&rgn=div8](http://www.ecfr.gov/cgi-bin/text-idx?SID=e725d2005679847d163190d5196aaaad&mc=true&node=se40.24.180_141&rgn=div8).

**Table 5: Crosswalk between 40 CFR and USDA NASS commodity field crops.**

Commodity (Representative)	NASS Usual Planting and Harvest Dates (2010)	NASS Crop Progress Reports (Annual)	NASS Cropland Data Layer (Annual)	40 CFR 180.41: Crop Groups
Barley	X	X	X	15 (cereal grains), 16 (cereal forage)
Beans, Dry Edible		X		6 (legumes)
Buckwheat			X	15 (cereal grains), 16 (cereal forage)
Camelina		X	X	
Canola		X	X	20 (oilseed)
Corn, Grain	X	X	X	15 (cereal grains), 16 (cereal forage)
Corn, Popcorn			X	15 (cereal grains), 16 (cereal forage)
Cotton	X	X	X	
Flaxseed		X	X	20 (oilseed)
Hay, Alfalfa	X	X	X	18 (non-grass feed)
Hay, Other	X		X	17 (grass for forage)
Hops			X	
Lentils		X	X	6 (legumes)
Millet		X	X	15 (cereal grains), 16 (cereal forage)
Mint			X	
Mustard		X	X	
Oats	X	X	X	15 (cereal grains), 16 (cereal forage)
Pasture Land			X	
Peanuts	X	X	X	
Peas (dry edible)		X	X	
Rapeseed			X	20 (oilseed)
Rice	X	X	X	15 (cereal grains), 16 (cereal forage)
Rice, Wild				15 (cereal grains), 16 (cereal forage)
Rye		X	X	15 (cereal grains), 16 (cereal forage)
Safflower		X	X	
Sorghum	X	X	X	15 (cereal grains), 16 (cereal forage)
Soybeans	X	X	X	6 (legumes)

<b>Commodity (Representative)</b>	<b>NASS Usual Planting and Harvest Dates (2010)</b>	<b>NASS Crop Progress Reports (Annual)</b>	<b>NASS Cropland Data Layer (Annual)</b>	<b>40 CFR 180.41: Crop Groups</b>
Sugarbeets	X	X	X	1 (root and tuber)
Sugarcane		X	X	
Sunflowers		X	X	20 (oilseed)
Taro		X		
Teosinte				15 (cereal grains), 16 (cereal forage)
Tobacco	X	X	X	
Triticale				15 (cereal grains), 16 (cereal forage)
Wheat, Durum	X	X	X	15 (cereal grains), 16 (cereal forage)
Wheat, Spring	X	X	X	15 (cereal grains), 16 (cereal forage)
Wheat, Winter	X	X	X	15 (cereal grains), 16 (cereal forage)

### 5.3 Crop Growth Models

Although the USDA CPR data provide crop phenological stages, these data are not available for all crops or for all crop stages that may be included on pesticide labels. USEPA OPP has considered the potential for using crop growth models to fill in where empirical NASS crop data are unavailable. This is only a preliminary exploration; before proceeding, USEPA OPP is asking the SAP to comment on the feasibility of using such models, the extent to which the models would be applicable, and the kinds of crop growth models to consider (Question 8).

Crop growth (phenology) models of varying complexities have been used for crop management (Miller et al, 2001; Sakamoto et al, 2013; Torrion et al, 2012) and water needs (Ines et al, 2001; McMaster et al, 2011), evaluating the impacts of different climate scenarios on crops (Murthy, 2003), and addressing pest management needs (Murray, 2008; Pruess, 1983)<sup>21</sup>. This is not meant to be an exhaustive search. A number of crop phenology models have been developed by USDA's Agricultural Research Service (ARS) and by various research institutions; some have been incorporated into broader models such as the Environmental Policy Integrated (EPIC) and Agricultural Policy/Environmental Extender (APEX) models<sup>22</sup>.

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<sup>21</sup> Additional phenology and growing degree-day models for use in pest management are available through the USDA IPM Pest and Plant Disease Models and Forecasting page at <http://uspest.org/wea/>

<sup>22</sup> These models are available through Texas A&M University at <http://epicapex.tamu.edu/>

For this scoping exercise, USEPA OPP used a simple growing degree day (GDD) model for corn. Additional models are available for other crops and may include additional environmental factors to model crop progress. The GDD model uses simple weather data that are available for SAM (daily maximum and minimum air temperature).

The GDD index used for this example is defined by the following equation:

$$\text{GDD} = \left[ \frac{(T_{\text{MAX}} + T_{\text{MIN}})}{2} \right] - T_{\text{BASE}}$$

Where  $T_{\text{max}}$  and  $T_{\text{min}}$  are daily maximum and minimum air temperatures at a given weather grid location, and

$T_{\text{base}}$  is the established threshold temperature at which a given crop becomes active and begins to accumulate GDD units.

For corn,  $T_{\text{base}} = 50$  F. Daily temperatures below this do not accumulate GDD units. Although not reflected in the equation, the upper temperature threshold is 86 F, above which GDD units do not accumulate. Since  $T_{\text{base}}$  and the upper threshold temperature vary for each crop, it is possible to determine the GDD value at any given day of the year and, hence, infer the stage for that particular crop.

This approach for determining crop stage does not take precipitation or available moisture into account; nor does it predict planting date. USEPA OPP compared the arrival of threshold air temperatures ( $T_{\text{base}}$ ) by weather grid to the published most active planting dates described in CPR data. The comparison showed that the dates in which threshold air temperatures dates occurred preceded published planting dates by one to two weeks. This may reflect soil temperature taking longer to reach the ideal  $T_{\text{base}}$  target. It is possible that the GDD model can stand by itself and use CPR data to seed planting dates for a given area in a hybrid approach. However this technique would bring with it the limitations of temporal, spatial and crop categories coverage inherent in the published reports. Another limitation of the GDD approach is widely different measures of time for a given crop to reach a given state of maturity. There are regional differences reflected by a states' cooperative extension bulletin on how many GDDs are needed for a crop to reach a given target stage.

#### 5.4 Model Demonstration Using Corn

To evaluate the impacts of using crop growth data as a reference for pesticide applications, USEPA OPP configured SAM to use corn growth stages defined by CPR and a GDD model for Missouri (MO) and Ohio (OH). The model was also updated to allow users to specify pesticide application dates relative to a particular growth stage (planting, emergence, maturity, harvest). Table 6 compares the test version of the model (baseline) to the two new approaches (CPR,

GDD+CPR). The actual CPR dates used for the years 2006-2013 are summarized in Tables 7 and 8 for MO and OH, respectively.

**Table 6: Alpha version, CPR, and GDD+CPR approaches: Definition of planting, emergence, maturity, harvest, and crop growth curve.**

Approach	Planting	Emergence	Maturity	Harvest
Alpha version (baseline)	USDA NASS, 2006, 2007, and 2010; PHZ (Sec. 3.1.4)	7 days after planting date	Midpoint of planting and harvest dates	USDA NASS, 2006, 2007, and 2010; PHZ (Sec. 3.1.4)
Crop Progress Report (CPR) Approach	CPR planting window for 2006-2013	At beginning of CPR emergence window for 2006-2013	At beginning of CPR maturity window for 2006-2013	At beginning of CPR harvest window for 2006-2013
Growing Degree Day (GDD) + CPR Approach	CPR planting window for 2006-2013	Cumulative GDD = 100, relative to planting date	Cumulative GDD = 1360, relative to planting date	At beginning of CPR harvest window for 2006-2013

**Table 7: Beginning date of corn stages from Missouri CPR for 2006-2013 in Julian days (range from 1 to 365).**

MO Crop Stage	2006	2007	2008	2009	2010	2011	2012	2013
Planting	98	97	102	101	93	92	90	103
Emergence	112	118	123	122	114	113	111	131
Maturity	229	235	242	241	233	230	228	243
Harvest	238	244	263	255	254	239	230	250

**Table 8: Beginning date of corn stages from Ohio CPR for 2006-2013 in Julian days (range from 1 to 365).**

OH Crop Stage	2006	2007	2008	2009	2010	2011	2012	2013
Planting	99	97	111	102	100	113	90	103
Emergence	118	119	124	122	114	120	111	125
Maturity	232	230	239	241	235	241	225	244
Harvest	260	231	263	269	254	242	226	245

In the Scenario Generator, the CPR and GDD+CPR approaches were applied in the years 2006-2013, and in the year 2014, the 2013 dates were used. The crop growth dates from the test version (baseline) were used for all other years simulated (e.g., 2000-2005).

The GDD+CPR approach used the CPR corn planting dates (2006-2013), since the GDD model requires a beginning planting date to start accumulating GDDs. The CPR corn harvest dates were also used as the GDD+CPR harvest dates.

The GDD approach relates the growth of a crop to the accumulation of heat over time (Barker et al., 2005). In the GDD calculations, boundary conditions are first applied to the daily minimum and maximum temperatures:

- 1) If the daily minimum temperature ( $T_{\min}$ ) is less than the base temperature for corn growth ( $T_{\text{base}} = 10^{\circ}\text{C}$ ), then  $T_{\min}$  set equal to  $T_{\text{base}}$ .
- 2) If the daily maximum temperature ( $T_{\max}$ ) is greater than the threshold temperature for corn growth ( $T_{\text{threshold}} = 30^{\circ}\text{C}$ ), then  $T_{\max}$  is set equal to  $T_{\text{threshold}}$ .

The average daily temperature ( $T_{\text{avg}}$ ) is calculated from daily maximum and minimum temperatures, after taking into account the above boundary conditions:

$$T_{\text{avg}} = (T_{\max} + T_{\min})/2$$

Then, the daily GDDs are calculated as an accumulation of the difference between  $T_{\text{avg}}$  and  $T_{\text{base}}$ , beginning from the CPR planting date.

$$\text{GDD}(d) = T_{\text{avg}} - T_{\text{base}} + \text{GDD}(d-1)$$

The emergence and maturity dates for each year are finally identified as the first days to reach 100 and 1360 GDDs, respectively.

#### **5.4.1 Model results**

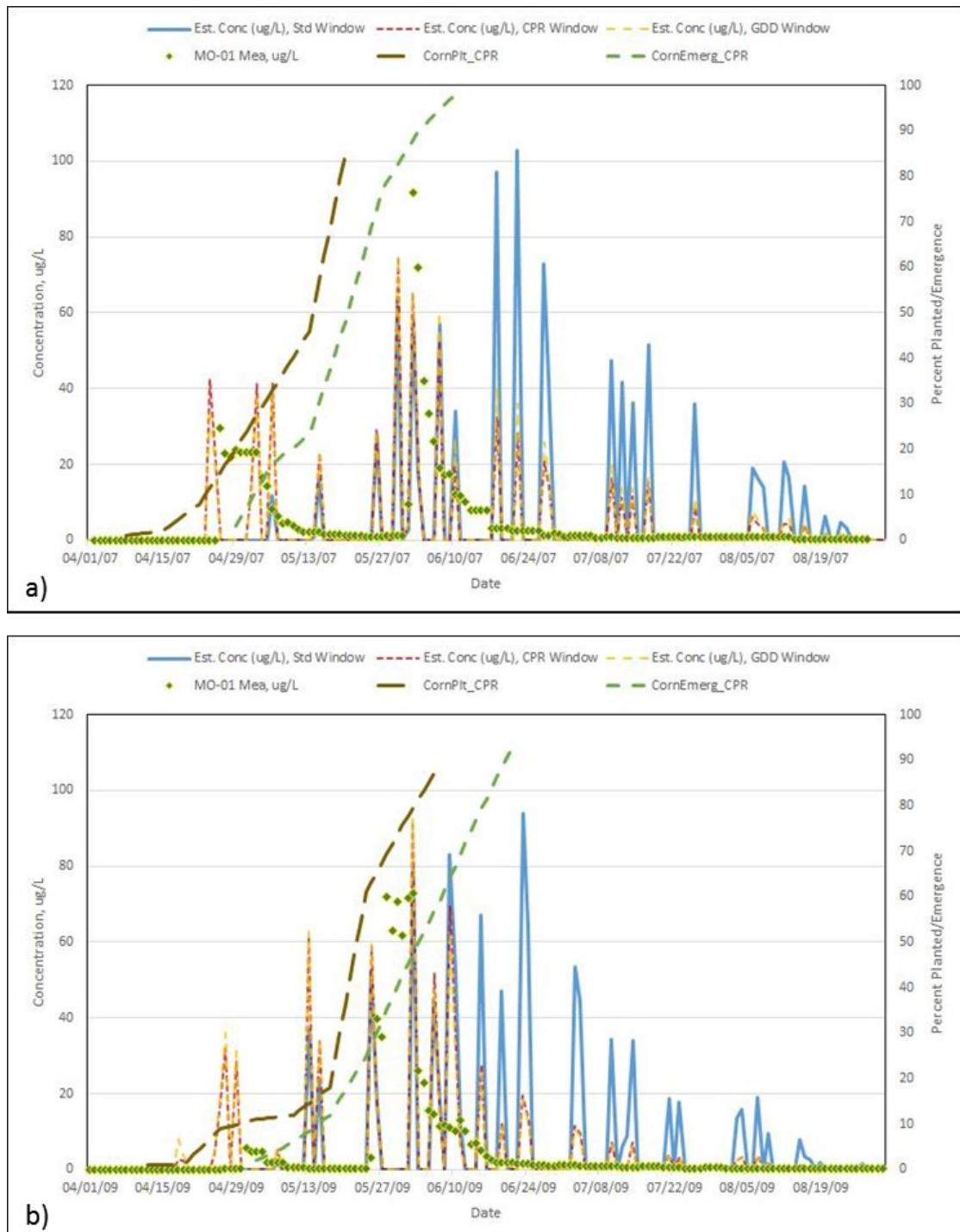
SAM use the CPR and GDD+CPR approaches for several test basins in MO and OH. Pesticide applications (Section 2.4) were assumed to be uniform over a 50-day window, beginning 14 days prior to the first day of emergence (i.e., one-fiftieth, or 2%, of the application was applied each day during the application window).

Results from the preliminary comparison showed that varying the start of the planting season (and subsequent crop stages) to coincide with dates reported in CPR improved pesticide concentration estimates (Appendix 5-A; Figure 35). These examples suggest that using CPR and/or crop growth models show promise for improving concentration estimates in SAM.

Appendix 5-A provides results of the comparisons for the test basins across all years. The results show that the CPR and GDD+CPR approaches shift the timing of simulated exposure concentrations closer to the occurrence of measured concentrations, given the updated crop growth stages based on CPR and GDDs. The simulated magnitudes for the CPR and GDD+CPR approaches also show closer agreement with measured concentrations.

In Figure 35 (and Appendix 5-A), the results for individual years are shown, including simulated concentrations from the three approaches, measured concentrations, and the CPR percentage planted and emerged. The CPR and GDD+CPR concentrations first appear ~14 days prior to the

first day of emergence (or 0% emerged), and correspond well with the measured concentrations in terms of magnitude and timing.



**Figure 35: Estimated concentrations for MO-01 (comid 4989415) from the test version, CPR, and GDD+CPR approaches compared to measured concentrations, with the CPR percentage planted and emerged also shown on right axis, for a) 2007 and b) 2009.**

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