UNITED STATES ENVIRONMENTA L PROTECTION AGENCY
WASHINGTON DC 20460

OFFICE OF
CHEMICAL SAFETY
AND POLLUTION
PREVENTION

December 17, 2015

MEMORANDUM

SUBJECT: Transmittal of Meeting Minutes of the September 15-17, 2015 FIFRA SAP Meeting Held to Consider and Review Scientific Issues Associated with the "Development of a Spatial Aquatic Model (SAM) for Pesticide Assessments"

TO: Jack Housenger
Director
Office of Pesticides Programs

FROM: Fred Jenkins, Jr., Ph.D.
Designated Federal Official FIFRA Scientific Advisory Panel
Office of Science Coordination and Policy

THRU: David Dix, Ph.D.
Director
Office of Science Coordination and Policy

Laura Bailey, M.S.
Executive Secretary FIFRA Scientific Advisory Panel
Office of Science Coordination and Policy

Please find attached the meeting minutes of the September 15-17, 2015 FIFRA SAP open public meeting held in Arlington, VA. This report addresses a set of scientific issues associated with the Development of a Spatial Aquatic Model (SAM) for Pesticide Assessments.

Enclosure

cc:
Jim Jones
Louise Wise
William Jordan
Yu-Ting Guilaran
Robert McNally
Donald Brady
Jacqueline Mosby
Steve Knizer
Dana Vogel
Susan Lewis
Richard Keigwin
Laura Bailey
James Cowles
Mark Corbin
James Carlton
Meridith Fry
Paul Mastradone
Michelle Thawley
Nelson Thurman
Cathy Milbourn
Linda Strauss
OPP Docket

FIFRA Scientific Advisory Panel Members
Stephen Klaine, Ph.D.
Dana Barr, Ph.D.
David A. Jett, Ph.D.
James McManaman, Ph.D.

FQPA Science Review Board Members
Paul Capel, Ph.D.
Chittaranjan Ray, Ph.D.
Bernard A. Engel, Ph.D.
Amor V. M. Ines, Ph.D.
Erica Fleishman, Ph.D.
Yuzhou Luo, Ph.D.
Keith A. Maruya, Ph.D.
Thomas Potter, Ph.D.
Geoffrey I. Scott, Ph.D.

FIFRA Scientific Advisory Panel Minutes No. 2015-03

A Set of Scientific Issues Being Considered by the Environmental Protection Agency Regarding Development of a Spatial Aquatic Model (SAM) for Pesticide Risk Assessments

September 15-17, 2015
FIFRA Scientific Advisory Panel Meeting
Held at the
EPA Conference Center
Arlington, VA

The Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) Scientific Advisory Panel (SAP) is a Federal advisory committee operating in accordance with the Federal Advisory Committee Act and established under the provisions of FIFRA as amended by the Food Quality Protection Act (FQPA) of 1996. The FIFRA SAP provides scientific advice, information, and recommendations to the EPA Administrator on pesticides and pesticide-related issues regarding the impact of regulatory actions on health and the environment. The meeting minutes represent the views and recommendations of the FIFRA SAP and do not necessarily represent the views and policies of the EPA or of other agencies in the Executive Branch of the Federal government. Mention of trade names or commercial products does not constitute an endorsement or recommendation for use. The meeting minutes do not create or confer legal rights or impose any legally binding requirements on the EPA or any party.

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1. NOTICE

The Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA), Scientific Advisory Panel (SAP) is a Federal advisory committee operating in accordance with the Federal Advisory Committee Act and established under the provisions of FIFRA as amended by the Food Quality Protection Act (FQPA) of 1996. The FIFRA SAP provides advice, information, and recommendations to the Agency Administrator on pesticides and pesticide-related issues regarding the impact of regulatory actions on health and the environment. The Panel serves as the primary scientific peer review mechanism of the Environmental Protection Agency (EPA), Office of Pesticide Programs (OPP), and is structured to provide balanced expert assessment of pesticide and pesticide-related matters facing the Agency. FQPA Science Review Board members serve the FIFRA SAP on an *ad hoc* basis to assist in reviews conducted by the FIFRA SAP. The meeting minutes have been written as part of the activities of the FIFRA SAP.

In preparing the meeting minutes, the FIFRA SAP carefully considered all information provided and presented by EPA, as well as information presented in public comment. The minutes represent the views and recommendations of the FIFRA SAP and do not necessarily represent the views and policies of the EPA, nor of other agencies in the Executive Branch of the Federal government. Mention of trade names or commercial products does not constitute an endorsement or recommendation for use. The meeting minutes do not create or confer legal rights or impose any legally binding requirements on EPA or any party.

The meeting minutes of the September 15-17, 2015 FIFRA SAP meeting held to consider and review scientific issues associated with "Development of a Spatial Aquatic Model (SAM) for Pesticide Assessments" were certified by James McManaman, Ph.D., FIFRA SAP acting on behalf of Stephen Klaine, FIFRA SAP Chair, and Fred Jenkins, Ph.D., FIFRA SAP Designated Federal Official, on December 11, 2015. The minutes were proofread by FIFRA SAP staff including Scott Lynn, Ph.D., FIFRA SAP Designated Federal Official and Steven Knott, FIFRA SAP Executive Secretary. The minutes are publicly available on the SAP website (http://www.epa.gov/scipoly/sap/) under the heading of "Meetings" and in the public e-docket, Docket No. EPA-HQ-OPP-2015-0424, accessible through the docket portal: http://www.regulations.gov. Further information about FIFRA SAP reports and activities can be obtained from its website at http://www.epa.gov/scipoly/sap/. Interested persons are invited to contact Fred Jenkins, Ph.D., SAP Designated Federal Official, via e-mail at jenkins.fred@epa.gov.

SAP Minutes No. 2015-03

A Set of Scientific Issues Being Considered by the Environmental Protection Agency Regarding:

Development of a Spatial Aquatic Model (SAM) for Pesticide Risk Assessment

September 15-17, 2015
FIFRA Scientific Advisory Panel Meeting
Held at
One Potomac Yard
Arlington, Virginia

James McManaman, Ph.D.
on behalf of Stephen Klaine, Ph.D.
FIFRA SAP Chair

Date: December 11, 2015

Fred Jenkins, Jr., Ph.D.
Designated Federal Official
FIFRA SAP Staff

Date: December 11, 2015

2. PANEL ROSTER

FIFRA SAP Chair

Stephen Klaine, Ph.D.
Professor, Department of Biological Sciences
Director, Institute of Environmental Toxicology
Clemson University
Clemson, SC

Designated Federal Official

Fred Jenkins, Jr., Ph.D.
U.S. Environmental Protection Agency
Office of Science Coordination and Policy
FIFRA Scientific Advisory Panel
EPA East Building, MC 7201M
1200 Pennsylvania Avenue, NW
Washington, DC 20460
Phone: (202) 564-3327
jenkins.fred@epa.gov

FIFRA Scientific Advisory Panel Members

Dana Barr, Ph.D.
Research Professor
Environmental and Occupational Health
Rollins School of Public Health
Emory University
Atlanta, GA

David A. Jett, Ph.D.
Director, National Institute of Health Countermeasures Against Chemical Threats Program
National Institute of Neurological Disorders and Stroke
National Institutes of Health
Bethesda, MD

James McManaman, Ph.D.
Professor and Chief
Section of Basic Reproductive Sciences
Department of Obstetrics and Gynecology, Physiology
and Biophysics
University of Colorado Denver
Aurora, CO

FQPA Science Review Board Members

Paul Capel, Ph.D.
Research Team Leader
US Geological Survey, National Water Quality Assessment Program
University of Minnesota, Civil Engineering and Geo-Engineering
Minneapolis, MN

Chittaranjan Ray, Ph.D.
Professor of Civil Engineering and Director
Nebraska Water Center
University of Nebraska-Lincoln
Lincoln, NE

Bernard A. Engel, Ph.D.
Head, Agricultural and Biological Engineering
Purdue University
Lafayette, IN

Amor V. M. Ines, Ph.D.
Assistant Professor
Department of Plant, Soil, Microbial Sciences/Biosystems
and Agricultural Engineering
Michigan State University
Okemos, MI

Erica Fleishman, Ph.D.
Researcher
Department of Environmental Science and Policy
University of California
Davis, CA

Yuzhou Luo, Ph.D.
Environmental Scientist
Department of Pesticide Regulation
California Environmental Protection Agency
Sacramento, CA

Keith A. Maruya, Ph.D.
Chemist and Environmental Fate Scientist
Southern California Coastal
Water Research Project Authority
Costa Mesa, CA

Thomas Potter, Ph.D.
Research Chemist
USDA-ARS, Coastal Plain Experiment Station,
Southeast Watershed Research Laboratory
Tifton, GA

Geoffrey I. Scott, Ph.D.
Clinical Professor and Chair
Department of Environmental Health Sciences at the Arnold School of Public Health
University of South Carolina
Columbia, SC

List of Commonly Used Acronyms and Abbreviations

Abbreviation	Description
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
DSSAT	Decision Support System for Agrotechnology Transfer
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 Soil Survey Geographic Database (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
NHD Plus	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
PA-PIPE	Pennsylvania Pest Information Platform for Extension and Education
PHZ	Plant Hardiness Zone (USDA map)
PRZM / PRZM5	Pesticide Root Zone Model / version 5 (the current version)
SAM	Spatial Aquatic Model
USDA-RMS	United States Department of Agriculture – Risk Management Agency
VVWM	Variable Volume Water Model

INTRODUCTION

On September 15-17, 2015 the US EPA Federal Insecticide, Fungicide, and Rodenticide Act Scientific Advisory Panel (FIFRA SAP) met in an open public meeting in Crystal City, VA to consider and review scientific issues associated with "Development of a Spatial Aquatic Model (SAM) for Pesticide Risk Assessments". The USEPA Office of Pesticide Programs (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. If estimated aquatic exposures indicate a potential for adverse effects, the assessment needs to characterize the likelihood of occurrence, including the range in magnitude of exposure, the frequency of exceeding toxicity thresholds, the location of likely exposures, and the potential for exposure to populations at risk. The goal of the Spatial Aquatic Model (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 context is needed to address common risk management questions regarding the likelihood of the exposure 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 at risk. Though much of SAM is based upon OPP's traditional water models (*i.e.*, Surface Water Concentration Calculator [SWCC] comprised of the Pesticide Root Zone Model version 5 [PRZM5] and Variable Volume Water Model [VVWM]), the model is new in its spatial approach to modeling the fate and transport of pesticides and has been optimized for speed and efficiency. The FIFRA SAP was convened to provide advice to EPA regarding the development of SAM.

US EPA presentations were provided during the FIFRA SAP meeting by the following Agency scientists (listed in alphabetical order):

Accounting for Time of Travel – James Carlton, Ph.D., (Environmental Fate and Effects Division, Office of Pesticide Programs), EPA

Welcome and Opening Remarks – James Cowles, Ph.D., Deputy Division Director, Environmental Fate and Effects Division, Office of Pesticide Programs, EPA

Model Components – Meridith Fry, Ph.D., Environmental Fate and Effects Division, Office of Pesticide Programs, EPA

Defining Likely Pesticide Application Window – Paul Mastradone, Ph.D., Environmental Fate and Effects Division, Office of Pesticide Programs, EPA

Data Inputs – Michelle Thawley, M.S., Environmental Fate and Effects Division, Office of Pesticide Programs, EPA

Background, Objectives, and Conceptual Model – Nelson Thurman, M.S., Environmental Fate and Effects Division, Office of Pesticide Programs, EPA

Wrap-up -- Nelson Thurman, M.S., Environmental Fate and Effects Division, Office of Pesticide Programs, EPA

PUBLIC COMMENTERS

Oral and written public comments were provided by:

Janet E. Collins, Ph.D., R.D., Senior Vice President, Science and Regulatory Affairs
on behalf of CropLife America

OVERALL SUMMARY

The Spatial Aquatic Model (SAM), like other watershed scale pesticide fate and transport models, spatially and to some degree temporally integrates landscape scale variation in soil properties, weather, runoff, and the timing and frequency of pesticide applications. While there was general agreement among the Panel that SAM has a sound scientific conceptual basis, it was emphasized that many important SAM components are at best in early development stages. This includes processes such as spray-drift, sediment transport, attenuation during transport, and crop growth and soil conditions as they relate to pesticide application. Limitations of SAM that were discussed were linked to both surface and subsurface hydrologic processes and how field and watershed scale conservation practices may impact fate and transport. The Panel recommended that the clarity of the conceptual approach in the documentation be enhanced and improved. The Panel felt that the separation of independent processes makes sense and results in improved computational efficiency that will likely be beneficial to continued scaling up of the model to large areas. The efforts to reduce and eliminate model computational inefficiencies are commendable, but there is a need for more careful assessment in scaling SAM. The Panel recommended that outputs from SAM be compared to outputs of other models used by the Agency and others (such as SWAT (Soil-Water Assessment Tool). Separate analyses of uncertainty in projections of flow and pesticide concentrations are necessary to examine parameter sensitivity since sorbing pesticides may move differently from aqueous pesticides.

The soil grouping that was conducted and used in the SAM application resulted in little difference in estimated runoff volumes, pesticide masses, and peaks of pesticide concentrations and therefore the Agency should consider disadvantages in grouping soil classes as model development continues. The feasibility of adjusting the resolution of spatial data and the physical, chemical, or biological rationale for adjusting the resolution of spatial data should be assessed separately. There was agreement among the Panel that the incorporation of travel-time based convolution would significantly improve SAM's modeling performance for pesticide simulation at the predefined watershed outlet. The Panel noted the potential impacts of the convolution on the SAM modeling capability for simulating pesticide spatial distribution.

The Panel was less convinced that the convolution approach, as described, could adequately account for pesticides that exhibit sorption or rapid decay in both water and sediment. The Panel identified additional compartments that need to be considered for representing chemical fate and transport in surface water. The Panel concluded that fate and transport of reactive and/or sorbing chemicals in the water column could be incorporated with the proposed convolution approach, while pesticide fate in bed sediment may require a separate computation module. The Panel provided a comprehensive list of data sources potentially useful for representing the benthic sediment layer and associated pesticides in surface waters at varying spatial scales. Growing degree days (GDD) and crop growth models may be more accurate for determining the planting window than the Plant Hardiness Zone map and weekly crop progress report. Trafficability of heavy equipment in the field is a key driver in herbicide applications and SAM can estimate the moisture profile in the soil, which can be used to determine equipment trafficability. The Panel agreed with the Agency that defining pesticide application windows and the distribution of applications within these windows would have a large impact on model outcomes. The Panel recommended other sources of data that are linked to crop insurance that, at minimum, can guide

crop planting and harvest dates. An alternative way to estimate first planting date suggested by Panelists focused on soil temperature. The Agency was encouraged to look for other examples where soil water content and trafficability were linked. Panelists noted that aerial applications must also be considered.

EXECUTIVE SUMMARY OF PANEL DISCUSSION AND RECOMMENDATIONS

Section 1: SAM Conceptual model

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.

The Spatial Aquatic Model (SAM), like other watershed scale pesticide fate and transport models, spatially, and to some degree temporally, integrates landscape scale variation in soil properties, weather, runoff, and the timing and frequency of pesticide applications. In that sense, the Panel felt that SAM has a sound scientific conceptual basis and that it will enhance the Agency's ability to evaluate pesticide aquatic exposures in comparison to currently used models. In addition, the Panel commended the Agency for efforts to reduce code inefficiencies in SAM's fate and transport sub-model PRZM 5 and to minimize SAM's parameterization requirements, and for plans to implement SAM on the internet. The Panel noted that making SAM publicly available on the internet will likely increase transparency in pesticide risk assessments and can potentially educate the public on processes that lead to regulatory decisions. However, the Panel encouraged the Agency to more carefully evaluate simplifying assumptions before they are implemented in SAM. In the case of internet implementation, one Panelist suggested that the Agency consider including a pesticide properties database. It was noted that databases of pesticide properties are commonly included in other pesticide fate and transport models and their inclusion can facilitate and enhance model use.

While there was general agreement that SAM has a sound scientific conceptual basis, it was emphasized that SAM is a work in progress. Many important SAM components, although discussed in the background document and in Agency presentations, are at best in early development stages. These include processes such as spray-drift, sediment transport, attenuation during transport, and crop growth and soil conditions as they relate to pesticide application. In short, SAM appears to be technically and conceptually sound, but as described by the Agency, further development and refinement are needed before SAM becomes a fully functional model.

Limitations of SAM that were discussed were linked to both surface and subsurface hydrologic processes, and how field and watershed scale conservation practices may impact fate and transport. Finally, the Panel indicated that there might be different versions and different conceptual models of SAM depending on desired model outcomes. It was recommended that the Agency consider creating a "SAM-MAX" version whose goal would be to predict maximum concentration to identify "hotspots". Another version could be described as SAM-Distribution; its goal would be to yield concentration predictions that are close to reality across the range of concentrations.

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?***

The Panel recommends the clarity of the conceptual approach in the documentation be enhanced and improved. Specific suggestions for improvement of the documentation include: (1) Clearly define and document the goals and likely applications of SAM; (2) Expand the description of how the Agency decided to pursue SAM, why currently available models were considered inadequate, and the choice of the methods included in SAM.

Section 2: SAM Model Components and Approach

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.***

Clarity regarding the model goals and likely applications should be used in guiding the appropriateness of separation of the model processes, and corresponding computational efficiencies, so that decisions made in these regards do not compromise the model for its intended use. A challenge in continued model development is to insure that the desire to improve model efficiency and reduce time for calculations does not interfere with future model additions or considerations, such as management practices, soil erosion, and subsurface drainage. Based on information available to the Panel, the separation of independent processes makes sense and results in improved computational efficiency that will likely be beneficial to continued scaling up of the model to large areas.

> ***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.***

Improvements in the computational efficiency of the model code and algorithms will be important in scaling SAM. The efforts to reduce and eliminate model computational inefficiencies are commendable, but there is a need for more careful assessment. More clearly articulated goals and requirements for the model would serve as a guide to help evaluate impacts of simplifications, such as use of the single soil layer example presented. Key questions that should be considered when evaluating potential simplifications in algorithms and code include whether assumptions made will limit future development and whether computational power will be a factor when the model is ready to be applied.

Q3. Section 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?

From earlier PRZM validation exercises, the Agency found that rainfall in periods when the pesticide is in the field or on the crop, runoff curve number, pesticide half-life, sorption coefficient, soil organic carbon fraction, soil bulk density, water content of the soil in the top horizon, and total pesticide mass applied were key parameters in estimating pesticide concentrations in runoff. The Agency also found that when pesticide properties were fixed, precipitation, followed by runoff curve number, were the most sensitive parameters in estimation of pesticide loads in runoff. Because watersheds are the units of analysis in SAM, soil heterogeneity, application area with respect to the pour point of the watershed, area of runoff-prone soils, and artificial drainage features (such as tile drains) also are expected to affect runoff concentrations. Additionally, soil mixing zone, short-term variability in rainfall intensity, inputs of water from sources other than precipitation, and biphasic degradation of pesticides may warrant consideration in additional sensitivity analyses. Moreover, the Panel recommended that outputs from SAM be compared to outputs of other models used by the Agency and others (such as SWAT (Soil-Water Assessment Tool). Finally, the Panel recommended that high-tier features of SAM should be preserved for internal valuations, and that systematic methods be developed to determine the relative strength of association between individual parameters and model outputs.

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 or 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?

Separate analyses of uncertainty in projections of flow and pesticide concentrations are necessary to examine parameter sensitivity. Strongly sorbing pesticides such as pyrethroids may move along with sediments to a greater extent than weakly sorbing compounds such as atrazine, which mainly are present in the aqueous phase. Sources of data include registrants, sometimes in partnership with local organizations or universities; research studies; studies conducted by the US Geological Survey (USGS) for the National Water Quality Assessment (NAWQA) program, and studies conducted by the USGS for estimating discharge and mass loads at different times and during different seasons.

Section 3: Input Data

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.

a. Please comment on any implications for using soil grouping classes for watershed-scale modeling.

Decisions about whether to group soil classes should be based on whether grouping is consistent with the objectives of the model. The rationale for grouping that appears in the charge question and background document is not primarily scientific but rather operational, and thus may not be consistent with the model objectives. The soil grouping that was conducted and used in SAM application resulted in little difference in estimated runoff volumes, pesticide masses, and peaks of pesticide concentrations. The results represent one pesticide; similar results may not hold for other pesticides with different properties. The Agency should consider disadvantages in grouping soil classes as model development continues and considers other pesticides and landscapes.

Q5. 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.

a. Please comment on the implications for aggregating spatial inputs across varying scales.

The feasibility of adjusting the resolution of spatial data and the physical, chemical, or biological rationale for adjusting the resolution of spatial data should be assessed separately. It is fairly common in spatial modeling to overlay data layers with different spatial resolutions. Whether doing so makes sense depends on the objectives of the analysis, the metrics being calculated, the variation in the variables represented in the data layers, and the resolution of the desired outputs. The resolutions of the soil and land-use data are similar, and combining these as the Agency has done likely would be well accepted. With the possible exception of montane areas, the density of weather observations should be sufficient for operational use of SAM. In the example application of SAM, the spatial resolution of the crop planting data used to identify the timing of pesticide applications does not match the resolution of the weather, soil, and land use data. Alternatives to the crop planting data used are suggested.

Section 4: Accounting for Time-of-Travel Effects

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.

a. 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.

There was agreement among the Panel that the incorporation of travel-time based convolution would significantly improve SAM's modeling performance for pesticide simulation at the predefined watershed outlet. The Panel requested clarification of the study objectives for incorporating mathematical convolution into SAM and justification of its implementation into the next version of SAM. Additional considerations on the flow and mass routing were suggested by the Panel, including baseflow and the transport processes from field to stream.

The Panel noted the potential impacts of the convolution on the SAM modeling capability for simulating pesticide spatial distribution. Water connectivity and watershed size could be critical factors on the implementation of convolution in SAM. In addition, the Panel recommended additional investigation on travel times in the NHD Plus version 2.

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.

a. ***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.***

The Panel was less convinced that the convolution approach as described could adequately account for pesticides that exhibit sorption or rapid decay in both water and sediment. The Panel identified additional compartments that need to be considered for representing chemical fate and transport in surface water. They include [1] dissolved organic carbon (DOC) or total organic carbon (TOC), and [2] total suspended sediment (TSS).

The Panel noted that sediment sources and transport are not sufficiently modeled in the current and proposed versions of SAM. They suggested a series of models for this purpose, including: [1] one for erosion to move the sediment from within the field to the channel; [2] a different model to move the sediment from the channel into the stream network (including long term

storage in various channels); and [3] an in-stream sediment transport model that accounts for deposition and resuspension in the stream and the floodplain.

The Panel concluded that fate and transport of reactive and/or sorbing chemicals in water column could be incorporated with the proposed convolution approach, while pesticide fate in bed sediment may require a separate computation module. Relevant algorithms can be taken from the USEPA Varying Volume Water Model (VVWM). Detailed simulations on pesticide fate in bed sediment would also support further chronic ecotoxicology risk assessment of pesticides.

b. 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.

The Panel provided a comprehensive list of data sources potentially useful for representing the benthic sediment layer and associated pesticides in surface waters at varying spatial scales. The Panel also noted that the transport of non-pesticide trace chemicals (such as trace elements, total phosphorous, hydrophobic organic chemicals) could be considered as surrogates to help inform the mechanisms affecting the fate of strongly-sorbing pesticides.

Section 5: Defining the Likely Pesticide Application Window based on Crops and Weather

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?

Growing degree days (GDD) and crop growth models may be more accurate for determining the planting window than the Plant Hardiness Zone map and weekly crop progress report. Sources of data on the former variables may include the weed science literature and university extension web sites. There also may exist regional data on soil moisture and temperature that can be used to estimate planting dates. For post-emergent herbicides or other chemicals, it may be useful to apply a crop growth model and other climate data to predict or validate disease intensity.

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.

Collaboration with industry (such as commercial applicators), extension service personnel, and USDA Risk Management Service will enable the Agency to better represent and understand planting decisions by farmers and typical planting windows over multiple years. Trafficability of heavy equipment in the field is a key driver in herbicide applications. SAM can estimate the moisture profile in the soil, which can be used to determine equipment trafficability.

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.

The Agency has the option to use different crop simulation models to examine the growth stage of a single plant or multiple plants in ecosystems throughout the country. The Agency can run these crop models with an early planting date and then can shift the planting date by days or weeks until the model-predicted concentrations match the observed data reasonably well. This calibration of the model with empirical data will allow the Agency to obtain a relatively accurate understanding of the window of application of pesticides in a given year.

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).

a. Please comment on the use of empirical data or models to define the distribution of pesticide applications within an application window.

The Panel agreed with the Agency that defining pesticide application windows and the distribution of applications within these windows will have a large impact on model outcomes. There was agreement that empirical data and models can be used to guide the distribution within application windows. The examples presented by the Agency in the SAM background document are a clear illustration of how this can be done. The Panel recommended other sources of data that are linked to crop insurance that at minimum can guide crop planting and harvest dates. Crop specific data are available from the USDA Risk Management Agency (USDA-RMA) for most counties in the USA. These data include the first and last dates when crops can be planted to be eligible for insurance. USDA-RMA also collects acreage planted data. If USDA-RMA can release this information to the Agency, it may be used to "ground-truth" crop acreage data obtained from crop data-layers.

An alternative way to estimate first planting date suggested by Panelists focused on soil temperature. Soil temperature is a key determinant that growers use to establish when crops can be planted. Soil temperature and recommendations for planting various crops can readily be obtained from State Agricultural Extension offices, while soil temperature data can be obtained from both local and national networks. These data likely can be compiled in a data-layer in the model. Alternatively, soil temperature can be estimated in PRZM. There is a routine in the model that estimates soil temperature that is linked to pesticide degradation kinetics. With minor

modification, the PRZM soil temperature estimates may be extracted and used to predict planting dates. Once soil temperature reaches the acceptable threshold for a given crop, it can be assumed that farmers will plant crops as quickly as possible. The logic behind this is that "late-planting" typically reduces yields. A factor that will retard planting is rain, because of "trafficability" issues that may limit the ability to drive heavy equipment such as tractors on a field. The Agency was encouraged to look for other examples where soil water content and trafficability were linked.

Regarding this point, the Panel focused on the use of tractors for pesticide application and pre-emergence herbicides. Panelists noted that aerial applications must also be considered. With aerial applications, large areas may be treated on a single "favorable" day. Consultations with commercial pesticide applicators about aerial applications may provide additional insight. In the case of fungicides and insecticides, it was suggested that crop growth models and decision support tools might be useful guides. There are many crop models available with varying levels of sophistication and data requirements and decision support tools that aid in determining when fungicides and or insecticides should be applied. In calendar-based spray programs once the crops reach a specific growth stage it is reasonable to assume applications will take place at a defined interval, such as weekly or biweekly. Growth stage can be defined empirically or with crop growth models.

Detailed Panel Recommendations

Section 1: SAM Conceptual model

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.

Conceptually, the Spatial Aquatic Model (SAM) is like other watershed scale pesticide fate and transport models (e.g., SWAT (Soil Water Assessment Tool) and MIKE-SHE (Système Hydrologique Européen), in that SAM spatially and, to some degree, temporally integrates landscape scale variations in soil properties, weather, runoff, and the timing and frequency of pesticide applications. In that sense, the Panel felt that SAM has a sound scientific conceptual basis. In addition, SAM will enhance the Agency's ability to evaluate pesticide aquatic exposures particularly in comparison to currently used models that evaluate runoff from a single field, and which assume uniformity/non-variance in soil properties, slopes, spatial rainfall differences, and timing of pesticide applications. Also, the Panel concurred with the advantages of SAM identified in the background document prepared for the FIFRA-SAP meeting. This included SAM's ability to account for: 1) the heterogeneity in soil, land cover, and hydrologic conditions within each contributing drainage area; 2) geographic and temporal differences in weather, crop growth and timing, watershed area, and type and flow characteristics of receiving waters; and 3) the interplay between catchment area and pesticide application dates.

In addition, the Panel commended the Agency for efforts to reduce code inefficiencies in SAM's fate and transport sub-model PRZM 5, to minimize SAM's parameterization requirements, and for plans to implement SAM on the internet. The Panel noted that making SAM publicly available on the internet will likely increase transparency in pesticide risk assessments and can potentially educate the public on processes that lead to regulatory decisions. However, the Panel provided the following cautions. In an example cited in the SAM background document, it was reported that to reduce processing time, the depth of runoff interaction with surface soil was uniformly set to 2 cm. As described in responses to question 2b, this assumption may not hold especially in regions with sandy surface soils. Panelists encouraged the Agency to more carefully evaluate this and other assumptions before they are implemented in SAM. In the case of internet implementation another Panelist suggested that the Agency consider including a pesticide properties database. Databases of pesticide properties are commonly included in pesticide fate and transport models, and their inclusion can facilitate and enhance model use.

While there was general agreement that SAM has a sound conceptual basis, it was emphasized that SAM is a work in progress. Many important SAM components although discussed in the background document and in Agency presentations are at best in early development stages. This includes processes such as spray-drift, sediment transport, attenuation during transport, and crop growth and soil conditions as they relate to pesticide application. In short, SAM appears to be

technically and conceptually sound, but as described by the Agency, further development is needed before SAM becomes a fully functional model.

Regarding conceptual model descriptions in the SAM background document, one Panelist felt that it was difficult to identify a single conceptual model noting that no figure or section in the background documents or in presentations at the meeting was characterized as "the conceptual watershed model." The Panelist further observed that the closest approximation to a conceptual model was Figure 3, and stated that in general, conceptual models present hypotheses about the series of causal relations between one or more response variables, and the natural or anthropogenic factors that directly or indirectly affect the values of those response variables. Quantitative implementation of conceptual models allows those hypotheses to be tested (i.e., confronted with data). Figure 3 appears to confound hypotheses about exposure to pesticides with data sources and methods for testing the hypotheses.

The Panelists linked these comments to the charge question that suggested that the response variables were spatially and temporally variable in pesticide concentrations in water. Accordingly, the Panel suggested that the conceptual model should identify the factors that directly and indirectly affect spatial variability in concentrations, and temporal variability in concentrations, and the relations among those factors. For example, one might hypothesize that precipitation (probably not restricted to rainfall)—an indirect effect on concentrations—affects runoff, which directly affects predicted pesticide concentrations.

It was also observed that many of the polygons in Figure 3 ultimately might become elements in the conceptual model. This was identified as a strength, with the recommendation that polygons be culled, and be presented in a relatively linear manner to highlight the main associations and relationships, which would be tested via quantitative models. For example, it is unclear how registrant studies directly or indirectly affect spatial and temporal variability in pesticide concentrations in water. The studies might contribute to parameterization of models, but the studies do not actually affect concentrations.

In addition to the recommendation to improve the clarity of the conceptual model descriptions, the Panel suggested that the model explicitly include interactions between pesticide concentrations and management practices. There is ample evidence that practices such as conservation tillage and edge-of-field buffers may control runoff and reduce pesticide loading into water bodies. The inclusion of these and other management practices in SAM was identified as an opportunity for the Agency to help internet SAM users gain insight to the value of these practices. It was acknowledged that to some degree, tillage is addressed in curve number selection in PRZM. However, this may not be the most effective surrogate, and management data of these types (tillage) are not effectively captured in crop data layers derived from USDA reports.

Other limitations of SAM discussed by the Panel were linked to hydrologic processes. One Panelist suggested that SAM could be described best as a semi-distributed model since it is not completely distributed in a hydrologic sense. This is a conceptual element that may limit SAM's adequacy to simulate watershed scale processes such as routing flows and residence time in streams and intermediate water bodies, among others. The weighting of soil, vegetation, and

climate in SAM is a shortcut to this type of hydrological modeling. This may be acceptable for rapid assessment, but more rigorous pesticide aquatic exposure evaluations will require more comprehensive hydrologic models including routines that explicitly account for elevation and runoff routing between landscape units and for subsurface flow. The latter is linked to widespread use of tile drains in the midwestern USA and the importance of lateral subsurface flow in the hydrologic cycle of the southeastern USA. It was recommended that both tile and lateral subsurface flow be explicitly described in SAM, since they contribute to baseflows in streams and rivers, and to seepage in ponds, lakes, and estuarine environments, and can carry substantial pesticide loads (Kladivko et al., 2001; Potter et al., 2015).

Related suggestions were to include a model compartment that specifically describes hydrologic responses of impervious areas and other non-cropped areas, and proper calibration. For example, a Panelist indicated that curve numbers used in PRZM can be calibrated and not assumed to be fixed. In addition, the importance of unpaved roads to sediment loads in some watersheds was described. It was also recognized that pesticide degradates are handled in PRZM, but this is not obvious to model users who may not be familiar with PRZM's inner processes. In the interest of transparency, a compartment in the conceptual model that shows that pesticide degradates are formed and that subsequent degradate transport is evaluated was recommended.

Finally, the Panel indicated that there might be different versions and different conceptual models of SAM depending on desired model outcomes. It was recommended that the Agency consider creating a "SAM-MAX" version whose goal would be to predict maximum concentration to identify "hotspots". This would be analogous to the current field-pond model conducted simultaneously for 10,000 catchments, and is very close to the SAM alpha 2.0 version. It was suggested that in this version, it might be better to use another more stable statistic, such as the 95th percentile. Maximum values are outliers. However, the choice of the statistic goes back to the goals of the model run. It was also noted that the amount of pesticide that is "applied" in the model is the greatest driver for the stream concentration (e.g., twice the amount applied should yield about twice the concentration), and the decision on how much is applied in SAM is much more complex than the currently used model with a single field. Thus application amounts, for example maximum label rates to all fields, should be considered carefully and linked to the goal of the model run.

A second version could be described as "SAM-Distribution" whose goal it would be to provide better spatial and temporal resolution throughout watersheds, and to yield concentration predictions that are close to reality across the range of concentrations. Here performance metrics such as the Nash-Sutcliffe coefficient or Root Mean Square Error could be used to assess model performance.

Switching between the two or more versions of SAM is made possible by the Agency's use of a modular approach and the ability for data layers to be interchanged. This could be taken a step further, where a menu of subroutines could be developed that could be selected depending on the goal of the model. This could be done for the hydrology portion, i.e., the current curve number routine may the simplest approach that fits SAM-MAX, but better estimates of runoff, based on a mechanistic model, could be substituted if greater accuracy is needed. The pesticide runoff

model routine is another example. These routines can be found in many models and can serve as the sources for the menu of options.

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?

The Panel recommended improving the clarity of the conceptual approach in the documentation. The discussion of the conceptual approach would benefit from additional background. For example, the Panel suggested providing a discussion and clarification of the goals for the model.

An expanded narrative is needed to describe how the Agency decided to pursue SAM, why other available models were considered inadequate, and what factors drove the choice of the methods included in SAM. Such discussion might address questions such as what outputs the model can and cannot provide, the physical and chemical processes or cases that the model cannot address, how the model will be used, and the primary model assumptions and limitations. Until these questions are addressed, it will be challenging to explicitly state the objectives for the model or to gauge when the model is ready for use.

A detailed written statement of the intended regulatory uses of SAM should be developed as recommended in EPA's guidance on the development, evaluation, and application of environmental models (USEPA, 2009). Intended uses of SAM in ecological and human health risk assessments are not well explained in the current documentation. Thus, it is difficult to assess whether increasing the model complexity will better meet modeling objectives, or whether the outputs provided by SAM will be sufficient for such assessments. Similarly, it is difficult to assess whether simplifications (addressed primarily in Charge Question 2b) are warranted.

The Panel recommended that the Introduction in the SAM background document be revised to include a review of the literature on watershed-level modeling of water quality. This is an area of substantial research and application that includes numerous water quality constituents, including pesticides. It is worthwhile to explain how SAM complements or builds on, rather than duplicates, existing models and methods, and is thus is an efficient use of limited government resources.

Several well-established and well-cited models of watershed-level hydrology and chemical transport can simulate movement of agricultural chemicals. The Panel recommends that the Agency describe how SAM compares to these existing models in terms of efficiency, accuracy of predictions, calibration potential, incorporation of Best Management Practices (BMPs), representation of water flows and routing, and so forth. Some of the approaches used within these models might be adopted for use in SAM.

The conceptual model (which is not synonymous with a conceptual approach) is not explained clearly. To maximize clarity and transparency, the response variables (e.g., pesticide concentration in water, spatial or temporal variance in the concentration), covariates hypothesized to directly affect response variables (i.e., direct drivers), and covariates hypothesized to affect direct drivers (thus to indirectly affect the response variables) should be

specified, and the rationale for the hypotheses explained. Margoluis et al. (2009) may be useful background in developing a more explicit conceptual model. The level of uncertainty associated with the relations between indirect and direct drivers, and between drivers and the response variables, also should be explained. That is, explain what is reasonably well known, what is assumed, which of the hypotheses represented in the model cannot adequately be evaluated at this point in time, and what would be necessary to evaluate those hypotheses.

Discussion of how the conceptual model will be evaluated quantitatively—in essence, a flow diagram for SAM—should be presented separately from the conceptual model of an aquatic system. Additionally, it might be useful to discuss the extent to which reduction of each uncertainty is likely to inform decision-making, and the level of investment of time and resources that the Agency feels is warranted to reduce these uncertainties. The latter two questions can be analyzed quantitatively as expected value of perfect information or expected value of partial information (e.g., Runge et al., 2011; Moore and Runge, 2012).

The simulation domain was not clearly defined. The Panel was provided examples of SAM application to agricultural watersheds, but the proposed simulation domain of the final model was unclear. For example, will highly impervious urban areas be considered? Will the model be applied to rice-production regions, and consider point sources such as discharge from wastewater treatment plants?

Documentation of assumptions and algorithms should be expanded and clarified. In particular, key equations in addition to the transport equation should be provided. Methods for quantifying processes in addition to runoff, including leaching and degradation, should be documented. The appendices are helpful and contain equations that perhaps should also be included within the main document.

The figures included in the background section of the document are useful. Additional figures that describe SAM and processes considered in SAM would also be useful. As the text is updated and revised, the Panel recommends considering which figures may help improve readers' understanding of the model. On a related note, it may be worthwhile to include some of the graphics from the presentation in the document.

Table 1, which compares the current aquatics screening models used by the Agency and SAM, was quite useful, but assumes considerable knowledge of the Agency's current methods. Additional references to current approaches would improve the utility of the table.

Other model documents (e.g. SWAT) may serve as good examples to emulate and improve upon as the SAM background and conceptual approach sections of documentation are revised.

Both PRZM and SAM are referenced in the text, and it was not always clear which model was being discussed. However, the presentation of the spatial approach of SAM compared to the previous modeling framework is clear. The connection among SAM sub-modeling units was not clear. The appendices are helpful, but key assumptions or equations should be included in the main text.

The background references both SAM scenarios and PRZM scenarios. To reduce confusion, the use of *scenario* may need to be qualified. For example, the sensitivity analysis for soil grouping is based on "IL corn scenario", might be changed to "PRZM scenario for IL corn".

The Panel suggested that the Agency not characterize model outputs as identifications of *vulnerable* locations *per se*, but SAM does help identify sensitive locations where highest pesticide concentrations may occur. The model estimates pesticide concentrations, not ecological, human health, or other responses to these exposure concentrations. Nevertheless SAM may be helpful in better defining where subsequent monitoring and other ecological and human health assessments should be focused to address these concerns. When the same rate of a pesticide application is used for the entire area of the model, then vulnerable locations are the same as sensitive locations. But when the varying application rate is used (which is the reality), then the two diverge.

The Panel also suggested that the Agency consider adding the capacity for users to estimate the sustainability of pesticide-application practices and support the objectives of reducing the amount of pesticides applied, reducing overall annual loadings, and reducing expenses. In South Carolina, planting of cover crops to maximize soil condition has the potential to not only to reduce N and P fertilizer applications but to also reduce pesticide use by up to 20% (Buzz Kloot, University of South Carolina, Arnold School of Public Health personal communication).

For a given input variable, it may be feasible to use sources that vary among regions yet collectively encompass the full extent of the United States. For example, the regional accuracy of different sources of 30-m land-cover data may vary.

The USGS Land Cover Institute (http://landcover.usgs.gov/) recently released a time series of data on land use and land cover from 1973 – 2000 for the conterminous United States (Falcone, 2015). These data may be useful for estimating past scenarios or exposures.

Groundwater contributions to surface flow, and associated pesticides carried with the groundwater, warrant consideration in some regions. In coastal areas, groundwater discharge may exceed surface runoff under certain conditions. For example, Moore (2007) estimated that > 60% of the freshwater input into the south Atlantic comes from subsurface flow. Case studies of pesticide use in the coastal zone, particularly in high-use areas such as golf courses, often with year round pesticide usage (average > 80 PAI/acre/year) and in irrigated areas, may provide opportunities to apply the model to evaluate subsurface pesticide inputs to receiving waters.

In graphs that compare the results of SAM to empirical data, the Panel recommends clarifying the discrepancy between modeled pesticide levels and surface water monitoring data, including the direction and magnitude (µg/L) of the discrepancy. These metrics will help evaluate whether SAM results are within the Agency's target range of acceptable variation (1-5X).

Section 2: SAM Model Components and Approach

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.***

Based on the information presented, the separation of independent processes makes sense and results in improved computational efficiency that will likely be beneficial to continued scaling up of the model to large areas. However, providing a comprehensive response to this question is challenging without additional details of the suggestions to Question 1 (e.g., better definition of the model goals, how it will be used).

Computing power is readily available, and will be even more available in the future. Thus it is not the issue that it once was and will be even less of an issue when the model is ready for deployment. A challenge faced by the SAM team is to insure the desire to improve model efficiency and to reduce time for calculations does not interfere with future model additions or considerations. For example, does separation of processes complicate or negate the ability to consider management practices, subsurface drainage, or other processes that may be desirable to include in SAM in the future?

Soil erosion is not currently reflected in the model. Shape of fields, size of fields, and other field properties are potentially important considerations in soil erosion estimation. Therefore, making computations independently may impact some factors shared between routines.

One potential problem with the use of independent components is that if one component's computational engine is erroneous because of over simplifications or omissions, the error propagates with the other subsequent components. So, in order for this to work, the higher order components should be somewhat 'fool-proof'. The potential for this to occur is minimized if flow and concentrations are solved simultaneously. The panel can see this propagation effect between SAM 1 and SAM 2. One must add a correction factor or process to better represent the results. For example, SAM 1 does not include travel time using convolution while SAM 2 does. The model could be expanded to 'routing' the runoff from the 'sub-computational' units, wherein topology is considered explicitly to better estimate the hydrography and hence both flow and concentration.

The spatial scale for SAM modeling capability is not well defined, i.e., how large of a watershed it will be applied to. The use of simulated flow data from NHD Plus actually sets an upper bound for the watershed size. Very large watersheds are usually associated with water diversion and controlled discharge from dams, so the simulated flow rates may not be consistent with NHD

Plus. A comparison between NHD Plus flow and USGS measured flow at watershed outlets at national scale may be needed to understand if this is a significant issue.

Clarification of what data will be stored on the cloud should be provided. Based on information in the documentation provided, this was unclear. This clarification should include what raw data will be stored as well as the types of pre-computed data from the process representations addressed in this question.

The baseflow approach documentation needs further attention, as it is somewhat unclear how this was done and whether results of baseflow within SAM match other approaches. Experience with the Curve Number (CN) runoff approach suggests it is often necessary to reduce CN when using certain baseflow separation approaches on observed flow data. Presentation of results of baseflow estimation from the model and comparison to baseflow data would be helpful.

The descriptions of SAM components are not consistent between the figure (Fig. 7) and the text. For example, page 31, "*Super PRZM Hydro uses recipes to define the scenarios...*" This is not reflected in Figure 7. In Figure 7, "scenarios" are labelled as input to Super PRZM Hydro.

The three components (scenario, hydrology, and pesticide) and the two modeling stages ("pre-processed" and "chemical/site specific", Fig 7.) are well established for the alpha version 1.0, but not for the newly developed functions for 2.0, such as soil grouping and water and pesticide routing. Figure 7 may need significant changes to include those new functions because they are associated with multiple components and modeling stages. For example, the water and pesticide routing algorithm is based on watershed hydrology data, but also is dependent on the user-specified location of watershed outlets (pour points).

"Hydraulic flow length (L)" is used in the calculation of time of concentration (appendix 2-A). How this parameter is estimated for each scenario in SAM is not mentioned in the documentation. Unlike runoff generation, which is mainly determined by field area, soil erosion is related to the shape, dimension, and flow pathway of a field. The Agency provided default L values for a farm pond scenario and an index reservoir scenario. Estimation of L values could be difficult for SAM scenarios because they could be spatially disconnected.

If the Agency determines SAM should consider subsurface drainage, areas with subsurface drainage might be identified in one of several ways. There are United States Geographic Survey (USGS) National Water-Quality Assessment (NAWQA) derived spatial data layers of estimated tile drainage and baseflow index (and many other spatial parameters). These can be obtained through the Spatially Referenced Regressions on Watershed (SPARROW - http://water.usgs.gov/nawqa/sparrow/) attributes model development team. In many Midwestern states, soils labeled such as B/D are typically subsurface drained if they are in agricultural production.

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.

While the Agency's efforts to reduce and eliminate model computational inefficiencies are commendable, there is need for more careful assessment. In this case it was reported that the zone was treated uniformly to a depth of 2 cm with regard to pesticide extraction. Model code in PRZM was modified to reflect this, and it was reported that this change had a negligible impact on model outcomes. This indeed may have been the case in the scenario evaluated, but metrics were not provided.

The improvements in the computational efficiency of the model code and algorithms will be important in scaling SAM as described. The primary example presented, which simplified soil surface into a single layer, indicates significant gains in efficiency are possible within the model. Such improvements are certainly worth exploring.

A more clearly articulated vision and requirements for the model (Question 1) would serve as a guide to help the Agency, the Panel, and others evaluate impacts of simplifications such as use of a single soil layer.

Key questions that should be considered when evaluating potential simplifications in algorithms and code include the following: Does this assumption limit future development? For example, does this impact the ability to consider pesticides leached that may be intercepted by subsurface drains and return to surface flow? Will computational power be a factor when the model is ready to be applied?

Porting the model to a cluster may be the best strategy, especially when SAM is applied at the national level. Simplifying the soil discretization, since it is only for the first 2 cm layer, may not have much of an effect on computational efficiency, especially at the watershed scale when all model computations are combined to produce watershed level results. Experimenting with the 2 cm mixing layer should be done to determine how important this assumption is for other cases, such as on sandy soils or when irrigation is used. The mixing layer depth could potentially be a calibration parameter of the model.

The 2 cm assumption routine is also probably not compatible when estimating pesticides that are strongly sorbed to sediment. This will involve an erosion-type model that will work on surface transport, but in which no pesticide is actually at the surface with the 2 cm assumption.

There are broad areas across the country where the assumption of 2 cm single soil layer may not hold, in particular where surface soils are sandy. Studies conducted in the Atlantic Coastal Plain of Georgia with rainfall simulation found that post-application irrigation incorporation, that did not generate runoff, reduced runoff losses of two mobile herbicides, metolachlor and fomesafen, by more than 50% during large simulated storms 1 day after application (Potter et al., 2008 and

2011). Irrigation incorporation for "activation" is commonly recommended on pre-emergent herbicide labels. In these studies, where surface soils were 85 to 90% sand, the reduction in losses could be linked to movement of the herbicides over short distances in the surface soil leading to the conclusion that pesticide extraction is sensitive with regard to depth over short distances (mm) in the surface soil. This issue was addressed in the late 1970's and 1980's (see review by Ahuja, 1986). It was recommend that extraction in the top 2 cm be described with a simple exponential decay function with depth. Some rate constants are available; thus implementation in SAM (via PRZM) would be relatively straightforward. It is highly recommended that the Agency pursue this. The depth of the extraction zone and extraction rates that occur within it are critically important to more accurate assessments of runoff losses.

The Agency may want to consider other soil layer depths or options that include other depths to account for practices such as incorporation, and seed treatment that results in placement of pesticides below 2 cm.

Differences in modeled results with and without the single 2 cm surface soil layer are presented. However, statistical analysis for comparison of modified and original results would be useful for the single 2 cm surface soil layer versus the current approach in PRZM.

The Panel noted that pesticide volatilization from soil and canopy is not considered in the simplified model. This may be an important fate process for some pesticides. Furthermore, according to the background document, pesticide application method (parameter "CAM" in the PRZM5) is not currently considered as an input in SAM. In this case, the initial distribution of applied pesticide between canopy and soil, and the soil incorporation of pesticide reaching the soil, should be documented. There is a need to consider the pesticide application method as part of the runoff calculation. Many methods of pesticide applications (such as foliar, seed treatments, surface applied to no-till, incorporation) are not compatible with the assumption of an equal distribution over the top 2 cm. The Panel understood these limitations would be addressed in the future.

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?

In SAM, the key parameters for estimating pesticide concentrations and loadings in runoff are: a) total pesticide mass applied, b) timing of pesticide application and rainfall, c) pesticide half-life and sorption coefficient, d) runoff curve number, and e) soil properties including organic carbon, available water, and bulk density. It was also noted that when the rates of application as well as the sorption and degradation parameters for the pesticides were fixed, rainfall with respect to the time of pesticide application appeared to be the most sensitive parameter, followed by the runoff curve number. The background document also notes the key sensitivities of the watershed (slide 48 – based on monitoring studies).

The Panel recommended that several additional parameters to be included in sensitivity analysis for future versions of SAM:

a) *Varying depth of soil mixing zone*: The current version of the model converts 10 distinct zones in PRZM 3/5 for soil to a fixed depth of 2 cm. Will it make any difference in runoff if the depth is reduced or increased? Will it matter if the number of zones is reduced from 10 to a smaller number (e.g. 3)?

b) *Short-term variability in rainfall intensity*: Currently, runoff volume is modeled on the basis of average daily precipitation data. However, rainfall intensity is not always uniform over a 24-h period, and mobilization of pesticides may be sensitive to intensity as well as total runoff volume. The Agency should consider investigating the availability of rainfall intensity data, and to determine if considering intensity makes a significant difference in estimated pesticide concentrations and loadings. The Agency could also consider combining precipitation for contiguous rain events over several days, and use the totaled precipitation for a single day precipitation amount to determine if the increased intensity has a significant impact in runoff volume. Another consideration for sensitivity analysis would be to vary the same amount of rainfall over different time periods (e.g., 24, 12 and 6 hours), to determine any effects of increased intensity.

c) *Non-precipitation water input* (such as irrigation and incidental runoff in arid areas): Currently, the model does not account for irrigation and other water input into the system. For sensitivity analysis, the impact of irrigation can be simulated by adding the amount of irrigation water to daily precipitation. However, in that case, the curve number needs to be adjusted to account for seasonality and antecedent moisture conditions.

d) *Uncertainty in soil and pesticide fate parameters* (f_{oc}, K_{oc}, $t_{1/2}$): These parameters should be varied across the reported ranges of values in SAM simulations. For example, atrazine may not represent strongly sorbing or highly stable pesticides and atrazine may not be the best choice of pesticide because of the potential for highly variable soil degradation. In many studies across the country, atrazine accelerated degradation following a single treatment has been observed. Half-life values in this case may decrease to 2 days or less (Krutz et al., 2008; Jablonowski et al., 2010; Potter et al., 2013). Furthermore, use of a first-order kinetic model to describe degradation under the above conditions considerably overestimates half-life. Biphasic models are much more effective under these conditions. Unfortunately the potential to use this approach was turned off in PRZM 5. This option should remain in SAM.

e) *Data on weather and climate*: The Panel recommended that the Agency evaluate the extent to which model outputs vary as a function of data sources—for example, the data sources currently used versus finer-resolution downscales from various sources and PRISM (not to be confused with PRZM; see http://www.prism.oregonstate.edu/). The quality of input data likely will vary depending on the geographic region (some sources are more accurate for the northeastern United States, others for the southwestern United States). Although Panel members agreed that data need to be available for the entire U.S., they also felt that data need not be from the same source or database, provided that the accuracy, applicability, and coverage of these data are well

understood. The Panel suggested that an incremental increase in the accuracy or resolution of a given source might not warrant the resources necessary to frequently update data inputs.

f) *Use of components of Hydrologic Simulation Program-Fortran (HSPF) or other Agency models*: Some Panel members feel that some hydrologic simulations within Hydrological Simulation Program – FORTRAN (HSPF) or Better Assessment Science Inegrating point and Non-point Sources (BASINS) models (EPA products) should be made available within SAM.

g) *Use of quantitative measures of model predictions*: The outputs from SAM are shown in graphical format. Visually, it is difficult to judge the relative degree of difference between the observed and simulation results. SAP members feel some quantitative measures such as root mean square error (RMSE), R^2, or Nash-Sutcliffe model efficiency (NSE) coefficient should be used to develop and illustrate relationships between observed and simulated results.

h) *Relative importance of parameters*: It has been hypothesized that rainfall, mass and rate of pesticide application, and runoff curve numbers are the most sensitive parameters. Although their influence seems intuitive, it is unclear how the Agency prioritized these parameters as presented in the background document. Techniques such as Latin Hypercube sampling or Analytic Hierarchy process (AHP) may be used to systematically evaluate the relative importance of these parameters.

i) *Preserving high-tier features within SAM for internal evaluation*: The Agency might consider a higher tier version of SAM for internal use or for sharing with specific researchers for testing and evaluation. In doing so, it will be able to preserve the distributed hydrology options as in other Agency models. The Panel thinks that developing a family of SAMs for various applications may be useful. A strategy to compare the results of SAM with other Agency products should be devised.

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?

The Panel feels that the Agency needs to separate the uncertainty in estimating runoff volume from the uncertainty in estimating pesticide mobilization, partitioning, and fate. Doing so will make it easier to conduct the sensitivity analysis described in the Panel's response to Q3a. For example, the Agency's model pesticide, atrazine, has weak sorption towards sediments. Whereas, strongly sorbing pesticides (e.g. pyrethroids) behave fundamentally different than atrazine. This points to the need for suspended and bedded sediment data, as well as water column data, when extending SAM to a broader universe of registered pesticides. Thus, the need exists for data sets that have observations of pesticides for both water column (dissolved) and sediment (sorbed) data at the same time. The Panel acknowledges that such paired data sets are rare.

To complement existing monitoring and fate information, the Panel members suggest that the Agency look into studies sponsored by pesticide companies or registrants. For example, some companies have monitored chemical application as well as runoff and surface water concentrations in specific watersheds. These data will be useful in future evaluations of SAM performance.

The effect of various management practices on water quality in well-instrumented sites or watersheds has been targeted by the research community. Such data are available in the literature, or by contacting the researchers directly. The Panel members also recommend that the Agency collaborate with state agencies and utilities that monitor pesticides in specific watersheds. As one example, the Ohio River Sanitation Commission (ORSANCO) monitors water quality in the Ohio River at regular intervals and during chemical spills. The Panel recommends the Agency look into the feasibility of obtaining pesticide data from cooperative organizations such as ORSANCO.

The USGS and other agencies and institutions are now monitoring nitrate in real time in selected watersheds. The Panel recognized that nitrate might not be an appropriate surrogate for many pesticides. However they recommended that the Agency examine whether such data for nitrate can be used to test model predictions for some pesticides. The real time nitrate data can also prove useful as a non-conservative reference chemical for areas with missing data.

Another source of data that could be used for model testing and evaluation is estimated daily concentrations from long-term, but infrequent stream measurements. Weighted regressions on time, discharge, and season (WRTDS) (Hirsch et al., 2010) is a US Geological Survey modeling approach that uses historical daily stream flows with measured chemical concentration to estimate daily concentrations and daily loads. Also, data from small-scale studies may be available through the Water Quality Portal http://waterqualitydata.us/.

Section 3: Input Data

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.

a. Please comment on any implications for using soil grouping classes for watershed-scale modeling.

Soil classes were grouped on the basis of factors that were believed to have the greatest effects on pesticide accumulation in water bodies due to runoff and erosion. The major factors affecting pesticide transport from agricultural fields in a given watershed to water bodies within that watershed that were considered by the Agency included hydrological soil group (A-D), slope (<2%, 2-5%, 5-10%, 10-15% and <15%), soil erodibility potential, which was based on the K factor (<0.1; 0.11-0.20; 0.21-0.32, 0.33-0.43, 0.44-0.66), and soil organic matter (<0.5%, 0.5-2%, 2-4%, 4-6%, 6-8% and >8%; these were values reported in documentation but ranges

overlap as reported in the Agency document. The Panel recommends a revision of these classes so they do not overlap. The number of levels of each factor resulted in 600 soil groups.

There was little difference between individual soil classes and groups of those classes with respect to estimated runoff volumes, pesticide masses, and peaks of pesticide concentrations. For station MO-01 (Missouri Watershed), 40% of model estimates of peak atrazine concentrations were based on either soil classes or soil groups that underestimated measured concentrations by 22-26 µg/L (a factor of 0.7); and 60% of estimates were based on either soil classes or soil groups that overestimated peak concentrations of atrazine by <32 µg/L (a factor of < 0.32) (Figure 10, page 63). This limited test indicates that estimates based on soil classes and soil groups are consistent, and that both methods are fairly accurate.

Decisions about whether to group soil classes should be based on whether grouping is consistent with the objectives of the model. The charge question suggests that the criteria for whether to group soils relate to runoff and erosion. However, the rationale for grouping that appears in the charge question and background document is not primarily scientific (e.g., "we think that multiple soil classes have similar relations with runoff and erosion") but operational (e.g., "lessen the number of scenarios and improve computational speed of the model"). Furthermore, it does not appear that an *a priori* value, or range of values, was established to determine whether soil groups captured the range of variation in the individual soil classes. Supporting material in Appendix 3-F does not clearly identify hypotheses, methods, results of tests of the hypotheses, and inferences about whether the criteria for grouping were met.

As noted above, the comparisons of pesticide estimates that were based on either soil classes or soil groups suggest that reducing the number of soil classes will not compromise reliability of model outputs or inferences. Providing more-comprehensive statistical analysis of the results of the comparisons would offer more insight than simply presenting the maximum differences in estimated pesticide concentrations.

The Panel recommends that the Agency consider trade-offs in grouping soil classes for future analysis. For example, will soil properties that may differ from those considered in the analysis of atrazine be highly relevant for projecting concentrations of other pesticides? Different grouping criteria may need to be explored for other pesticides (such as those with high sediment adsorption) or other environmental conditions. If many grouping criteria or many groups are necessary, the value of grouping may decrease.

Hydrologic soil groups such as B/D potentially should be maintained rather than subsumed in larger groups. Hydrologic soils may be subsurface drained and will behave differently than other soils within hydrologic group D.

The Panel suggested that the Agency compare model-projected and measured concentrations of a pesticide with a higher sorption coefficient than atrazine, and evaluate the extent to which use of soil groups affects the modeled concentrations of such a pesticide. Atrazine behaves differently than many other pesticides.

The Panel also recommended that the Agency consider use of one or more case studies to assess how irrigation may change the relation between grouping of soils and model projections.

Different soil-grouping criteria may be required for modeling concentrations of different pesticides, for modeling in irrigated systems, and so forth. If different applications of SAM require use of different soil groups, grouping soils may not be warranted.

The current Agency method overlays a single soil group (e.g., hydrologic group C or D) that has high runoff potential with a single major crop to predict pesticide loading across a watershed. By contrast, SAM overlays all soil groups on the cropland. The new SAM method is perhaps a more accurate approach for assessing interactions between soil groups and crop types because it uses different soil groups to derive loading on the basis of curve numbers. The method for assessing interactions between soil groups and crop types in SAM is a more accurate approach because it uses different soil groups to derive loading on the basis of curve numbers. The approach in SAM is similar to that of Blair et al. (2014), who developed the Surface Water Runoff Modeling Systems (SWARM), which uses curve numbers and the unit hydrograph methods of USDA's Natural Resources Conservation Service. Blair et al. (2014) found that imperviousness in urban areas greatly increased runoff volumes and thus used it as a covariate in derivation of modified curve numbers (Blair et al. 2014).

The USDA's Cropland Data Layer recognizes 111 agricultural land-cover classes and a total of 133 land-cover classes. The Agency proposed to derive curve numbers on the basis of a much smaller group of classes. Given the similarities in agricultural land uses to be grouped, the Panel expected that the effects of grouping land-cover classes on modeled runoff would be negligible.

It may be useful for SAM to account for no-till farming methods that typically reduce surface runoff and techniques, such as plasticulture, which will increase runoff for crops such as tomatoes and strawberries. Comparisons of simulated runoff of organochlorines and pyrethrins, applied at maximum label rates to conventional and nonconventional (e.g., plasticulture) tomato fields, suggested that runoff volume during a rainfall event may be 70% greater in areas where plasticulture was applied (Carver, 1988).

The Agency should carefully consider the effects of runoff from urban areas within SAM. The methods of Blair et al. (2014) may be useful for estimating urban pesticide use and resulting aquatic concentrations. In that study, the percentage of impervious cover ranged from <1% (North Inlet) to 55% (New Market Creek), and impervious cover had a substantial effect on curve numbers. Another consideration for applying SAM to urban areas is the proliferation of retention ponds in urban areas. In the coastal zone of South Carolina, for example, more than 21,000 ponds of ≥ 1 acre are now used to capture nonpoint source runoff. Retention ponds substantially reduce runoff volume and contaminant mass. Moreover, there is increasing use of ponds by farmers to provide irrigation during drought. In previous studies funded by the Agency (Scott et al., 1990, 1992, 1999; Scott, 1997), the use of ponds for pesticide non-point source (NPS) runoff control resulted in > 90% reduction in maximum instream pesticide concentrations of organic phosphate, organochlorines, and pyrethroids. If SAM is used in a regulatory context, retention ponds may reduce runoff of pesticides into larger water bodies in locations where pesticide loads are relatively high.

SAM uses major crop groups such as corn, soybeans, wheat, vegetables and ground fruits, and orchards and vineyards (Appendix 3B), and the methods of the USDA NRCS (1986) to generate curve numbers. The Panel suggests that evaluation of the grouping method should address whether the land-use classes within each group have similar relations to runoff. For example, it would be helpful for the Agency to assess whether the land uses within each group are associated with similar slopes, soil classes, quantities and timing of pesticides applied, and harvest and planting dates.

Q5. 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.

a. Please comment on the implications for aggregating spatial inputs across varying scales.

Scale includes extent and resolution. In this instance the Agency referenced resolution only. The Panel recommended that the feasibility of adjusting the resolution of spatial data and the physical, chemical, or biological rationale for adjusting the resolution of spatial data be assessed separately. It is fairly common in spatial modeling to overlay data layers with different spatial resolutions. For example, one might overlay land-cover data at 30-m resolution, elevation data at 10-m resolution, and climate data at 2-km resolution, and then derive values of those variables for pixels or polygons of still different sizes. Whether doing so makes sense depends on the objectives of the analysis, the metrics being calculated, the variation in the variables represented in the data layers, and the resolution of the desired outputs. For example, if an area largely is flat, estimating the slope of a 10 km^2 polygon as the average of the slopes of the 10-m pixels within that polygon will have little effect on the values. If there is considerable variability in values of a given variable among pixels, it might make sense to calculate a measure of variance in addition to a summary measure for the polygon. Without a more explicit explanation of the objectives of SAM, or more knowledge of sources of variation within data layers and mechanisms driving such variation, it is difficult to make generalizations about either resampling (subdividing a pixel), which appears to be have been done during development of SAM, or aggregating among crop types and geographic areas.

The rules of thumb for combining spatial data at different resolutions apply to combining data for use in SAM, and thus a review of the current literature on spatial analysis or landscape ecology may be useful. In general, when combining spatial data, the level of resolution of the resulting product will be as fine as that of the coarsest-resolution input.

The resolutions of the soil and land-use data are similar, and combining these as the Agency has done likely would be well accepted. However, deriving integrated soil and land-use classes at 30-m rather than 10-m resolution might make more sense given that the native resolution of the land-cover data is 30 m. Use of a 30-m rather than a 10-m grid also would likely reduce model computational time.

Results from aggregation of data at different scales or resolutions can be misinterpreted. Some of the gridded data layers used in SAM represent a point, and some represent averages of points within a grid. The empirical data and methods of interpolation or extrapolation need to be considered prior to aggregation or regridding.

The Panel recommended that the Agency not present high spatial resolution as synonymous with high accuracy or complexity.

With the possible exception of montane areas, the density of weather observations should be sufficient for operational use of SAM. For operational application of SAM, the use of a sufficiently long period of weather data (e.g., 30 years) will allow estimation of the magnitude and frequency of pesticide concentrations needed by the Agency. Precipitation can have high spatial heterogeneity, which may affect the ability to accurately model runoff and pesticide concentrations. Because climate is changing, the Panel recommended that the Agency use the most recent 30 years of weather data to estimate climate normals, or the most recent climate normals provided by national climate data centers.

The Agency is using data for 30 recent years to represent weather within SAM, whereas data from 1961 through 1990 were used in PRZM. The experience of Panel member Dr. Engel's research team in analyzing national rainfall and temperature data in the process of updating a weather-generation program (CLIGEN) identified 30 years of daily weather records as an appropriate period of record.

In the example application of SAM that was presented to the Panel, the spatial resolution of the crop planting data that were used to identify the timing of pesticide applications does not match the resolution of the weather, soil, and land use data. The Agency has explored the use of crop planting data and USDA Plant Hardiness Zone data to estimate planting dates and corresponding pesticide application rates. The spatial extent and resolution of the crop planting and hardiness zone data differ greatly from those of other spatial data used in SAM. The resolution of these data generally is coarser than that of other data used in SAM, and the spatial extent and quality of the different types of data also vary. Beyond these caveats, the accuracy of the crop planting data and corresponding estimates of pesticide application dates is likely lower than the quality of other data sources used in SAM.

Although the dates of pesticide application are useful when comparing model outputs to observed data, other approaches should be considered when using SAM operationally. Crop planting dates have high spatial and temporal variability. In theory, use of multidecadal averages could be used to estimate crop-planting dates. However, there are no reliable, long-term crop planting data at the extent of the conterminous United States or large regions. An alternative that would facilitate operational modeling might be to conduct sensitivity analyses in which the functional forms of the planting-date distribution are unchanged, but the temporal window of the planting dates is shifted. Doing so would increase computational time but could improve estimates of the potential magnitudes and distributions of pesticide concentrations in runoff.

The current design of SAM allows for incorporation of new or different data with higher accuracy. Because input data may affect model outputs, the Panel recommends archiving the data that were used for each operational application of the model.

The Panel recommends that the Agency attempt to run the sensitivity analysis referenced in section 3.2.1 of the background document ("Differing spatial resolutions will likely impact modeling results, although quantifying the impact of this effect may be difficult, and has not yet been attempted"). If it is too difficult to quantify the effects of the aggregation, then the Panel cannot fairly be expected to comment on "the implications." If the sensitivity analysis is not feasible, the Panel recommends including an explanation in the background document.

It was unclear how values of each data layer were treated to develop covariates or scenarios for a given watershed when applying SAM. For example, were values of each data layer averaged within a watershed? How were data on all of the weather variables described in the background document and appendices incorporated into the scenarios? More-explicit methods and descriptions of covariates would be helpful.

If it is desirable to consider future climate change scenarios with SAM, other methods for estimating weather patterns may be required. The CLIGEN weather generation software, data, and methods developed by Trotochaud et al. (2015) may be useful. Numerous downscaling methods and model outputs are available, and the Panel suggests consulting with climatologists to match the objectives of SAM with any downscaled data that may be used. For example, the localized analog statistical downscaling method (LOCA; Pierce et al. 2014) produces estimates that can be incorporated into hydrological simulations by selecting analogs that are defined statistically on the basis of historical observations of variation in local versus regional precipitation or temperature. The LOCA method contrasts with other methods that use a weighted 30-day average for the full spatial extent of analyses. The Panel recommended that the Agency ensure that the error of any downscaled data incorporated into SAM be evaluated rigorously.

Given that SAM will use 30 years of weather data, if precipitation increased in some areas during the past decade, will the SAM results for the last decade differ from those for the preceding two decades? That is, will annual variation in model outputs represent the variability of one population, or two or more populations? If the latter, how will the Agency interpret the differences?

Section 4: Accounting for Time-of-Travel Effects

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.

a. 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.

The principle and benefits of convolution were clearly explained by the Agency's SAM development team. The Panel endorsed further development of convolution for addressing travel time of dissolved pesticides within model watersheds. The Panel also felt that the study objectives of the SAM model development were not clearly defined in the documentation provided to the Panel. The usefulness of travel-time based convolution depends on the purpose of the model.

If the goal of SAM is indeed to identify hot spots of pesticide occurrence that lead to elevated risk, especially for water soluble pesticides such as atrazine, then the consideration of travel time will not be very useful. In the Panel's experience, maximum concentrations will usually occur in small watersheds. The mixing and dilution afforded in higher order rivers will serve to decrease aqueous pesticide concentrations, so the focus on locations that integrate watershed outlets ("pour point") will not likely identify such hot spots. On the other hand, if the goal is to obtain more realistic distributions of concentrations in space and time (over an annual time period of flow regime), as demonstrated in the results of the initial alpha version of SAM, then the incorporation of travel time and flow and mass routing play critical roles. Consequently, other relevant components of the model, such as estimating runoff, considerations of baseflow, and transfer and transport phenomena from field to stream, should be developed simultaneously with the convolution approach. Some of these modeling components were not explicitly stated or discussed in detail by the development team.

Travel-time based convolution is a new function to be included in the next version of SAM. While this function is expected to improve model performance compared to earlier versions that did not include convolution, it may also significantly change SAM modeling capability and output structure. For example, the initial alpha version generates results for all HUC12 watersheds in the simulation domain, which provides a spatially continuous mapping of potential pesticide risks over the landscape. Thus, a pre-defined location for pesticide evaluation is not needed, but SAM will simply provide results for every location according to the spatial resolution (i.e., HUC12 in the initial alpha version).

The implementation of the proposed convolution approach requires a single user-defined "pour points" because the time of travel is currently defined between the pour point to each NHD catchment. If other pour points within the watershed are of interest (e.g., a series of monitoring sites along a river), one must re-run the convolution for each location because travel times change. To incorporate convolution while retaining the capacity to conduct spatially continuous

simulations, the Panel suggested a more modular approach that can define time of travel between any two connected hydrologic units such as NHD catchments or HUC's at a certain level. Convolution can then be performed for all hydrological units of interest within the watershed, resulting in complete hydrographs and chemographs for all potential pour points. In addition, the size of watersheds could be a critical factor for the implementation of convolution in SAM because of the proposed use of integer-day stream travel-time zones. That is, the travel times estimates between watersheds at HUC-12, HUC-8, HUC-6 and larger levels will be more meaningful, compared to smaller units of NHD catchment.

This suggested modeling approach has been demonstrated in previous studies (Luo and Zhang, 2009; 2011), that were based on PRZM simulations scaled up to a watershed, and have been tested for streamflow, suspended sediment concentration, and pesticide concentrations in water and in sediment for multiple locations in an agriculture dominated watershed in California.

There is some uncertainty about the validity of the travel times that are part of NHD Plus ver 2 (at least the version of NHD Plus ver 2 that USGS NAWQA is using). One possibility is that the basic travel time equations may have been coded incorrectly. This is currently a topic of investigation in the NAWQA program. The Panel recommends the Agency work collaboratively with the USGS NAWQA Program to investigate the use of travel time data retrieved from NHD Plus ver 2.

Q7. USEPA OPP has not yet investigated possible adaptations of the approach referred to in Question 6 to simulate reactive and/or sorbing chemicals.

a. 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.

The dual-compartment (aqueous and benthos) system is currently applied in two Agency models: the Exposure Analysis Modeling System (EXAMS) and the Variable Volume Water Model (VVWM). Since these models were developed for pesticide evaluation at small spatial scales (e.g., a single agricultural field), water quality parameters including dissolved organic carbon (DOC) and total suspended sediment (TSS) are assumed constant. For example, default values for DOC and TSS are 5 and 30 mg/L, respectively, in the USEPA's Surface Water Concentration Calculator (Fry et al., 2013).

In reality, organic carbon (measured by DOC or total organic carbon, TOC) and suspended sediment may change significantly over time and space between, and perhaps even within, watershed units. Regardless of the approach to estimate time of travel within a watershed, hydrophobic pesticides delivered into the watershed will partition and sorb to dissolved and suspended organic matter, as well as to bed sediments. The rate at which a pesticide travels through a watershed reach will affect the rate of partitioning into organic carbon, suspended sediment, and bed sediments within a watershed. Clearly, sorption of hydrophobic pesticides

will reduce surface water concentrations measured in field monitoring and national assessment programs. Unfortunately, the ability to adapt the model to address the multimedia fate of pesticides has not been rigorously addressed in the current version of SAM. Thus, as an initial step towards inclusion of pesticides with a wide range of physicochemical properties and environmental behavior, the Panel recommends the addition of [1] organic carbon (measured by DOC for the aqueous phase, and TOC for the suspended or bed sediment compartments), and [2] suspended sediment (measured by TSS) in future versions of SAM. Addition of these compartments will be essential for application of SAM to strongly sorbing pesticides (e.g., pyrethroids, fipronil). Furthermore, allowing for organic carbon and suspended sediment to vary for model parameterization and simulation is consistent with SAM's development goal for pesticide evaluation at higher spatial resolution. Suspended sediment concentrations in streams can be obtained through the USGS sediment data portal (http://cida.usgs.gov/sediment/).

The process of modeling sediment sources and transport is not sufficiently addressed in SAM documentation and development plans. This process can be divided into one for lake/reservoirs and a parallel flow question for lotic systems. There is an abundance of work that can be drawn upon to allow the lake/reservoirs to be addressed by SAM. Incorporation of sediments for lotic systems is likely an order of magnitude greater challenge because sediment transport must be modeled. The convolution integral approach is probably not applicable since sediment transport is an episodic process. Storage in the stream network and travel times can be on the time scale of decades as evidenced by the observation of DDE and other organochlorine pesticide long after their use.

In addition to soil erosion from fields and uplands to channels, stream bank and *in situ* contributions of sediment can be significant (Simon and Klimetz, 2008; Wilson et al., 2008). To model sediment transport from the field through the stream network, a series of sub-models are needed to account for: [1] soil erosion within the field to the channel; [2] sediment transport from the channel into the stream network (including long term storage in various channels), and [3] in-stream sediment transport that accounts for deposition and resuspension in the stream and the floodplain. Although much work has been done to address the impact of sediments on water quality, there remain many issues and few useful models. This will represent a formidable challenge to the SAM team, given the large areas and diversity of streams to be addressed. The Panel's initial recommendation for modeling of channel-derived sediment and sediment transport in channelized flows is to consider existing models, e.g., the Soil and Water Assessment Tool (SWAT, 2015).

The description by the Agency's SAM development team, both in the background paper and Panel meeting presentations, of modification of the convolution equation lacked a logical and tangible connection to fate mechanisms established in lab and field studies, and which are routinely modeled using other well-established approaches (e.g., box (mass balance) models). Whether or not modification of the convolution approach is deemed valid and moves forward, additional development, definition, and translation of the adopted approach relative to the processes and mechanisms represented in a conceptual fate model, is highly recommended. As incorporation of a more comprehensive fate component in SAM evolves, the Panel recommended that the following steps be taken to maximize clarity and transparency of the approach taken:

1) Define the scope of pesticides to be addressed (i.e., water soluble, strongly sorbing, or both), and define what compartments are relevant (total concentration, aqueous, suspended sediment, bedded sediment, biota, air).
2) Outline all mechanisms and processes that are relevant for modeling fate. Utilize graphics to illustrate the fate of pesticides among the different conceptual model compartments.
3) Present and discuss the current literature on aquatic fate modeling, contrasting the different options available for modeling fate. Provide a compelling rationale for selecting the approach adopted for SAM.
4) Select an approach that best addresses the modeling objectives.
5) Cross-calibrate preliminary model output with output from other similar or candidate modeling efforts.

For the currently proposed convolution algorithm in SAM, two model approaches are suggested to account for pesticide dissipation in the water column:

- Approach 1 (aggregated dissipation rate constant): An aggregated decay factor can be easily incorporated into the response function "G" in the convolution calculation (section 4.2). For example, overall dissipation rate constants for chlorpyrifos and diazinon were incorporated into a convolution-based linear routing model (Luo and Zhang, 2009).
- Approach 2 (simulation of individual fate processes). Modeling of individual fate processes, e.g., hydrolysis, photolysis, biotransformation, and air-water exchange, as considered in VVWM.

The Panel believes that modeling of the fate of pesticides in bed sediment may not be readily incorporated into the convolution approach proposed for SAM. As a result, a separate computational module will likely be needed. In each time step (one day), this module is expected to predict sediment settling, re-suspension, and associated pesticide fate within each catchment based on suspended sediment concentrations. Most of the VVWM equations for pesticide partitioning and exchange between suspended and bed sediment are applicable, with modifications needed to account for variable TSS. In addition, the original analytical solution may have to be replaced by a numerical approach.

The Panel feels that addressing the chronic ecotoxicology risk of pesticides in sediments is beyond the current scope of SAM but should be considered in future sensitivity analysis and evaluations of the SAM Model. Analyzing data on pesticide measurements along with data on important factors such as grain size, TOC and benthos will enable the Agency to assess hazards posed by sediment sorbed pesticides to benthic organisms in rivers, lakes, streams and estuaries. In addition, the use of benchmark sediment toxicity tests with key benthic organisms would be appropriate to complement benthic community assessments, as benthic assessments do not always permit direct predictions of toxicity *per se*. NOAA and the Agency use this approach in their current monitoring programs (e.g. National Status & Trends and EMAP). These protocols are also used in part in the National Coastal Condition reports prepared jointly by the Agency and NOAA. A variety of sediment toxicity tests have also been proposed by the Agency for sediment-associated pesticides, PAHs and trace metals (Fulton et al., 1999). Current Agency pesticide risk assessments are focused primarily on aquatic assessments that compare the

estimated environmental concentrations (EEC) with aquatic hazard levels. This provides a more acute exposure focus and, therefore, assessing pesticide levels in sediments would be a more chronic focus and may be beyond current Agency assessment methods used with SAM.

b. 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.

Data sets for inclusion in this type of analysis would include:

1. National Datasets

NOAA National Status and Trend (NS&T) and EPA Environmental Monitoring & Assessment Program (EMAP): The NS&T program conducted by NOAA regularly reports the trends in levels of contaminants in the coastal environment in sediments and in certain organisms, including mussels and oysters, over distances and over time. Started in 1984, NS&T is the only long-term coastal and estuarine contaminant monitoring effort in the U.S. One component of the NS&T Program, the Mussel Watch Project, started in 1986, is the longest continuous contaminant monitoring effort ever conducted in the country. Today, the number of contaminants that are routinely analyzed in the Mussel Watch Project has grown to around 170 and improved technology enables detection of even lower concentrations at over 280 sites across all 50 states and Puerto Rico.

NOAA's Bioeffects Program is a nationwide program of environmental assessment and related research designed to describe the current status of environmental quality in our nation's estuarine and coastal areas. More than thirty multidisciplinary projects have been carried out since 1991 in close cooperation or partnership with coastal states or regional organizations. Field studies examine the distribution and concentration of over 100 chemical contaminants in sediments, measure sediment toxicity, and assess the condition of benthic communities. This information is integrated into a comprehensive assessment of the health of the marine system. Sediment contaminant data, including grain size analysis, total organic carbon (TOC), nutrients and benthic analysis, are available at selected locations around the US. This includes contaminant data for > 83 legacy pollutants including pesticides and PCBs as well as some contemporary use pesticides. Most locations are within coastal watersheds as well as offshore watersheds on the continental shelf. EPA's EMAP and subsequent coastal and national assessment programs have conducted similar studies throughout the US and often in collaboration with NOAA.

Figure 1 below depicts examples of data locations for NOAA NS&T and EPA's EMAP in the southeastern US. A total of 697 estuarine and 50 continental shelf stations are in NC, SC, GA and northern FL. These types of data sets exist for most coastal regions of the US.

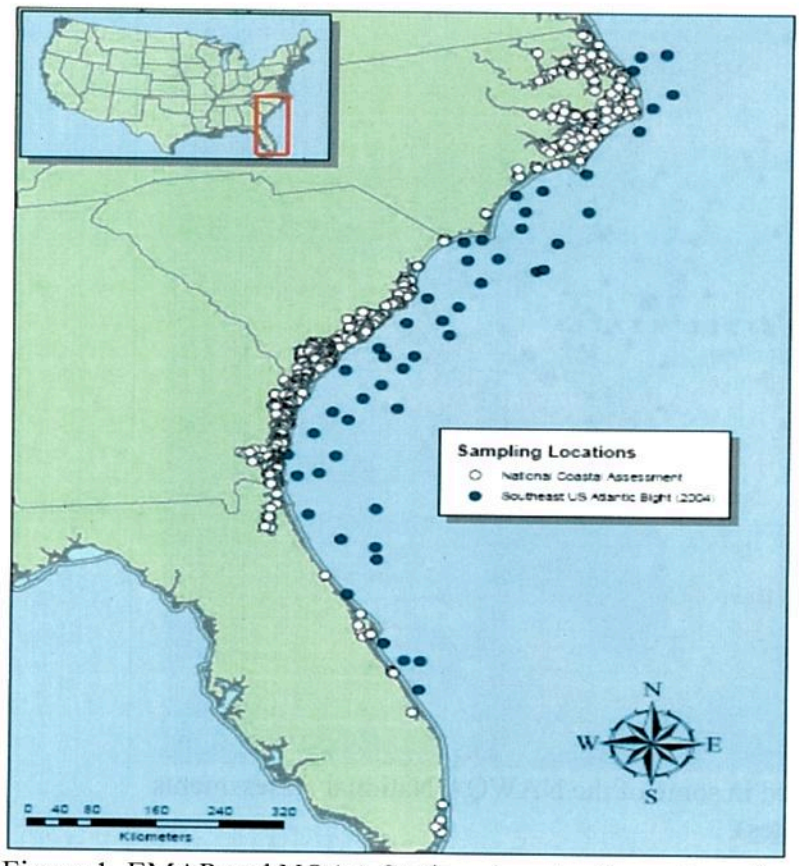

Figure 1. EMAP and NOAA Stations in estuarine and continental shelf areas of the southeastern US. TOC, benthos and chemical contaminant data are measured at each location. (Scott, 2012)

The National Water Quality Assessment (NAWQA): NAWQA is a national monitoring program conducted by the USGS that provides an understanding of status of water-quality conditions throughout the US. This program specifically assesses whether conditions are getting better or worse over time, and it evaluates the impact of natural and anthropogenic factors on environmental conditions. Both regional and national assessments are conducted. The study design entails uniform methods of data collection and its analyses permit assessments over a broad range of geographic conditions. Monitoring data are integrated with geographic information on hydrological characteristics, land use, and other landscape features in models to extend water-quality measurements from station locations to unmonitored areas. Figure 2 depicts the network of stations used in some of NAWQA National Assessments.

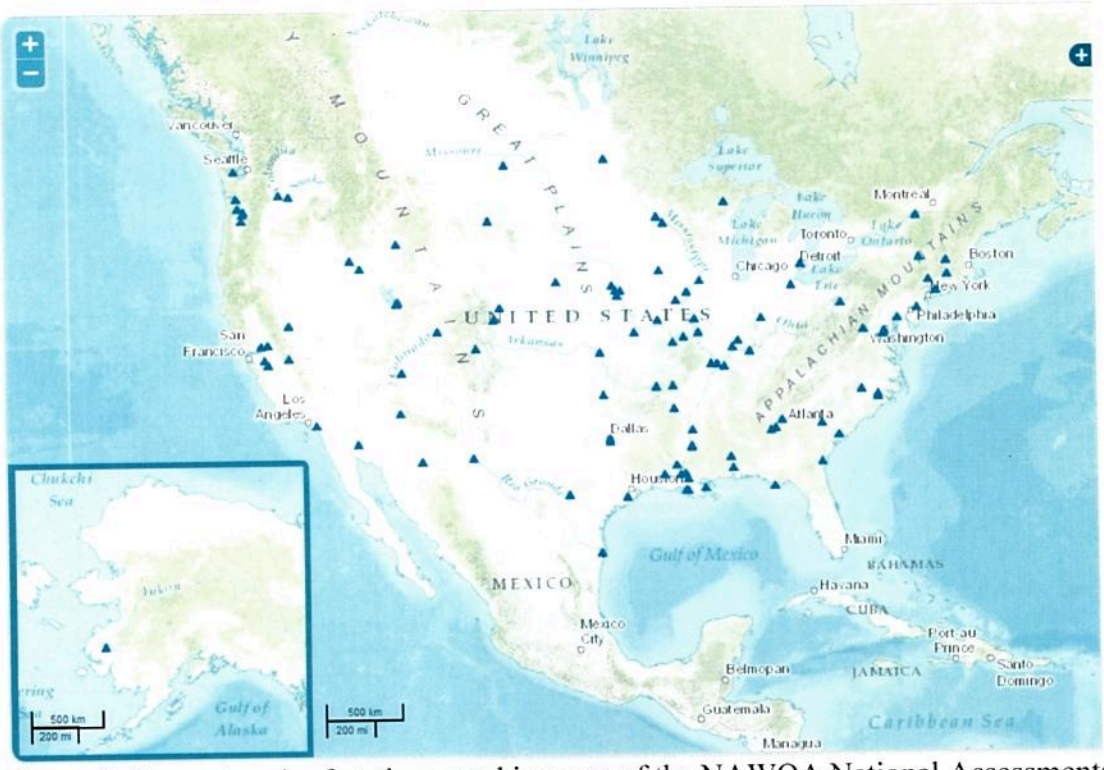

Figure 2. The network of stations used in some of the NAWQA National Assessments (http://cida.usgs.gov/quality/rivers/sites).

In a recent NAWQA report (Stone et al., 2014) assessing the 2002–2011 time period, only one stream assessed throughout the US had an annual mean pesticide concentration that exceeded a human health benchmark. During the 1992-2001 time period, some 17% of agriculture land-use streams and one mixed land-use stream had annual mean pesticide concentrations that exceeded human health benchmarks. During 2002–2011, nearly two-thirds of agriculture land-use streams, nearly 50% of mixed land-use streams and 90% of urban land use streams exceeded chronic Aquatic Life Benchmarks (ALB). Fipronil, metolachlor, malathion, cis-permethrin, and dichlorvos exceeded chronic ALBs in more than 10% of the streams under monitoring. Figure 3 depicts these results summarized in these reports.

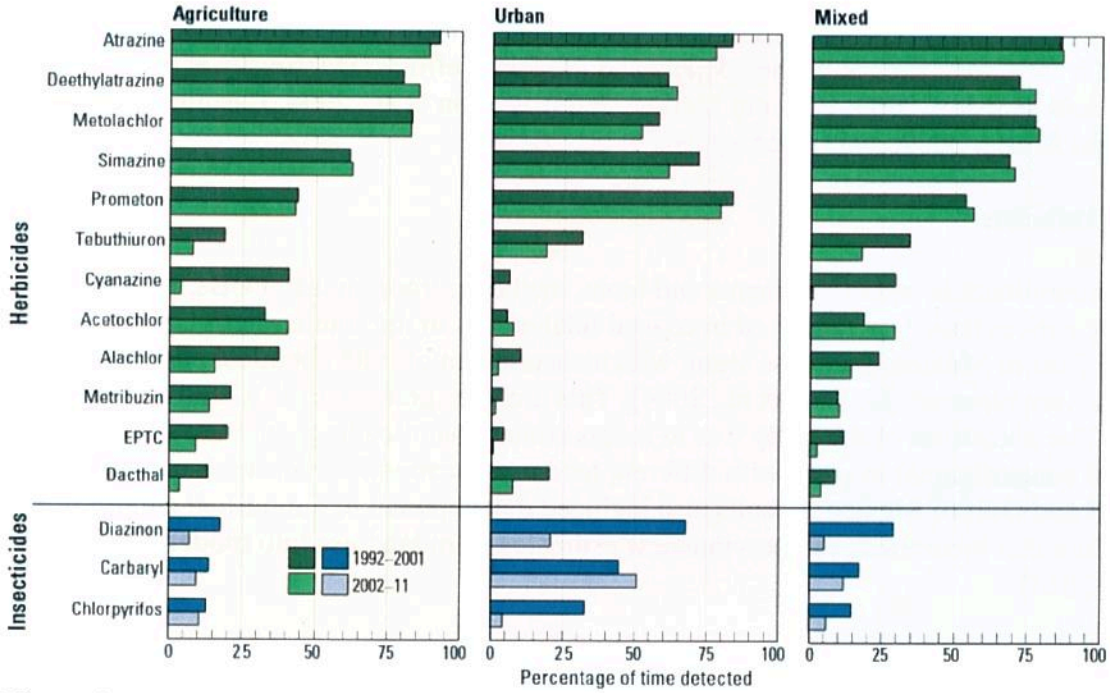

Figure 3. Results of national stream and river pesticide assessment reported by USGS in NAWQA (Stone et al., 2014). This study includes pesticde monitoring data in sediments along with grain size and TOC measurements.

In addition, NAWQA has more in depth core analysis of sediments of pesticides and other contaminants in lake and stream sediments (Van Metre and Mahler, 2005), which permit time series analysis of pesticide levels.

2. Statewide Datasets

Many states have long term trend monitoring stations that measure chemical contaminants in sediments along with grain size, TOC, and benthos. These data can be accessed by contacting state regulatory agencies. For example, concentrations of current-use pesticides (e.g. pyrethroids and fipronil and its degradates) in the top 2 cm of bed sediment of wadeable streams, coastal embayments, and the continental shelf for the southern California region are available from the California Surface Water Ambient Monitoring Program (SWAMP) (http://www.waterboards.ca.gov/water_issues/programs/swamp/), the Stormwater Monitoring Coalition (SMC) (http://www.socalsmc.org/) and the Southern California Bight Regional Monitoring Program (http://sccwrp.org/ResearchAreas/RegionalMonitoring.aspx).

The US Geological Survey (USGS), the California Department of Pesticide Regulation, and other agencies and universities have performed long-term surface water monitoring for dissolved and sediment-bound pesticides at some small watersheds in California. For example, Orestimba Creek in California's San Joaquin River basin would be a good candidate for model testing. Pesticide use data for the watershed are available with sufficiently high temporal and spatial resolution (daily time step for each 1 mi^2 section) through the California PUR (Pesticide Use Reporting) system. In addition, streamflow, water quality, and toxicity are intensively monitored by multiple entities. Most importantly, occurrence measurements in both the water column and

bed sediment are available, e.g. for pyrethroids. This watershed is a well-studied model system as evidenced by the numerous published papers and modeling efforts (Dubrovsky et al., 1998; Domagalski and Munday, 2003; Chu and Marino, 2004; Weston et al., 2004; Ensminger et al., 2009; Luo and Zhang, 2009; 2011; Domagalski et al., 2010).

3. Regional Datasets

Chemical contaiminant levels in sediments and biota, including trace metals, PCBs, PAHs, PPCPs, and pesitices have been assessed in coastal tidal creeks in the southeastern US (NC, SC, GA) and the Gulf of Mexico. Land use along with measurement of > 85 chemical contaminants in sediments were reported (Holland et al., 2004). This includes grain size, TOC and benthic assessment. The objectives of the study was to assess contaminant loadings (nutrients, microbes, and chemical contaminants) in areas with different land uses surrounding coastal estuaries of the southeast US and Gulf of Mexico. Results also included development of a modified curve number method that incorporates imperviousness estimates from land use into model predictions (Blair et al., 2014).

Numerous regional assessment studies conducted by state or regional regulatory agencies and academia may contain data on chemical contaminant levels in sediments along with grain size, TOC, benthos, and other important and relevant data that would be useful to the Agency. Conducting regional workshops with state and regional partners would be a good way to identify these data sets. Small scale case studies were conducted by the Southern California Coastal Water Research Project Authority (SCCWRP) (Lao et al., 2010; 2012) University of California at Riverside (Gan et al., 2005) and USDA (Potter et al., 2008) for sediment measurments of pyrethroids.

4. Other non-pesticide chemicals with available data in sediment

Many tracer chemicals could be considered to help with the strongly-sorbed pesticide transport question, such as trace elements, total phosphorous, and hydrophobic organic chemicals (PCBs, PAHs, and others). Work on sediment fingerprinting might also provide some insight in to the sources of sediment (and sorbed pesticides) in stream. The transport of total phosphorous (TP) is a similar question to the transport of sorbed pesticides. The EPA Chesapeake Bay Program has worked on incorporating the transport of TP into the Chesapeake Bay model. (http: //ches.communitymodeling.org/models/CBPhase5/documentation.php#p5modeldoc) This might be a useful resource to the Agency as they think about sorbed pesticide transport.

Section 5: Defining the Likely Pesticide Application Window based on Crops and Weather
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, USEPA OPP tested the potential for using empirical data and, where such data are incomplete, crop growth models.

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?

There are no easy answers to these questions. However, the Panel suggests doing a thorough search of the weed science literature. For example, two references: i) Predicting Emergence of 23 Summer Annual Weed Species (Werle et al. 2014a); and ii) Environmental Triggers of Winter Annual Weed emergence in the Midwestern United States (Werle et al. 2014b) provide some information about weed germination within the windows of temperature relevant to SAM simulations.

Since in many parts of the USA, no-till or minimum till corn and soybean rotations are practiced, one must recognize that there are also weeds that do not completely die at harvest and remain in the field throughout winter in dormant stages. This is particularly true if the soil temperature remains above some threshold after harvest. In this case, the Agency must be careful about the types of applications of herbicides. If one browses through websites of large agricultural extension programs, such as those at The Pennsylvania State University or Iowa State University, one will find that the classification for timing of application for herbicides can be grouped into categories (e.g., preplant, pre, delayed pre, early post, mid post, post, etc). These websites typically describe when herbicides are applied and particularly at what stages of plant growth for post emergent applications.

Weed emergence, like emergence of corn or soybeans, is tied to soil temperature. In Werle et al. (2014a), the authors describe emergences of about 23 summer annual weed species. They report emergence ranging from 2-17 °C with most centered around 10 °C (which is about 50 °F). This can be used as the T_{base} temperature as proposed in SAM. In the Werle et al. (2014a) paper, the authors refer to growing degree days (GDD) based on soil temperature at the top 2 cm. In order to get information on planting and germination, the Agency needs to obtain temperature and soil moisture data and these data are available from various universities and government entities. For example, the agricultural extension website for The Pennsylvania State University (Pennsylvania Pest Information Platform for Extension and Education – PA-PIPE), has maps of GDD and temperature of the top 2-cm of soil. Soil moisture data are available for a smaller number of stations (than for weather data) at various regional climate centers. The High Plains Regional Climate Center in Lincoln, NE has soil moisture data for more than 50 locations covering depths up to 4 feet (typically measured at 4 depths). Regionally, there may be holes in data – for example the Midwestern RCC has soil moisture data gaps for MN and IN – but has data for most other states for various durations. These data may be useful to the Agency to determine planting dates. Another data source that the Agency might consider is: Agweb.com

Simulations were done by the Agency using the Plant Hardiness Zone (PHZ) map for application of chemicals; however, this map seems to be off by several weeks or more. The Panel suggested that the Agency correlate the PHZ map with crop insurance mandated planting dates (USDA Risk Management Services identifies planting dates and the Agency should review certain years of records to identify the earliest planting dates and to assess differences between the dates specified by the PHZ and the USDA Risk Management Service).

The GDD requires baseline temperature data. For corn and other crops, data on baseline temperature may be available from various states or universities. State extension sites (e.g., Iowa State University, University of California Davis, The Pennsylvania State University) have such information. With GDD, the Agency must correlate application with rain events. The window of time between the likely date of pesticide application and the next big storm as well as the soil moisture profile at the time of application or storm are useful types of information in this regard.

For post-emergent chemicals, one needs to know the growth stage of the plant and a crop model is needed for this. For example, the Iowa State University extension, University of Nebraska extension, California Integrated Pest Management (IPM) for non-major crops, and The Pennsylvania State University (PA-PIPE) sites refer to crop models.

Dr. Haishun Yang of the University of Nebraska has a crop model for hybrid maize: (Hybridmaize.unl.edu). This crop model calculates biomass, growth, and yield under rain fed and irrigated conditions and calculates yield on the basis of weather and soil data assuming no deficiency in nutrients. Many post-emergent insecticides are applied in response to pest pressure. One may examine the correlation between precipitation and temperature to determine any relationships with pest outbreak. Currently NOAA provides a number of weather forecasts that use predictive variables, such as temperature, precipitation, etc., for agricultural uses (e.g., Runoff Risk Advisory Forecast produced for Wisconsin Manure Producers on the basis of weather records from 1948-2008). Decision tools for the application of fungicides to peanuts that are based on weather and soil moisture are available. Often farmers do not use or follow the recommendations of these forecasting tools because conflicts of convenience and economics.

The Agency uses a 50-day planting window. This number seems reasonable. However, checking against empirical data (available from extension service or cooperators) and correlating planting dates with weather data for areas where such data exist will enable determination of the shape of application window (e.g., triangular, left skewed, right skewed).

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.

The Panel suggested that collaboration with industry, extension service researchers and county agents, and the USDA Risk Management Service would be beneficial to obtain such information. For heavy machinery use, often researchers use a "trafficability" index with levels (e.g., dry workable, wet workable, optimal) based on soil moisture regimes which indirectly

estimates the ability to move in the field (Helms, 2009). PRZM 3/5 can estimate the soil moisture profile at a given time and that information can be used to estimate "trafficability".

The Agency might consider two other sources of information in this regard: a) California Integrated Pest Management:
http://www.ipm.ucdavis.edu/WEATHER/ddvideos.html
and b) National Drought Monitor at the University of Nebraska:
http://droughtmonitor.unl.edu/
These sites provide educational and scientific information for decision making.
Commercial applicators often spray chemicals on contract basis to farmers. They can be a good source of information on planting and chemical application.

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.

Decision Support System for Agrotechnology Transfer (DSSAT) is a crop modeling software program that uses data on soil, weather, and management to simulate the growth, development, and yield of 28 crops. Various user trainings are offered by the developers of DSSAT:
http://dssat.net/

Additionally, the Panel has described single species crop simulation models (see section 8.a). Because SAM uses 30 years of weather data, the Agency should consider running the model for 30 years and capturing the output. In subsequent simulations, the Agency can shift the planting window by a week or a few days. By doing such simulations, the Agency may be able to match the simulation output with observations.

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).

a. Please comment on the use of empirical data or models to define the distribution of pesticide applications within an application window.

As indicated in responses to several charge questions, the Panel agreed with the Agency that defining pesticide application windows and the distribution of applications within these windows will have a large impact on model outcomes. Thus, careful assessment is needed. The Panel also agreed that empirical data and models could be used to guide the distribution within windows. The examples presented by the Agency in the SAM background document are clear illustrations of how empirical data such as crop progress reports can be used for this purpose. The Panel recommended other sources of data that are linked to crop insurance that at minimum can guide crop planting and harvest dates. Crop-specific data are available from the USDA Risk Management Agency (USDA-RMA) for most counties in the USA. These data include the first

and last dates when crops can be planted to be eligible for insurance. See http://www.rma.usda.gov/aboutrma/fields/rsos.html for regional office locations and http://webapp.rma.usda.gov/apps/actuarialinformationbrowser2015/DisplayCrop.aspx for information on specific crops by county. It is reasonable to assume that the first and last planting dates for crop insurance can define application windows of products such as pre-plant and pre-emergence herbicides. USDA-RMA also collects acreage planted data. If USDA-RMA can release this information to the Agency, it may be used to "ground-truth" crop acreage data obtained from crop data-layers.

The Panel also suggested that soil temperature could be used as an alternative way to estimate first planting date. Soil temperature is a key determinant that growers use to establish when crops can be planted. Soil temperature and recommendations for planting various crops can readily be obtained from state agricultural extension offices while soil temperature can be obtained from both local and national networks (e.g., http://www.wcc.nrcs.usda.gov/scan/). These data likely can be compiled in a data-layer in the model. Alternatively, soil temperature can be estimated in PRZM. A routine in PRZM that estimates soil temperature is linked to pesticide degradation kinetics. With minor modification, the PRZM soil temperature estimates may be extracted and used to predict planting dates.

Once soil temperature reaches the acceptable threshold for a given crop, it can be assumed that farmers will plant crops as quickly as possible. Farmers are well aware that late planting typically reduces yields. Precipitation may delay planting because it may be difficult to drive heavy equipment on wet fields. The Agency was encouraged to look for examples where soil water content and ability to operate planting equipment were linked (e.g., Helms, 2009). Once such relations are established, observed or projected soil water content can be used to estimate the feasibility of planting. Relations between estimated or measured soil temperature and water content can be further evaluated and compared to crop-progress data for selected watersheds to determine whether a predictive relation can be identified. Such a relation can guide assumptions regarding the functional distribution of crop planting within temporal windows (triangular, linear, etc.) for specific crops in a given region. Precipitation data also may be useful. Precipitation above a certain threshold will affect farmers' decisions to plant crops and apply pesticides. Thus application can be turned "on" or "off" as a function of total precipitation.

Panelists noted that aerial applications also must be considered. Aerial applications typically are used to treat large areas on a single day. Consultations with commercial pesticide applicators may provide insight. In the case of fungicides and insecticides, crop-growth models and decision-support tools may be useful guides. There are many crop models with varying levels of complexity and data requirements, and many decision support tools for determining when fungicides or insecticides should be applied to a given crop. Drivers in decision-support systems include temperature, precipitation, and crop growth stage. For example, the AU-Pnuts system, developed at Auburn University (AU) for peanuts, uses the number of days with precipitation greater than 2.5 cm and weather service predictions of precipitation probabilities to adjust timing of fungicide applications to control leaf-spot (Jacobi et al., 1995). The AU-Pnuts system has been compared to calendar-based spray programs and has proven effective both in disease management and in reduction of fungicide applications (Hagen et al., 2007). However, it appears that calendar-based schedules continue to be widely used. This in part reflects logistics demands

at the farm level. In calendar-based spray programs, once the crops reach a specific growth stage it is reasonable to assume that applications will take place at a defined frequency. Growth stage can be defined empirically or with crop growth models.

In response to the question, one Panelist found it odd to use "pesticides" with reference to plants. This Panelist felt that it would be clearer to use "biocides" as a generic term, herbicides for chemicals that are targeted to kill plants, and pesticides for chemicals that are targeted to kill animals, sometimes including insects. It was suggested that the window for application might depend in part on whether the target of the pesticide is a plant or an animal. The phenology of insects often is less predictable than that of plants. Insects may affect a crop at a certain stage in the crop's development, but as a generalization, insect populations are somewhat more dynamic than those of plants. The Panelist added that social information (e.g., decisions about use of calendar-based or other application schedules for fungicides) might be helpful in identifying potential sources of information for identifying application windows.

In concluding remarks, several Panelists returned to a point made in response to Question 1a: it would be possible to develop multiple versions of SAM to meet different objectives. The objectives will affect how pesticide applications are distributed over time. If the objective of using SAM is to maximize the agreement between measured and modeled concentrations, then application dates will need to be estimated. However, if the objective is to estimate maximum concentrations or the upper 95% confidence interval, then application dates become less important.

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