

US EPA ARCHIVE DOCUMENT



UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, DC 20460

OFFICE OF CHEMICAL SAFETY AND POLLUTION PREVENTION

January 12, 2012

MEMORANDUM

SUBJECT: Transmittal of Meeting Minutes of the FIFRA Scientific Advisory Panel Meeting held October 25-26, 2011 on the Two-dimensional Exposure Rainfall-Runoff Assessment (TERRA) Watershed Model and its Use in the FIFRA Ecological Risk Assessment for Antimicrobial Uses of Copper

TO: Steven Bradbury, Ph.D.
Director
Office of Pesticide Programs

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

THRU: Laura Bailey, MS *Laura Bailey 1/24/12*
Executive Secretary
FIFRA Scientific Advisory Panel
Office of Science Coordination and Policy

Frank Sanders *Frank Sanders 1/24/12*
Director
Office of Science Coordination and Policy

Attached, please find the meeting minutes of the FIFRA Scientific Advisory Panel open meeting held in Arlington, VA on October 25-26, 2011. This report addresses a set of scientific issues associated with "The Two-dimensional Exposure Rainfall-Runoff Assessment (TERRA) Watershed Model and its Use in the FIFRA Ecological Risk Assessment for Antimicrobial Uses of Copper."

Enclosure

cc:

Jim Jones
Louise Wise
Vicki Dellarco
William Jordan
Margie Fehrenbach
Keith Matthews
Donald Brady
Jack Housenger
Joan Harrigan-Farrelly
Lois Rossi
Jay Ellenberger
Karen Whitby
Richard Keigwin
Jennifer Mclain
Nader Elkassabany
Rebecca VonDem-Hagen
James Hetrick
Siroos Mostaghimi
Donna Randall
Stephen Wente
Dale Kemery
Douglas Parsons
Vanessa Vu
OPP Docket

FIFRA Scientific Advisory Panel Members

Kenneth M. Portier, Ph.D.
Janice Chambers, Ph.D., DABT, Fellow ATS
Stephen Klaine, Ph.D.
Martha Sandy, Ph.D.
Daniel Schlenk, Ph.D.

FQPA Science Review Board Members

Linda Abbott, Ph.D.
Xuefeng Chu, Ph.D.
Richard H. Coupe, Ph.D.
Bernard A. Engel, Ph.D.
Robert J.M. Hudson, Ph.D.
Ian A. Kennedy, Ph.D.
Yuzhou Luo, Ph.D.
Thomas L. Potter, Ph.D.

SAP Minutes No. 2012-01

The Two-dimensional Exposure Rainfall-Runoff Assessment (TERRA)
Watershed Model and its Use in the FIFRA Ecological Risk
Assessment for Antimicrobial Uses of Copper

October 25-26, 2011

FIFRA Scientific Advisory Panel Meeting

Held at the

Environmental Protection Agency Conference Center

Arlington, VA

NOTICE

These meeting minutes have been written as part of the activities of the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA), Scientific Advisory Panel (SAP). The meeting minutes represent the views and recommendations of the FIFRA SAP, not the United States Environmental Protection Agency (Agency). The content of the meeting minutes does not represent information approved or disseminated by the Agency. The meeting minutes have not been reviewed for approval by the Agency and, hence, the contents of these meeting minutes do not necessarily represent the views and policies of the Agency, nor of other agencies in the Executive Branch of the Federal Government, nor does mention of trade names or commercial products constitute a recommendation for use.

The FIFRA 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, 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. Further information about FIFRA SAP reports and activities can be obtained from its website at <http://www.epa.gov/scipoly/sap/> or the OPP Docket at (703) 305-5805. Interested persons are invited to contact Fred Jenkins, Jr., Ph.D., SAP Designated Federal Official, via e-mail at jenkins.fred@epa.gov.

In preparing these meeting minutes, the Panel carefully considered all information provided and presented by EPA, as well as information presented by public commenters.

TABLE OF CONTENTS

PARTICIPANTS	3
INTRODUCTION	5
PUBLIC COMMENTS.....	6
SUMMARY OF PANEL DISCUSSION AND RECOMMENDATIONS.....	7
DETAILED PANEL DELIBERATIONS AND RESPONSE TO CHARGE.....	11
REFERENCES	32

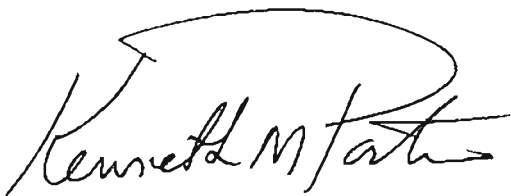
SAP Minutes No. 2012-01

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

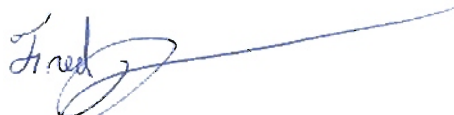
**The Two-dimensional Exposure Rainfall-Runoff
Assessment (TERRA) Watershed Model and its
Use in the FIFRA Ecological Risk Assessment for
Antimicrobial Uses of Copper**

October 25-26, 2011

**FIFRA Scientific Advisory Panel Meeting
Held at the
Environmental Protection Agency Conference
Center
Arlington, VA**



**Kenneth M. Portier, Ph.D.
FIFRA SAP Session Chair
FIFRA Scientific Advisory Panel
Date: JAN 12 2012**



**Fred Jenkins, Jr., Ph.D.
Designated Federal Official
FIFRA Scientific Advisory Panel
Date JAN 12 2012**

**Federal Insecticide Fungicide and Rodenticide Act
Scientific Advisory Panel Meeting
October 25-26, 2011**

PARTICIPANTS

FIFRA SAP Chair

Kenneth M. Portier, Ph.D.

Managing Director, Statistics & Evaluation Center, American Cancer Society,
National Home Office, Atlanta, GA

Designated Federal Official

Fred Jenkins, Jr., Ph.D.,

FIFRA Scientific Advisory Panel, Office of Science Coordination and Policy, EPA

FIFRA Scientific Advisory Panel Members

Janice Chambers, Ph.D., DABT, Fellow ATS

Director, Center for Environmental Health Sciences, College of Veterinary Medicine,
Mississippi State University, Mississippi State, MS

Stephen Klaine, Ph.D.

Professor
Department of Biological Sciences
Director Clemson Institute of Environmental Toxicology
Clemson University
Clemson, SC

Martha Sandy, Ph.D.

Senior Toxicologist and Chief
Cancer Toxicology and Epidemiology Section
Office of Environmental Health Hazard Assessment
California Environmental Protection Agency
Oakland, CA

Daniel Schlenk, Ph.D.

Professor of Aquatic Ecotoxicology & Environmental Toxicology
Department of Environmental Sciences
University of California, Riverside
Riverside, CA

FQPA Science Review Board Members

Linda Abbott, Ph.D.

Regulatory Risk Analyst
U.S. Department of Agriculture
Office of Risk Assessment and Cost Benefit Analysis
Washington, DC

Xuefeng Chu, Ph.D.

Assistant Professor, Department of Civil Engineering
North Dakota State University
Fargo, ND

Richard H. Coupe, Ph.D.

Associate Water Science Director
U.S. Geological Survey
Pearl, MS

Bernard A. Engel, Ph.D.

Head, Agricultural & Biological Engineering
Purdue University
West Lafayette, IN

Robert J.M. Hudson, Ph.D.

Associate Professor
Department of Natural Resources & Environmental Sciences
University of Illinois
Champaign, IL

Ian A. Kennedy, Ph.D.

Senior Evaluator/Pesticide Modeler
Pest Management Regulatory Agency, Health Canada,
Ottawa, Canada

Yuzhou Luo, Ph.D.

Environmental Scientist
Department of Pesticide Regulation
California Environmental Protection Agency
Sacramento, CA

Thomas L. Potter, Ph.D.

Research Chemist
U.S. Department of Agriculture
Agricultural Research Service
Southeast Watershed Research Laboratory
Tifton, GA

INTRODUCTION

The Federal Insecticide, Fungicide and Rodenticide Act Scientific Advisory Panel (FIFRA SAP) has completed its review of a set of scientific issues associated with the Two-dimensional Exposure Rainfall-Runoff Assessment (TERRA) Watershed Model and its use in the FIFRA Ecological Risk Assessment for Antimicrobial Uses of Copper.

Advance notice of the consultation meeting was published in the *Federal Register* on August 3, 2011. The review was conducted in an open Panel meeting held in Arlington, VA, on October 25-26, 2011. Dr. Kenneth M. Portier chaired the meeting and Dr. Fred Jenkins Jr. served as the Designated Federal Official.

EPA's Office of Pesticide Programs performs ecological risk assessments under the authority provided in the Federal Insecticide, Rodenticide, and Fungicide Act (FIFRA) as amended by the Food Quality Protection Act (FQPA) to ensure that a pesticide does not pose any unreasonable risks to the environment. The Agency utilizes a combination of data submitted by pesticide manufacturers, open literature, and computer models to conduct risk assessments and to evaluate the potential hazards posed by a pesticide to non-target species and the environment. Models are an essential part of the risk assessment process because they allow the Agency to perform nationwide environmental exposure assessments in the absence of nationwide spatially explicit monitoring data for each chemical.

The most recent ecological risk assessment for antimicrobial uses of copper, completed in 2010 as part of its' Reregistration process, used the "Biotic Ligand Model" (BLM) to estimate aqueous exposures from wood preservative and roofing shingle uses and the "Marine Antifoulant Model to Predict Environmental Concentrations" (MAM-PEC Model; version 2) to evaluate exposure from antifoulant uses of copper. The Agency anticipates conducting a complete ecological risk assessment, including an endangered species assessment, for all pesticidal uses of copper through its' Registration Review process. The Final Work Plan for the Registration Review of copper was published in March 2011. Documents related to the Reregistration and Registration Review of copper can be found at regulations.gov in dockets EPA-HQ-OPP-2005-0558 and EPA-HQ-OPP-2010-0212, respectively.

The Two-dimensional Exposure Rainfall-Runoff Assessment (TERRA) Watershed Model has been proposed by the American Chemistry Council (ACC) as a refined model for estimating environmental exposure from the use of copper as an antimicrobial pesticide. The TERRA Model uses a generalized watershed rainfall-runoff, sediment transport, and contaminant transport modeling framework. It is a spatially distributed watershed model which allows for multiple use patterns of antimicrobial copper to be simulated simultaneously across a watershed, thereby providing a cumulative aqueous exposure profile from antimicrobial uses of copper at any point in the watershed.

The purpose of the SAP Consultation was to obtain an independent evaluation of the TERRA watershed-scale model and to gain advice on the application of TERRA specifically as applied to the antimicrobial copper risk assessment.

Opening remarks at the meeting were provided by Dr. Steven Bradbury, Director, Office of Pesticide Programs (OPP, EPA). Presentations were made during the meeting by Dr. James Hetrick (OPP, EPA), Dr. Siroos Mostaghimi (OPP, EPA), Dr. Mark Velleux, HydroQual on behalf of the American Chemical Council (ACC), Dr. Stephen Wente (OPP, EPA), and Ms. Donna Randall (OPP, EPA)

PUBLIC COMMENTS

There were no written or oral statements provided by the public for this meeting.

Summary of Panel Discussion and Recommendations

Charge Question 1a: What does the Panel believe are the advantages and/or limitations of assessing antimicrobial uses of copper from roofing shingles and wood preservatives with TERRA, a spatially-explicit, watershed scale model? Are there other models that the Panel feels should be considered for use by OPP in estimating exposure to copper from its use as an antimicrobial pesticide, specifically in roofing shingles and wood preservative?

Transport and fate simulations of copper were conducted with the TERRA model to demonstrate the potential of the model for urban pesticide exposure assessment analysis. The TERRA model, a grid-based distributed parameter hydrologic/water quality model, was applied to a hypothetical urban watershed to assess movement of copper to the watershed outlet from uses on shingles, utility poles, and wood decks. The model has strengths and limitations that are consistent with characteristics of grid-based, distributed parameter hydrologic/water quality models. Strengths include the ability to represent spatial variability and processes, the provision of spatially variable results, and the potential to improve simulated results. Limitations of these approaches include extensive spatial data requirements, model and calibration complexity, and results that vary depending on grid cell size used.

The TERRA model has further advantages and limitations for assessing losses of copper from antimicrobial use on shingles and as a wood preservative in an urban watershed setting. Advantages include the potential for improved simulation of copper losses relative to simpler models and flow routing approaches that scale over a range of conditions. Limitations include the lack of TERRA's applications to real urban watersheds, the approach used in represented grid cells with mixed properties such as land uses, inadequate representation of impervious connected surfaces, and the long computational time required to complete watershed simulations.

Charge Question 1b: In the opinion of the Panel, what attributes of an urban watershed model are the most critical and why does the Panel regard these attributes as critical? Does the TERRA model possess these attributes?

The Panel discussed several attributes which they deemed as important in urban watershed models for estimating pesticide exposure. These included:

- Representation of connected impervious areas and engineered water conveyances
- Ability to represent the spatial complexity of urban areas
- Ability to represent best management practices (BMP) for stormwater such as detention basins and other low impact development practices

They noted that TERRA currently does not have these attributes; however, it appears that the model could be adapted to include such capabilities.

Charge Question 1c: Please discuss whether TERRA has the modeling capabilities necessary for it to be applied to other urban metal exposure assessments for antimicrobial pesticides as well as what modifications, if any, would be needed to assess exposure to other metals used as pesticides.

The Panel recommended several modifications to TERRA that should be considered to improve its ability to conduct urban metal exposure assessments for antimicrobial pesticides and to assess exposure to other metals used as pesticides. These include:

- Simulation of water-sediment mass transfer
- Improvement of pesticide wash off representation
- Consideration of impacts of other copper sources in the watershed
- Representation of impervious surfaces
- Modeling of re-initializing between events including soil antecedent water conditions
- Representation of subsurface flow
- Representation of engineered structures like storm drains and detention ponds
- Computation of organic carbon (OC) enrichment as a function of sediment delivery ratio

Charge Question 1d: In the opinion of the Panel what further development and/or assessment is necessary to prepare the TERRA model for use as an exposure assessment tool by the EPA?

The Panel agreed that some further development and assessment is necessary to prepare the TERRA model for use as an exposure assessment tool. Thus, they discussed and suggested that further development and assessment include:

- Consideration of how mixed land use and other mixed parameter grids are handled
- Representation of connected impervious areas and engineered conveyances
- Consideration of advective or diffusive metal transport out of stream sediments
- Representation of Low Impact Development (LID) and other practices that reduce runoff and trap pollutants
- Consideration of base flow for longer time steps than currently considered
- An account of spatial-temporal dissolved organic carbon variations
- Consideration of background copper loading
- A parallelization of model code using multi-core processors and CPUs and/or optimization of the code
- Calibration and validation of the model in urban watersheds
- An evaluation of the model's behavior through sensitivity and error analysis

Charge Question 2a: *Are the appropriate pathways (e.g. engineered water conveyance structures) for modeling urban antimicrobial uses of copper within the Goodwin Creek scenario currently included in the framework of the TERRA model? What, if any, additional pathways are necessary to appropriately estimate exposure concentrations?*

The model does not include several important pathways. Given that the TERRA model was originally developed for rural watersheds, the Panel advised that the following additional pathways are required for its application to urban environmental settings. They include: 1) shallow concentrated flow, 2) subsurface flow to streams, and 3) the direct water path from the antimicrobial roof shingles to gutter to road to storm drain and lastly to holding pond.

Charge Question 2b: *What are the most important attributes to consider when selecting and designing an urban watershed modeling scenario? In the opinion of the Panel, where does the Goodwin Creek watershed fall within a distribution of the nation's urban watersheds? Also, given that the model does not account for storm drains, how does this compare to watersheds nationwide?*

The Panel identified and discussed the following as the most important attributes to consider when selecting and designing an urban watershed modeling aquatic exposure scenario:

- Urban or suburban soils
- Man-made conveyance structures and impervious surfaces
- Consideration of urban/suburban organic matter sources and other urban or suburban contaminants (e.g., road salt)
- Increased temperature of runoff; and
- Timing to peak flow changes with increasing impervious area

The Panel noted that the urban landscape imposed upon the Goodwin Creek watershed probably represents a point on the entire continuum of rural—suburban-urban landscapes in the United States but is not typical of an urban or suburban watershed. They concluded that the land use pattern used in the hypothetical urbanized Goodwin Creek (30% 1 house/ac; 30% 4 houses/ac; 30% 8 houses/ac; 9% open space; and 1% total for all commercial, educational, and governmental developments) is not necessarily representative of suburban or urban land use in the United States (US).

Charge Question 3a: *Please discuss the implications of watershed land use patterns on model calibration. What types of impacts could these have on the estimated exposure concentrations of copper?*

There was agreement among the Panel that an essential requirement for water quality model calibration and validation is a dataset that includes hydrologic, sediment, and water quality measurements spanning at least several years. In the case of the simulated urban watershed scenario described, TERRA calibration and validation were not possible since there are no measured hydrologic, sediment, or copper transport measurements available for this watershed simply because the watershed does not exist.

The Panel concluded that the Agency needs realistic scenarios in addition to index, high exposure scenarios. The Panel was not able to agree on whether the Goodwin Creek scenario was an appropriate index scenario but seemed to agree that it did not have all the components needed to have a realistic scenario. Another complicating factor noted was the issue of understanding the quality of fit for within site versus between site validation. Calibration can occur using the first part of a time series and then this fitted model can be validated against the second half of the period. Similarly the model can be calibrated to a couple of different sites (scenarios) and then run with minor changes to predict for adjacent or similar sites. It might also be possible to calibrate a site to part of the target landscape and then validate it to the remainder of the landscape.

Charge Question 3b: Please indicate any unique calibration issues that should be considered when simulating an urban, residential watershed.

The Panel identified several unique calibration issues that should be considered for urban and residential watersheds. They include the:

- Storm water drainage systems including detention ponds
- High percentage of impervious areas and complex relations or connectivity
- High variability in hydrographs, sedigraphs, and chemographs
- Variation of temporal and spatial scales
- Rapid changes in land use
- Inability to capture DEM-based flow directions and accumulations which reflect the real conditions, due to man-made channels, dikes, freeway, bridges, etc.
- Comparison of simulated values against observed data
- Quantification of drainage from urban landscapes including leaks from water supply, drainage, and irrigation systems
- Determination of contaminant buildup and wash-off factors
- Data describing properties of soils in developed areas
- Simulation of pesticide applications

DETAILED PANEL DELIBERATIONS AND RESPONSE TO CHARGE

Charge Question 1

The three most prevalent antimicrobial uses of copper include antifoulant paints, roofing shingles and wood preservatives. The Antimicrobials Division used a basic field scale modeling approach, including maximum use rates, realistic heavy rainfall events, the assumption of high leaching rates, and storm-water conveyance via impervious surfaces, to estimate potential high end aquatic exposure from copper's use as an antimicrobial pesticide in roofing shingles and treated wood. The American Chemistry Council (ACC) has proposed the TERRA Model as an alternative and more refined way to assess aquatic exposure due to the two major urban antimicrobial uses of copper, in wood preservatives and in roofing shingles, on a watershed scale level.

a) What does the Panel believe are the advantages and/or limitations of assessing antimicrobial uses of copper from roofing shingles and wood preservatives with TERRA, a spatially-explicit, watershed scale model? Are there other models that the Panel feels should be considered for use by OPP in estimating exposure to copper from its use as an antimicrobial pesticide, specifically in roofing shingles and wood preservative?

General Advantages and Limitations

TERRA is a grid-based, distributed parameter hydrologic/water quality model and thus has the advantages and limitations of this type of model. Advantages of this type of model, and therefore TERRA, include the:

- Ability to capture spatial variability in a watershed
- Consideration of spatial variability in some hydrology and associated water quality processes
- Ability to obtain some model outputs spatially
- Potential for improved model prediction

The disadvantages of grid-based, distributed parameter hydrologic/water quality models, and thus TERRA, include its':

- Extensive spatial data requirements
- Model complexity
- Calibration complexity
- Potential to obtain different results when model input data are provided with different cell sizes (e.g. results may be different if data are input to the model with 30 m cells compared to 150 m cells)

A grid-based model such as TERRA may actually be less complex than other models. The major modeling effort takes place in the cell. Typically, this scale is where we have the most understanding. Once the cell is modeled, the movement among cells is relatively easy to handle. Thus, overall, the model is potentially more realistic as well as easier to understand. However, it

should be emphasized that accurate landscape scale elevation data are required because it may be difficult to apply this model to landscapes in which little or none of this data are available.

Additional advantages and limitations of TERRA are examined in the paragraphs that follow. Other sections of this report also provide some discussion of advantages and limitations of TERRA as these sections provide suggestions for enhancements to TERRA for application in urban settings.

Advantages

An advantage of TERRA is its spatially-explicit modeling approach for hydrology and associated water quality processes. The approach *may* generate more accurate estimates of water and contaminant transport at the watershed scale, and help with source identification. It is worth noting that the spatial variability represented in TERRA is mainly associated with the water and chemical transport between modeling cells, while each model cell is considered to be homogeneous. Within a cell, the location of houses and copper sources may have no effect on the simulation results.

Another advantage of TERRA is that the diffusive wave based flow simulations implemented in TERRA are suitable for various conditions, including overland flow, shallow concentrated flow, channel flow and even flows in storm drain systems. Thus, the model has the potential to be applied to a range of watershed conditions.

Limitations

There are several current limitations of the TERRA model or the approach with which it was applied to the urban antimicrobial copper case study. In many instances, these limitations could be overcome. Suggestions for overcoming many of these limitations are identified in responses to other charge questions in this report.

TERRA has limited application to urban watersheds (limited calibration, validation, and sensitivity analysis). The application and publication record of TERRA for urban watersheds is limited. A significant limitation of TERRA is that the model was originally designed for a non-urban watershed hydrology with fate/transport algorithms for organic chemicals. Thus, the model's performance in urban watersheds is unknown, and there is an unknown potential for errors in the model, especially when applied to watersheds with extensive urban land uses. For the application to urban environmental settings and copper pesticides, an averaging approach was used for the landscape characterization. Mixed land use grids present challenges in urban areas for processes important to fate and transport of some pesticides such as copper used in antimicrobial pesticides. Land uses, as well as other parameters, are represented with a single value in each grid. This potentially results in inaccuracies in modeled values within grids.

Model parameters within each grid cell are assumed homogeneous. Thus, grid cells in which a parameter, such as land use, is not homogeneous can create challenges. For example in the TERRA urban case study presented, the TERRA model was run with a 90 m (approximately 2 acre) grid, which is considerably larger than the assumed suburban lot sizes. At eight houses/acre, approximately sixteen lots with houses are contained within each cell. The parameters in these cells are thus an average of the properties of the different areas (lawns, bushes, roofs, driveways, decks, fences, poles, streets) within each lot. For the TERRA urban case study presented, TERRA is less spatially explicit than it seems, and groups parameters in the same manner as the Pesticide Root Zone Model (PRZM).

The use of polygons to represent land uses could potentially overcome the limitation of grid cells with mixed parameters such as land uses. Although this is feasible, such an approach will complicate the model by making movement among polygons more difficult. An alternative approach is to reduce the size of grid cells so they become homogeneous, or nearly so. However, this could greatly increase the computational time for the model.

Connected impervious surfaces are an important aspect in estimating movement of copper in antimicrobial pesticides used in urban areas. Currently, this aspect is not well represented in TERRA.

The TERRA model appears to be clearly written, and compiles and runs the example data on different systems. However, one Panelist experienced difficulties in compiling the code, and consequently the Panelist was unsuccessful in being able to run the model.

The TERRA model is complex and computationally time-consuming to run. In addition, some work within Geographic Information Systems (GIS) is required prior to using the model in order to prepare spatial inputs for TERRA. Thus, the time required to complete a model scenario run with TERRA may be a barrier to its use. However, as computer capabilities continue to grow, models like TERRA become increasingly more feasible to run.

Other Models

Other models the Agency may consider for urban pesticide exposure modeling, including copper's use as an antimicrobial agent, were reviewed in materials provided to the SAP (Literature Review: Comparison of Common Watershed Models for Rainfall, Runoff Sediment Transport, and Contaminant Transport and Fate). In addition, the Agency presented results from PRZM for two extreme scenarios (impervious and pervious assumptions). It is possible that PRZM could be enhanced to more realistically represent urban pesticide situations.

The Storm Water Management Model (SWMM) represents many key features and transport routes within urban areas and thus should be considered by the Agency for future urban pesticide runoff assessments. Note however, that SWMM would require modification for this purpose. Another possibility to leverage SWMM capabilities would be to incorporate portions of SWMM (e.g., engineered water conveyance structures) into other models.

b) In the opinion of the Panel, what attributes of an urban watershed model are the most critical and why does the Panel regard these attributes as critical? Does the TERRA model possess these attributes?

There are other model attributes that may be important for other urban hydrology and water quality assessments. However, the important attributes which specifically apply to modeling pesticide exposure in urban areas include the ability for the model to represent the: 1) connected impervious areas, and engineered components, 2) spatial complexity of urban areas, 3) best stormwater management practices, 4) variability of soil properties, and 5) level of urbanization.

The representation of connected impervious areas and engineered water conveyances within urban watershed models is important. Pollutants moving from roof tops or other impervious areas in urban areas can move across impervious surfaces and to engineered water conveyances, reaching streams or water impoundments without contact with soil or vegetation. Currently, the TERRA model does not represent these conditions. However, it could be modified to consider these issues.

The ability to represent the spatial complexity of urban areas is important. The urban landscape can have mixtures of impervious areas and vegetated areas that vary greatly within a few meters. The hydrological behavior of these features with respect to pesticide fate and transport, varies greatly. While the TERRA model has the potential to capture some of this level of spatial complexity, this level of detail was not captured in the TERRA urban watershed case study presented to the SAP. Attempts to capture this level of spatial variability may not be readily supported by available data and may result in significant computational requirements within TERRA if grid cell sizes are decreased to better represent land cover variability.

The ability to represent best management practices such as detention basins and low impact development practices may be important in some urban pesticide modeling applications. These practices are often designed to reduce runoff by infiltrating or detaining water. Further, some of these practices may remove pollutants from the runoff. TERRA has the potential to represent many of these practices, although currently they are not explicitly represented in TERRA.

Soil properties can be highly variable in urban areas as a result of soil disturbances that occur during urban and suburban development. The ability of models to consider this variability may be important for some situations. TERRA can represent the variability in soil properties. However, obtaining soil data representative of disturbed areas in urban and suburban areas is likely a significant challenge.

The critical attributes of an urban watershed for modeling its behavior are based on the level of urbanization. Urban watershed scenarios should be developed for various levels of urbanization, and used to evaluate either the watershed as a whole or different portions of the watershed. Listed below are some considerations in characterizing a watershed in modeling approaches:

1) **Watersheds with low population density** (the average household density of 0.03/acre in Panola County, MS). The natural hydrologic processes are not significantly affected by development, and the watershed and stream network could be delineated from a digital elevation model (DEM).

2) **Watersheds with an intermediate population density** (up to 3 houses/acre). Modifications of hydrologic parameters (e.g., Manning's n, curve numbers, if applicable) are required. Impervious surfaces may affect the hydrograph. For identification of watershed boundaries and flow paths, some human interaction may be required in addition to the DEM-based watershed delineation and stream generation approaches.

3) **Watersheds with high population density** (4+ houses/acre). These areas may be more appropriately termed a "community" rather than a watershed, because the traditional definition of the surface drainage area may not be suitable in this case. Conventional DEM data may not be very useful in determining the community boundaries, and pervious areas may only be associated with disturbed and amended soils, especially for the top soil layers (rather than those parameterized in soil databases such as Soil Survey Geographic (SSURGO) the database or State Soil Geographic (STASGO) database. Simulations of hydrologic flow and associated transport processes should consider the effects by the quick formation of shallow concentrated flow and the existence of storm drainage systems. The K_d (partition coefficient) value should be adjusted for environmental and field conditions.

c) Please discuss whether TERRA has the modeling capabilities necessary for it to be applied to other urban metal exposure assessments for antimicrobial pesticides as well as what modifications, if any, would be needed to assess exposure to other metals used as pesticides.

As confirmed by the following statement in the TERRA model background materials distributed to the Panel, the chemical processes module in TERRA was originally developed for organic chemicals:

"Chemical transport and fate algorithms in TREX (TERRA model) are derived from those in WASP5 (Water Quality Analysis Simulation Program) and IPX (In-Place Pollutant Export Water Quality Modeling Framework)" (page 8-251; Velleux, Parquin, Redman, & Sanfore, 2009).

Neither WASP5 or IPX were specifically designed for metals. As mentioned in the IPX manual, IPX was "*designed explicitly for organic chemicals*" (USEPA, 2001). These models use an approach generally referred to as the " K_d approach." This approach describes the distribution of the metal between water and soil or sediment using a single empirically defined constant. In

addition, by comparing to common K_d approach-based models, the Panel has identified the following concerns and recommendations regarding the TERRA model:

- Water-sediment mass transfer is not simulated in the model.
- Wash off of pesticides is assumed to be linearly related to rainfall. Data is needed to support this assumption. Generally, wash off processes can be best described with exponential decay functions.
- For organic pesticides, the model also should account for degradation, etc.; a pesticide processing module which includes all the primary pesticide fate processes is needed (Wauchope et al., 2004).
- The TERRA model uses single unit values for copper soil/sediment partition coefficients. The Panel recommends that this value be adjustable based on organic matter and pH. Other parameters to consider include clay content and mineralogy and/or Cation-Exchange Capacity (CEC). Use of an adjustable parameter based on soil/sediment properties is common practice when evaluating the fate and transport of conventional pesticides (e.g., Koc concept). Sauve et al. (2000) indicated that adding organic carbon (OC) substantially improved model fit; for Cu just pH; $R^2=0.288$, with OM $R^2=0.419$; $\text{Log}K_d = \text{constant} \cdot \text{pH} + \text{constant} \cdot \log(\%OC) + \text{constant}$ (R^2 was 0.419 to 0.758 for Cd, Cu, and Ni).

In addition, as stated in the USEPA workshop review (Caruso et al., 2008), “the K_d approach in the Water Quality Analysis Simulation Program (WASP) is not the optimum way to model reactive metals fate and transport where pH-dependent sorption and precipitation reactions are involved in response, USEPA developed the Metals Exposure and Transformation Assessment (META4) module for WASP4. META4 simulates equilibrium reactions and slower kinetic processes, including metals adsorption/desorption, precipitation, ion exchange, and complexation.”

Therefore, if simulation capabilities of metals are expected, the two chemical processes of water-sediment mass transfer and K_d adjustments should be incorporated into the TERRA model. In addition, the metal fate simulations implemented in META4 or other relevant models should also be considered for further development.

To further address the question of the applicability of TERRA for other metal antimicrobials, it is helpful to leave aside the spatial resolution issue and compare TERRA and PRZM process representations that affect metal transport. Table 1 displays a comparison of TERRA and PRZM process representations that affect metal transport, a generic metal is denoted as “Me.”

Table 1. Comparison of TERRA and PRZM Process Representations that Affect Metal Transport

Process	PRZM Representation	TERRA Representation	Comments
Me binding to Dissolved Organic Matter (DOM)	Not included	Linear (when activated)	Use of this added realism in TERRA requires careful attention to calibration. It will be to the long-term benefit of TERRA.
Inorganic complexation of Me	Not included	Not included	Can be partially accounted for in site-specific K_p and K_b values.
Me adsorption	Linear adsorption	Linear adsorption	
Dissolved Me transport in surface runoff	Based on Curve Number	Spatially-resolved and based on Green-Ampt	Strength of TERRA is dependent on the site-specific conditions (King et al., 1999).
Erosive transport of particulate Me	Included based on Universal Soil Life Equation (USLE)	Spatially-resolved based on USLE	Strength of TERRA
Mineral phase precipitation/dissolution	Not included	Not included	Only relevant for a few metals
Transport via infiltration/groundwater	Included	Loss term only	Strength of PRZM
In-stream sediment deposition/resuspension	Streams not included	Included	
Sediment deposition/resuspension in floodplains	Streams not included	Included	Relevant mainly for larger river systems.
Advective/diffusive exchange with in-stream sediments	Process not relevant	Not included	Correctable shortcoming of TERRA

The similarity of many processes in the two models suggests that TERRA is as suitable for other metals as PRZM as long as subsurface transport can be reasonably neglected. It may be noted parenthetically that TERRA is not suitable for mercury (an important metal, but no longer an antimicrobial) in its current form due to the need for multiple non-equilibrium metal species. The Panel recommends moving beyond the constant K_p (K_d) approach and basing K_p values on fundamentally-sound, equilibrium chemical speciation models. This would greatly aid in site-specific calibration (explaining differences between geochemically-distinct watersheds) and in accounting for temporal variations (e.g., flow- or season-dependent) at a given site. While this is an important long-term goal, currently adding an explicit complexation sub-model for copper or other metals is not realistic for a spatially resolved model such as TERRA due to the immense increase in required input data (time-dependent concentrations of interacting ions and pH and the

computational requirement for many added equilibrium calculations). It may be more appropriate to start by implementing such an approach in PRZM. For either model, it would be valuable to implement a systematic approach to using Windmere Humic Acid Model (WHAM) or EPA's geochemical equilibrium model (MINTEQA2) to predict site- and season-specific K_p values (Tipping, 1994; EPA, 1999).

Another factor to be considered in modeling scenario design is the presence of other copper sources in the watershed. This is necessary due to the non-linear nature of copper-DOM (dissolved organic matter) interactions, which causes copper to be bound less strongly at high copper: DOM ratios than at low ratios. Such non-linearity is incorporated into WHAM, used in the Biotic Ligand Model (BLM), but not in the constant K_p (K_d) approach used in both PRZM and TERRA. Since it would be a simple matter to check how sensitive K_p is to total copper levels by using WHAM or BLM, such a check should be performed prior to continuing with the current approach, which neglects background copper.

In addition to the chemical process considerations, the Panel recommended the following hydrology and sediment simulation considerations for improvements to the TERRA model.

- **Proper consideration of impervious surface.** In simulations presented to the Agency, impervious surface was accounted for by adjusting saturated hydraulic conductivity K_{sat} values within grids based on the percentage of the grid area covered by impervious surface. This approach has not been evaluated to determine whether it adequately describes hydrologic response. This is testable at least at small scales by using rainfall simulation, varying soil/impervious surface ratio, and by examining rainfall partitioning.
- **Linkage of water balance to re-initializing between events and computing soil antecedent water conditions.** The Panel recommends that there be a linkage between water balance and the re-initialization between events and the computation of soil antecedent water conditions. This will require simulation of evapotranspiration (ET). ET is a large component, thus uncertainties can have large impacts on other hydrologic processes such as runoff and stream flow.
- **Subsurface flow.** This is a significant hydrologic process in many watersheds. For example, in the Little River Experimental Watershed located in south-central Georgia, subsurface flow typically exceeds surface runoff. This process is especially important for the south east USA where Ultisols are the predominant soil order. Characteristic features of these soils are dense subsoil horizons (30 to 50 cm) that redirect flow down slope. Another consideration is that strongly-sorbing substances are not typically transported far into soil profiles. If this is the case for copper, then the lack of subsurface flow in TERRA is tolerable for the prediction of total copper loadings. However, the impacts of subsurface flow on hydrologic simulation and in-stream copper concentrations need to be documented with relevant field data.
- **Engineered structures such as storm drains and detention ponds.** These practices should be represented within TERRA.
- **Numerous studies have shown that organic carbon (OC) enrichment (ER_{oc}) in runoff sediment is related to the sediment-delivery-ratio (SDR).** For example Schiettecatte et al. (2008) found $ER_{oc} = 1 + 1.931 \exp(-5.367 * SDR)$ for sediments in runoff from silt-loam soils. In short, the organic carbon content of sediment in runoff varies with erosion intensity and deposition processes during transport. This must be taken into account when evaluating

transport of elements like copper since most of the metal is transported sorbed to sediments and binding intensity to sediment is strongly dependant on organic carbon content. Sauve et al. 2000 developed the following regression equation for sorption of copper on soil using results from numerous published studies. $\text{Log}(K_d) = 0.21 * \text{pH} + 0.51 * \text{log}(\% \text{OC}) + 1.75$.

d) In the opinion of the Panel what further development and/or assessment is necessary to prepare the TERRA model for use as an exposure assessment tool by the EPA?

TERRA is an intriguing model and this type of model could provide important exposure estimates for the Agency that are not available from other models and techniques. It may also prove useful for Total Maximum Daily Loads (TMDL) analysis. A spatially explicit watershed model could be useful in assessing exposure of endangered or threatened species to pesticides. TERRA's fundamental strengths in modeling both dissolved and particulate metal transport in a spatially-explicit manner are in the long term essential for establishing confidence that realistic assessments are being made. When people can see Doppler radar images and obtain accurate weather forecasts days ahead every night on TV, the days of using simple models as final products for environmental pollution management have to be considered limited. TERRA application was demonstrated in an exposure assessment case study to assess antimicrobial uses of copper in the simulated urban or suburban environment. An analogy was made to the Tier 1 and 2 tools used by the Agency to evaluate agricultural pesticide uses. Evaluation of single use patterns, similar to the single crop exposure assessments conducted using the agricultural screening tools, should be possible with an exposure tool for antimicrobial uses in urban or suburban settings. It appears that TERRA can estimate water, sediment, and soil concentrations of copper resulting from the use of algae resistant shingles or treated wood as the sole use pattern in an urban or suburban watershed, although enhancements to the model are suggested. However, the quality of these estimates is unknown.

Several enhancements to TERRA are needed to improve its predictive abilities for pesticide exposure assessment in urban areas.

Model Enhancements

Further consideration on how to address mixed land use and other mixed parameter grids within TERRA should be explored. Land uses, as well as other parameters, are represented with a single value in each grid. This potentially results in inaccuracies in modeled values within grids when parameters such as land use are not homogeneous.

Connected impervious areas and engineered conveyances need to be better represented. Both connected impervious areas and engineered water conveyance structures allow water carrying pollutants to move to the outlet of the watershed without interaction with soil and plants. In the TERRA case study presented to the SAP, the interaction of runoff carrying copper with soil resulted in significant retention of copper in the soil. Thus, runoff carrying pollutants such as copper that are conveyed via impervious surfaces to water bodies may result in significantly greater pollutant delivery than was predicted in the case study presented to the SAP.

TERRA does not currently consider advective or diffusive metal transport out of stream sediments. Such processes may be important in some exposure assessments, and thus these capabilities should be added to TERRA. The importance of LID and other practices in reducing runoff and pollutants may need to be considered (depends on how the model will be used) in TERRA. Practices such as detention basins may be important points of pesticide exposure assessment. Other practices such as rain gardens may be important in capturing and retaining pesticides within small basins. Such representation methodologies should that consider groundwater-fed wetlands as hydrologic flows passing through these systems may behave distinctly differently than flows through upland soils.

Several additional improvements are needed to increase the realism of several processes within the TERRA model. A methodology for describing base flow (and simulating it using longer time steps) should be added to the model. Although some description of base flow is possible in the model as a point source, an approach to specifying base flow inputs that is consistent with the rainfall data needs to be incorporated in the model. This is important for exposure assessment as this process would transport metals from stream sediments back into the water column.

A methodology to account for spatio-temporal dissolved organic carbon (DOC) variations should be incorporated in the model. From Dr. Velleux's (of HydroQual presenting on behalf of the American Chemical Council) comments during the public meeting, dissolved copper transport seems to be the main mechanism of transport for the case study presented. Since in many environments copper is strongly bound to DOC, modeling the dynamics of this variable may be more important than predicting erosion. Perhaps modeling DOC separately, as done for sediments, would be the best approach.

The non-linearity of copper adsorption/binding means that background copper loading should be considered in the model. In some instances, these processes may be an important source of pollutants.

The TERRA model could be made more accessible by parallelization of the code using multi-core processors and GPUs (Graphics processing units) and/or optimization of the code. Decreasing the computational time for the model may prove to be an inexpensive means of making TERRA more accessible.

TERRA capabilities for estimating copper losses need to be explored further by applying it to additional sites with other soils and precipitation rates to provide estimates of exposure in ecosystems relevant to the Agency's ecological risk assessments. TERRA could be applied to some of the 811 monitoring sites with copper data to further demonstrate its predictive capabilities with respect to copper. Given the limitations of many of these datasets, it may be necessary to embark on an urban watershed study in which copper and other urban pesticide data are collected.

Calibration and validation of the TERRA model in urban watersheds is desirable and should be considered. TERRA has a limited record of application in urban watersheds and thus its predictive abilities in such watersheds are largely unknown. Given the limited nature of

pesticide data sets for urban areas, model validation for urban watersheds may need to rely on hydrology and pollutants other than pesticides.

The model behavior should be thoroughly evaluated through the use of sensitivity analysis (to assess model response to small changes in mean values of the parameters) and error analysis (to assess model response to changes in the variance of model parameters) for urban watersheds. Such analyses may have been performed with nonurban watersheds but analysis on urban watersheds is also necessary. Presentations to the SAP and materials provided to the SAP indicate the hydraulic conductivity (K_h) is an important parameter; sensitivity analysis would provide the user with the complete set of important parameters in the model.

Several sources of uncertainty were identified during the presentations: rate of copper release from the various antimicrobial building materials, the applicability of using the original soils for the urbanized version of the watershed, and modeling judgment. Uncertainty should be characterized for the exposure tool to alert the tool users with the range of uncertainty associated with the output. The uncertainty associated with the tool output will be needed for the input of exposure estimates into risk assessments.

From a practical standpoint, an exposure assessment tool used by the Agency eventually will be available to the public on the web. As such, the model should be available as an executable file. Not all Panel members who tried were able to build a working executable file from the source code files provided. A detailed user's manual should be available. The user's manual should transparently list the input data required, methodology used to derive the estimated environmental exposure concentrations, source code, assumptions made by the model and an evaluation of model behavior (sensitivity analysis, uncertainty analysis). The model should also not be resource prohibitive to run, in either time or data requirements. The output produced by the model should be labeled and easily identifiable.

The Agency may be missing an opportunity to have the SAP perform model evaluation by not providing an executable version of the model and typical input parameters. The SAP could perform sensitivity analysis, uncertainty analysis and more easily opine on model behavior if the executable version of models under review are supplied.

Urban Pesticide Watershed Modeling Scenario

In addition to enhancements to the TERRA model, enhancements to the urban watershed case study should be considered. In some instances, enhancements to the urban watershed case study interact with TERRA enhancements and thus the model is also included in the discussion.

An exposure tool used by the Agency should predict exposure over a spatial and temporal scale relevant to the biota potentially exposed. The use of the Goodwin Creek outlet as the water concentration output provides an aggregated estimate of copper concentrations that may occur in the watershed but may not provide the exposure estimate most relevant. Water concentrations from lower order streams may include higher concentrations that are diluted at the outlet. The exposure assessment tool should be used to provide estimates at other points in the watershed.

The urban watershed scenario presented and models such as TERRA used in these settings should represent, and allow the user to manipulate, components of the urban/suburban environment important to the fate and transport of copper from antimicrobial uses. TERRA should address how other urban contaminants influence water quality and concentrations of copper (e.g., salts from snow removal). The urban/suburban land use pattern should be amenable to manipulation by the user.

As an aspirational goal, ecological exposure from simultaneous use patterns, both antimicrobial and conventional, should be examined in the watershed. Suburban/urban areas may have the antimicrobial uses examined in TERRA, conventional uses in sewer systems to control mollusks, as well as lawn and garden application of conventional copper pesticides. The model and modeling scenario should address multiple sources of copper in watersheds such as shingles, fence posts, decks, utility poles, as well as pesticide applications to sewer systems, lawns, homes, gardens and agricultural uses, if present in the watershed. There are approximately 575 products registered as pesticides containing copper (National Pesticide Information Retrieval System (NPIRS) search of active registrations – 10-24-2011). While exposure assessment could involve estimating only the incremental exposure due to the deployment of antimicrobial copper in the types of uses currently addressed by the model (shingles, decks, fences and utility poles), the model would serve as a more useful tool if it also considered the total exposure from all other sources of copper, such as naturally occurring copper as well as copper from other non-antimicrobial pesticides and other man-made sources of copper. The model should be expanded to assess exposure resulting from all sources of copper.

Without further comparison between the predicted copper concentrations in the hypothetical urbanized Goodwin Creek and other hypothetical urbanized watersheds in other geographical locations, it is difficult to confirm that an urbanized Goodwin Creek is a conservative assessment or that other urbanized watersheds will not be necessary for the Agency's ecological risk assessments. TERRA needs to demonstrate the capacity to assess other geographical areas. A conservative scenario may be the simultaneous installation of antimicrobial building materials within a small sub-watershed. If the maximum short-term release rates occur during the first 250 mm of precipitation, simulating all installations to occur at the same time, as in a new

development, would represent a conservative scenario for terrestrial and aquatic exposure. Providing water and sediment concentrations in the lower order stream draining the development would be preferable to the concentration at the outlet.

The distribution of different land use types should be representative of a worst case urbanized area. It is unclear whether the distribution of 30% of the watershed in 1 house/acre land use; 30% in 4 houses/acre; 30% in 8 houses/acre; 9% in open space; 0.4 % in commercial; 0.6% in education and 0.5% in government is representative. Commercial uses typically have a high proportion of impervious surfaces; more than in a 1 house/acre or 4 house/acre land use. Velleux, Paquin, Redman, & Santore (2009), (document supplied to the SAP entitled *The "Exposure Assessment for Potential Risks from Antimicrobial Copper in Urbanized Areas"*) states that the distribution used in the model represents land use where the use of antimicrobial copper building products is estimated to be the greatest. It is unclear whether this land use pattern also represents the greatest transport of copper into aquatic environments or the greatest accumulation of copper in soil. An urban watershed scenario should include conditions likely to produce a high-end or upper bound exposure in the aquatic environment and a separate set of conditions likely to produce a high-end terrestrial soil exposure.

Urban or suburban soils are often not the soils originally occurring in the area. Soils consolidated from several sources may be used in urban areas. Suburban soils often have the topsoil layer removed. The current configuration of the TERRA model application to the watershed case study appears to assume that urban land uses do not alter most of the soil properties of the undeveloped soil originally found in the urban area. The example input files for the TERRA case study presented to the SAP show many of the same values for soil parameters in undeveloped soils and 35 urbanized soils used in the Goodwin Creek simulation. The availability of soil property variability data in urban watersheds will remain a challenge.

Presentations to the SAP focused on estimating concentrations of copper in water, sediments and soil. Presumably the exposure assessment currently possible with TERRA would include aquatic organisms in the water column and sediments and terrestrial organisms in the soil. The spatially-explicit watershed design of TERRA presents other opportunities to assess exposure of different types of organisms. A spatially explicit model could provide estimates of exposure for mobile organisms that might spend time in different parts of the watershed, perhaps directly contacting antimicrobial building materials, soil underneath the building materials, sediments or water in streams. This may include organisms flying from one building material to another, or fossorial organisms excavating the soil beneath building materials or amphibians moving from one stream section to another. As different types of ecological risk assessments become necessary, endangered species assessments in particular, spatially explicit watershed models may provide a method to assess these mobile, intermittently exposed species. Although the presentation on TERRA did not discuss these types of exposures and the spatial scale used in the model might preclude calculating these exposures in the current configuration, a spatially explicit model like TERRA could form the basis for different types of exposure assessments not previously attempted.

Charge Question 2

The Agency employs a tiered strategy to assess aquatic exposure. The first tier facilitates the rapid screening of pesticide uses for potential risk issues, while the second tier refines exposure estimates by utilizing a field scale model and site specific properties. This process is designed to incorporate additional data (e.g., site specific properties) for each progressive tier. The Agency has historically employed field scale models to assess aquatic exposure in support of national pesticide registrations. The TERRA model, unlike other models used by OPP, is a fully distributed, spatially-explicit watershed model. It has model capabilities of distributing differences in hydrology, meteorology, soil properties, and pesticide uses across a watershed. These model capabilities require consideration in terms of the proper scale of the exposure assessment.

a) Are the appropriate pathways (e.g. engineered water conveyance structures) for modeling urban antimicrobial uses of copper within the Goodwin Creek scenario currently included in the framework of the TERRA model? What, if any, additional pathways are necessary to appropriately estimate exposure concentrations?

The Agency's analysis of the need to represent engineered water conveyances in TERRA is compelling. There seems to be no debate that there are two parallel routes that runoff from antimicrobial shingles could take. Even if TERRA is modified to include engineered conveyances, e.g., by adding storm drain networks, likely it will always be a challenge to assess exactly how much roof runoff makes it to these conveyances. Thus, to some extent, the type of bounding approach used by the Agency may still need to be employed to assess how much copper reaches streams.

It may be worth exploring methods that permit TERRA to partially overcome this objection without major modifications to the code. Although the Agency showed the difficulties that arise from creating engineered conveyances in TERRA while retaining the logic of spatially explicit modeling, it may be possible to aggregate impervious areas in a way that approximates engineered conveyances, e.g., by selecting a set of cells connected to the stream whose number reflects the average impervious area for a relatively homogeneous region of the simulated basin. A methodology for doing this in a non-arbitrary fashion would need to be developed. Of course, for a hypothetical urban watershed, doing something like this should pose fewer objections.

The TERRA model was originally developed for rural watersheds. Additional pathways are required for its application to urban environmental settings. Shallow concentrated flow should be considered in the simulation as an additional flow type. The current TERRA model considers only two types of flow: overland flow and channel flow. Overland flow generated in one modeling cell may be transported over multiple downstream cells for a long travel distance. The typical distance for overland flow transport in the model application could be estimated based on the watershed delineation and stream network generation. For the Goodwin Creek watershed, the watershed delineation threshold is 0.4 km^2 , indicating a travel distance of 600+ m ($\sqrt{0.4 \text{ km}^2}$) of overland flow before reaching the stream. However, according to TR-55 (USDA, 1986) "*After a maximum of 300 feet, sheet flow usually becomes shallow concentrated flow.*" For urban environments, the travel distance is even shorter: "*Typically, urbanization*

reduces overland flow lengths by conveying storm runoff into a channel as soon as possible (USDA, 1986).” This indicates that the overland flow may already be converted into concentrated flow before leaving the model cell. Given the fact that TERRA does not simulate storm drainage systems, the inclusion of shallow concentrated flow could be used to account for some of the effects of the un-simulated drainage system on the hydrograph.

An additional pathway that may need to be considered because it has the potential to be important is a direct water path from the antimicrobial roof shingles to gutter to road to storm drain to holding pond. This pathway has the potential to deliver copper without much time for sorption and sedimentation.

Infiltration of water and the subsurface movement of this water to streams and ponds are important in some watersheds and therefore may need to be considered by the model. Further discussion of the importance of subsurface flow can be found in the response to question 1c.

b) What are the most important attributes to consider when selecting and designing an urban watershed modeling *scenario*? In the opinion of the Panel, where does the Goodwin Creek watershed fall within a distribution of the nation’s urban watersheds? Also, given that the model does not account for storm drains, how does this compare to watersheds nationwide?

As in most contaminant studies of this nature, there are several factors that must be correct in order for the model results to be of use. These are source, hydrology, and the interactions between the source and hydrology. Source of the contaminant is important for if there isn’t a source for the contaminant, then there isn’t any need to model its movement. The source must be well characterized in its behavior, i.e. how much is applied or available, where it is located on the landscape, and when it is applied or available. The second component (hydrology) is as important as the first, because in order for the contaminant of interest to move, water is needed to move it (excluding those contaminants that are transported atmospherically). It is important to be able to accurately model the hydrology to understand where and when water moves over the landscape. The model must interpret the interaction between the source and hydrology: how the contaminant is entrained in the water and the subsequent processes that affect the contaminant (i.e. degradation, sedimentation, volatilization, or other loss mechanisms). If the source or the hydrology of the study area or the fate of the contaminant is poorly understood, then the results from the model could give misleading or erroneous information. The model could even give accurate results because the poor assumptions that have been made would cancel each other out, but that may not be readily apparent.

Examining the results from the urban watershed model scenario presented using TERRA, the model suffers from some issues with characterizing the source and modeling the hydrology of the study area. First, there is a lack of literature on the release of copper from shingles and treated wood; it appears that it is not very well characterized or understood nor is the amount of houses with copper treated shingles and/or copper treated decks or fencing well known. Although it appears that reasonable assumptions were made in the model for the amount and distribution of copper sources, this remains an assumption. There really is no way of indexing the results from this model with actual environmental scenarios. If we consider what a

maximum scenario might look like, it can give an idea of where this scenario might fit compared to real world situations. The TERRA model showed that 90% of the copper is lost to infiltration into the soil so a maximum scenario might be to sample at the outlet of a heavily urbanized small subbasin that has 50 to 75 % impervious surfaces with stormwater conveyances as well as a majority of the roofs made with antimicrobial shingles and many with wood decks and fencing. There is some information that the release of copper from shingles and decks is larger in the beginning (many compounds show an exponential decay pattern) and so a larger export value could be used. The results from the TERRA model presented to the Panel probably do not represent a worse case scenario. Additionally, while TERRA seemed to simulate the hydrology of Goodwin Creek at least adequately while it was an agricultural watershed, there is no evidence that the way impervious surfaces were simulated in the model accurately represents urban hydrology. Further, the model does not have features that most urban landscapes have such as storm water conveyances, detention ponds, soil structural changes, and changes in vegetation cover. Nor does the model account for subsurface flow. The results from this model have to be filtered through this knowledge on its limitations.

The land use pattern used in the hypothetical urbanized Goodwin Creek (30% 1 house/ac; 30% 4 houses/ac; 30% 8 houses/ac; 9% open space and 1% total for all commercial, educational, government) is not necessarily representative of suburban or urban land use. Suburban and urban areas could be expected to have more commercial land use, recognizing that commercial areas have a larger proportion of impervious area than residential or open space. The Goodwin Creek watershed does not have the amount of impervious found in urban and suburban environments, and is completely lacking in storm drains and man-made water channelization structures, which are commonly present in urban and suburban environments.

The rainfall regime for the study watershed area probably represents the high end of rainfall amounts which may or may not be important in understanding the fate and transport of copper. Other rainfall regimes should be explored.

Rather than talking about a distribution of urban residential watersheds, the Agency should be considering a “continuum” of residential watersheds – ranging from residences in primarily agricultural landscape through suburban to urban landscapes. As one goes from rural to urban, a number of characteristics change simultaneously: housing density, size of lots, percent area in permeable (or impermeable) surfaces, increasing likelihood of runoff conveyance systems, changes in automobile traffic, levels of soil disturbance, etc. In addition, the nature, size, number, and degree of isolation of runoff management structures will change as well. It is understood that few if any of these characteristics will change uniformly and in fact some of these characteristics, such as soil permeability or percent impermeable surface, may plateau at some level of housing density that falls far short of inner-city levels. Another parameter to consider is the level of dry deposition occurring in rural versus urban settings.

An aquatic exposure scenario for an urban watershed should realistically account for attributes of the urban setting that may augment or alter the bioavailability of the hazard. The urban environment differs from an agricultural setting or rural setting in several important ways relevant to biogeochemical cycling and transport of micronutrients, metals and contaminants. These include: 1) urban or suburban soils; 2) man-made conveyance structures and impervious

surfaces; 3) consideration of urban/suburban organic matter sources and other urban or suburban contaminants (e.g., road salt); (4) increased temperature of runoff; and 5) timing to peak flow changes with increasing impervious area.

1) Urban soils may be consolidated from several other sources and may no longer resemble the original soil that once occurred in the urban area. Urban soils may be more compacted than rural or agricultural soils and may be more likely to result in runoff than the undeveloped soil of the urbanized area. It is unclear how representative undeveloped soils original to the area are in characterizing urban or suburban hydrology or erosion.

2) Runoff water in urban areas is likely to enter man-made channels or conveyance structures. Water carried by storm drains or storm sewer systems will have different flow pattern and peak flows than water in an undeveloped watershed. A greater amount of discharge may be generated over a shorter time period after a rainfall event in the urban environment than in an undeveloped watershed. The timing of the runoff and the amount will influence the flushing or scouring regime in watershed streams.

3) Organic material produced by fallen leaves, tree limbs, and debris will be carried to streams as will road salt, sand, oils, grease, nutrients, pesticides and other contaminants.

4) Water temperatures may increase due to runoff from impervious areas. Runoff water from heated impervious surfaces (e.g., roadways and parking lots exposed to sunlight) may raise the temperature of the receiving waters. Water temperature could play a role in the dynamics of metal or other contaminant transport in the aquatic system.

5) A generic urban watershed exposure scenario would address the change in timing and peak flow of urban runoff relative to undeveloped watersheds. The percent impervious surfaces in the watershed should be at the upper end of the distribution of impervious surfaces in urban areas. The degree of soil compaction should also be at the upper end of the distribution of compacted soils in urban areas to provide an urban aquatic exposure scenario.

Both photochemical decomposition and autochthonous production of DOM in lakes/ponds may cause them to exhibit different distributions of DOC concentrations than observed in streams. Since the 811 USGS sites were largely streams, it should be shown that this does not bias exposure calculations.

In general, correlations between discharge and season and geochemical variables that affect copper toxicity and transport (DOC, pH, cations, etc) need to be considered. Such correlations exist in small watersheds, and may be present in urban watersheds as well. These may affect the approach to coupling with BLM as well as specification of time-dependent K_p values.

Charge Question 3

Watershed-scale models require calibration to account for complex watershed-dependent hydrology and environmental fate processes. Model calibrations have been conducted by altering saturated hydraulic conductivity, Manning's *n*, soil erodibility factors, land cover factors, and chemical partitioning coefficients. In contrast, the OPP field-scale models such as PRZM/EXAMS are not calibrated for site-specific hydrology, *etc.* The TERRA model utilizes a simulated urban watershed that was calibrated to the hydrology and sediment loads of Goodwin Creek. Because the Goodwin Creek watershed is a predominately pastured/forested watershed, the EPA has concerns that the calibration processes may not adequately represent urban hydrologic and chemical transport processes.

a) Please discuss the implications of watershed land use patterns on model calibration. What types of impacts could these have on the estimated exposure concentrations of copper?

The model calibration process broadly defined is the iterative adjustment of sensitive model parameters to improve the agreement between simulated and observed values. Unambiguous performance metrics should be used in this process and include metrics such as Root Mean Square Error (RMSE) and Nash-Sutcliffe Efficiency (NSE). Calibration is typically hierarchical with model hydrologic response evaluated first, followed by sediment transport, and water quality constituents. A companion process, validation, should follow calibration to provide confidence to model users that the calibrated model appropriately assesses watershed conditions and model parameters and provides simulated results that agree with observed outputs. Watershed data records are often split with one portion used for calibration and one for validation. The goal in this case is to enhance model credibility by showing that a single set of parameters identified during model calibration provide simulated outputs that meet performance goals for measurements made during the period of record used for validation.

There was consensus among the Panel that an essential requirement for water quality model calibration and validation is a dataset that includes hydrologic, sediment, and water quality measurements spanning at least several years. As described in documents provided to the Panel, the hydrologic and sediment transport components of TERRA were calibrated using measurements provided by the USDA-Agricultural Research Service for the Goodwin Creek Watershed. Well-known metrics such as RMSE and NSE that quantitatively assess the goodness-of-fit between the observed and simulated values were not reported. Calibration and validation of the hydrologic components of the well-known watershed model, SWAT, was reported in a 1999 publication (King et al., 1999) using the Goodwin Creek dataset, and these metrics would be useful for comparing TERRA performance to this and other watershed models. TERRA validation was not described in the material provided to the SAP. No copper measurements were reported for the study watershed, thus calibration and validation associated with the ability of TERRA or other models to effectively predict copper fate and transport in the watershed were beyond the limits of available data.

In the case of the simulated urban watershed scenario described, TERRA calibration and validation were not possible since there are no measured hydrologic, sediment, or copper

transport measurements available for this watershed. Simply, the watershed does not exist. The effective evaluation of TERRA performance requires that the model be tested using an urban/suburban watershed dataset. Data sets for such a test may be available from researchers at Oregon State University, University of California at Riverside, and or the University of Connecticut.

Urban/suburban watersheds have unique hydrologic characteristics and chemical transport processes. In particular, elevation within these landscapes may be impacted through modifications associated with construction of water conveyances, roads, and other structures. Elevation changes in combination with storm drains and other structures may significantly alter hydrologic flow paths and mass exchange and deliver surface runoff directly to surface waters without interception and or transport across soil surfaces.

A recently released version of the model PRZM, called "super-PRZM", may be useful in simulating these urban/suburban scenarios since it is a scalable model whose outputs can be routed through the landscape using digital elevation data. In essence this makes the model useable at the watershed scale. Participants in a 2007 EPA OPP EFED Pesticide Exposure Modeling Public Meeting recommended that the Agency consider use of the SWMM Model in assessing pesticide fate and transport in urban and suburban environments. Presentations made at the meeting are available on-line in a public docket: <http://www.regulations.gov> (DOCKET NO. EPA-HQ-OPP-2007-0319).

TERRA may be used to assess the assumptions used for averaging cell properties. TERRA could be run at a fine scale on a single lot to see if the overall, infiltration matches the aggregate infiltration used for the 90m cells in the full watershed TERRA run. This wouldn't solve the urban watershed calibration problem, but it may provide some insight on these particular assumptions.

Calibration may not be needed as the Agency generally does generic modeling, such as for the scenarios used for PRZM/EXAMS. If the Agency were to use the TERRA model, it would likely use some sort of "index" watershed (to serve as a guide), which might not be a real watershed. This doesn't mean that calibration to a particular watershed is unnecessary, but it might be used mostly for insights into how to make a generic scenario for the Agency to use.

The Agency may wish to consider use of a suburban watershed located in southern California for an index watershed. University of California in Riverside scientists have studied a watershed in this region for several years and performance of the USEPA model SWMM in describing pesticide runoff will be reported in an upcoming American Chemical Society publication (Jackson and Winchell, 2011).

The spatial relationship of copper sources to impervious areas and to runoff-generating grid cells and to streams is crucial. In the Goodwin Creek scenario, riparian buffer areas were prevalent. On the contrary, impervious surfaces were not well connected to the streams. Accurately representing particle-water partitioning of copper is an important consideration. The relative importance of copper transport by water runoff and erosion (controlled by K_p) likely would strongly interact with the distribution of land use types since water and sediments

transport differently across pervious and impervious surfaces. It would be best to calibrate the model to the observed distribution of copper between water and particles in relevant runoff samples.

The Agency needs realistic scenarios in addition to index, high exposure scenarios. The Panel was not in agreement on whether the Goodwin Creek scenario was an appropriate index scenario but seemed to agree that it did not have all the components needed to have a realistic scenario. Another complicating factor noted was the issue of understanding the quality of fit for within site versus between site validation. Calibration can occur using the first part of a time series and then this fitted model can be validated against the second half of the period. Similarly the model can be calibrated to a couple of different sites (scenarios) and then run with minor changes to predict for adjacent or similar sites. It might also be possible to calibrate a site to part of the target landscape and then validate it to the remainder of the landscape.

b) Please indicate any unique calibration issues that should be considered when simulating an urban, residential watershed.

As noted in discussion for question 3a, the most significant challenge for urban simulation modeling is the limited number of appropriately robust datasets that are available for calibration and validation. TERRA calibration using the Goodwin Creek dataset should not be confused with calibration of the simulated urban/suburban scenario described.

Unique calibration issues were identified for urban and residential watersheds were:

- Storm water drainage systems including detention ponds.
- High percentage of impervious areas and complex relations or connectivity (directly connected and non-directly connected impervious areas).
- High variability in hydrographs, sedigraphs, and chemographs.
- Varying temporal and spatial scales. Smaller time interval should be used to capture short-duration storm peaks and small spatial scale and high-resolution data should be used to characterize the high variability in land use/land covers (LULC) and flow routing. This issue makes the model calibration difficult.
- Rapid changes in land use, e.g. construction of additional housing units, may contribute to high variability in impervious surface and other model parameters. Frequent recalibration of the model may be required.
- DEM-based flow directions and accumulations may not be able to reflect the real conditions, due to man-made channels, dikes, freeway, bridges, etc. Manual modification of watershed delineation may be needed to account for the changes in flow routing controlled by these engineering infrastructures in urban settings.
- During the calibration process, simulated values need to be compared against observed data. Note that the observed data come from local grab samples while the simulated values may be based on coarse resolution (such as a 90-m grid size) GIS data and represent the average over a 90 x 90 m grid. It can be difficult to make them comparable for model calibration purposes.
- Drainage from urban landscapes including leaks from water supply, drainage, and irrigation systems needs to be quantified. This is often termed “urban drool.”

- Determining contaminant buildup and wash-off factors. Improved models are needed that reflect responses of engineered materials like roofing shingles in various settings, e.g. where small storms may leave residual contaminants. Also, there is a need to account for dry deposition on roofs and other hard surfaces.
- Soils in developed areas are often disturbed. Data are needed describing their properties.
- Simulation pesticide applications. Pesticide applications in modeling differ from buildup and washoff functions that are commonly used. The well known SWMM model does not allow pesticide inputs to be made instantaneously. It is important that the amount of impervious surface treated be quantified since this may dominate contaminant loss. Another factor is the unpredictable way in which chemicals may be applied by homeowners.

One Panel member emphasized that “all models are wrong, some models are useful.” The role of model building is to integrate what is known into a coherent whole that allows better understanding of the relationships among complex components. Model building should integrate available data with expert knowledge to produce a logic construct that others consider valid. Data is needed to calibrate and validate the model at some point, but not always at the model building stage. An issue arises as to whether the whole model must be validated or whether it is enough to just validate the components of the model. The Panel seemed to prefer that the model needs to be validated as a whole and not just as individual components.

The Agency may wish to consider identifying a location that could serve as a mesocosm of an urban residential system. Such a mesocosm could be highly instrumental in having measurements taken over time to allow full calibration and subsequent calibration and validation of TERRA and other models.

References

- Caruso, B.S., Cox, T.J., Runkel, E.L., Velleux, M.L., Bencala, K.E., Nordstorm, D.K. Julien, P.Y., Butler, B.A., Alpers, C.N., Marion, A., Smith, K.S. (2008). Metals fate and transport modeling in streams and watersheds: state of the science and USEPA Workshop Review. *Hydrological Processes*, 22: 4011-4021.
- HydroQual, Inc. (2010). Literature Review: Comparison of Common Watershed Models for Rainfall, Runoff Sediment Transport, and Contaminant Transport and Fate. Document Provided in SAP Materials.
- Jackson, S. & Winchell, M. (2011). Use of the EPA Storm Water Management Model (SWMM) for Diagnosis of Pesticide Off-target Movement from Residential Areas. In Goh, K.; Bret, B.; Gan, J.; Potter, T.L. (eds.), *Pesticide Mitigation Strategies for Surface Water Quality*. American Chemical Society Symposium Series, Washington, D.C. (in press).
- King, K.W. Arnold, J.G. & Bingner, R.L. (1999). Comparison of Green-Ampt and Curve Number Methods on Goodwin Creek Watershed Using SWAT. *Trans ASAE* 42(4), 919-925
- Sauve, S., W. Hendershot, & H.E. Allen. (2000). Solid-solution partitioning of solution of metals in contaminated soils: dependence in pH, total metal burden, and organic matter. *Environ. Sci. Technol.* (34), 1125-1131.
- Schiettecatte, W., Gabriels, D., Cornelis, W.M. Hofman, G. (2008). Impact of deposition on the enrichment of organic carbon in eroded sediment, *CATENA*, 72 (3), 340-347.
- Tipping, E., (1994). WHAM – A Chemical Equilibrium Model and Computer Code for Waters, Sediments and Soils Incorporating a Discrete Site/Electrostatic Model of Ion Binding by Humic Substance, *Computational Geosciences*, (20), 973-1023.
- USDA. (1986). Urban hydrology for small watersheds, USDA Technical Report (TR) 55. U.S. Department of Agriculture, Natural Resources Conservation Service, Washington, DC.
- USEPA (1999). MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems: User Manual Supplement for Version 4.0. U.S. Environmental Protection Agency, National Exposure Research Laboratory, Ecosystems Research Division Athens, GA. Available at: <http://www.epa.gov/osw/hazard/wastetypes/wasteid/hwirwste/pdf/risk/reports/s0536.pdf>, verified 11/2011
- USEPA. (2001). A user's guide to IPX, the In-place pollutant export water quality modeling framework. EPA/600/R-01/074, U.S. Environmental Protection Agency, Washington, DC.
- Velleux, M., Redman, A., Paquin, P. & Santore, R. (2009). Copper Transport and Fate Simulations and Evaluation of Estimated Environmental Concentrations for Copper-Based Antimicrobial Compounds, American Chemistry Council Copper Task Force Washington, DC

Wauchope, R.D., K.W. Rojas, L.R. Ahuja, Q.L. Ma, R.W. Malone, L. Ma. (2004). Documenting the pesticide processes module of the ARS RZWQM Agroecosystem Model. *Pest management Science*, (60) 222–239.

