SAP Minutes No. 2004-01

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

REFINED (LEVEL II) TERRESTRIAL AND AQUATIC MODELS PROBABILISTIC ECOLOGICAL ASSESSMENTS FOR PESTICIDES: Level II Aquatic Model Session

APRIL 1 and 2, 2004
FIFRA Scientific Advisory Panel Meeting,
held at the Crowne Plaza Washington-National Airport Hotel,
Arlington, Virginia

NOTICE

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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 EPA, Office of Pesticide Programs (OPP), and is structured to provide balanced expert assessment of pesticide and pesticide-related matters facing the Agency. Food Quality Protection Act 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 Myrta R. Christian, SAP Designated Federal Official, via e-mail at christian.myrta@.epa.gov.

In preparing the meeting minutes, the Panel carefully considered all information provided and presented by the Agency presenters, as well as information presented by public commenters. This document addresses the information provided and presented by the Agency within the structure of the charge.

CONTENTS

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Myrta R. Christian, M.S.
Designated Federal Official
FIFRA Scientific Advisory Panel
Date: June 16, 2004

Stephen M. Roberts, Ph.D.
FIFRA SAP, Session Chair
FIFRA Scientific Advisory Panel
Date: June 16, 2004

Scientific Advisory Panel Meeting
April 1 and 2, 2004

REFINED (LEVEL II) TERRESTRIAL AND AQUATIC MODELS PROBABILISTIC ECOLOGICAL ASSESSMENTS FOR PESTICIDES - Level II Aquatic Model Session

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INTRODUCTION

The Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA), Scientific Advisory Panel (SAP) has completed its review of the set of scientific issues being considered by the Agency pertaining to refined (Level II) aquatic model probabilistic ecological assessment for pesticides. Advance notice of the meeting was published in the *Federal Register* on February 20, 2004. The review was conducted in an open Panel meeting held in Arlington, Virginia, on April 1 and 2, 2004. Dr. Stephen M. Roberts chaired the meeting. Mrs. Myrta R. Christian served as the Designated Federal Official.

The FIFRA SAP met to review the Agency's Level II Terrestrial and Aquatic Models (Version 2.0). The previous version of these models was reviewed by the SAP during a session held March 13 - 16, 2001. The terrestrial and aquatic models are a key component of the Agency's initiative to revise the ecological risk assessment process, focusing on the development of tools and methodologies to conduct probabilistic ecological risk assessments for pesticides.

Some modifications to the models were in response to the 2001 SAP comments and recommendations. Other modifications were based on the suggestions made by the Ecological Committee on FIFRA Risk Assessment Methods, a stakeholder workgroup which provided recommendations to the Agency when this initiative first began. These suggestions, which were evaluated in the context of the 2001 SAP review, were discussed within the Agency and in national and international scientific professional meetings.

The Agency was interested in any general comments and recommendations from the SAP regarding the modifications to the models. In addition, the Agency requested that the SAP respond to specific questions regarding the Terrestrial and Aquatic Level II Models.

In preparing these meeting minutes, the Panel carefully considered all information provided and presented by the Agency presenters, as well as information presented by public commenters. This document addresses the information provided and presented at the meeting, especially the response to the charge by the Agency.

CHARGE

1. <u>Varying Volume Water Model</u> (VVWM). For aquatic risk assessments, OPP currently uses a water body fate model that has a fixed volume and does not consider hydrologic inputs and outputs. The SAP 2001 suggested that adding volume variations and overflow to the Level II fate model would improve the characterization of the water body and improve estimates of aquatic pesticide concentrations.

In response, a new model has been developed that allows volume variations and overflow in the water body. The new model also allows for meteorologically-dependent parameters, such as temperature and wind speed, to vary on a daily basis, rather than a monthly basis, to better capture temporal variability. In addition, the model was constructed to improve runtime because of the potential use in Monte Carlo simulations.

a.) Please discuss the new model's capability to capture the most salient processes influencing the variations in water body volume, and also discuss the modification allowing daily variations in meteorologically-dependent variables.

b.) Inputs of mass on a given day are assumed to occur instantaneously. Please discuss the advantages and disadvantages of this assumption with specific consideration for the trade-off between runtime, accuracy and the consideration that input data are given as daily values. What, if any, additional approaches regarding modeling input mass would the SAP recommend? Please provide a discussion of the pros and cons as compared to the current method.

c.) What additional model characterization or documentation is required to ensure clarity and transparency?

2. Exposure Model Testing. The QA/QC testing of the aquatic Level II Version 2.0 exposure model demonstrated that the refined risk assessment shell is consistent with the Level II Version 1.0 shell (PE4) for launching PRZM and is compatible with all crop scenarios and meteorological files. The testing also showed that the dissipation algorithms in the VVWM are consistent with EXAMS and that the volume and overflow algorithms are correct. Evaluation of the VVWM showed the potential effect that a varying volume water body, using current standard field size and water body volume and surface area, can have on estimated environmental concentrations due to dilution, evaporation, and overflow.

a.) What additional testing, evaluation and/or sensitivity analysis can the SAP recommend to ensure that the aquatic Level II exposure model meets the Agency objectives of transparent processes, and clear, consistent and reasonable products suitable for risk characterization?

b.) Based on the evaluation performed using the VVWM under standard field (10 ha) and standard surface water scenario conditions (1 ha surface area, 20,000 m^3 volume), please discuss the advantages or disadvantages to characterizing risk by replacing a single standard with multiple, crop scenario-specific standards at Level II.

3. Field Drainage Area and Water Body Size Selection. At Level II, the risk assessment approach is aimed at addressing the risk to aquatic species in high exposure, edge-of-field situations. The surrogate surface water used for Level II consists of a small, perennial surface water body at the edge of an agricultural field. This water body is capable of being supported by agricultural field runoff alone, and of supporting an aquatic community. Crop scenario-specific input values for field size, surface water volume, surface area, and depth were developed and systematically explored using three methods. The methods used readily available drainage area to volume capacity (DA/VC) ratios and

associated water depth guidance for construction of small permanent surface waters of the continental U.S.

a.) The U.S. Department of Agriculture's (1997) DA/VC ratios and depth guidelines for construction of small permanent water supplies (e.g., irrigation, livestock, fish and wildlife) were used as the source of national and regional DA/VC ratios and associated water depths. What additional existing sources of national or regional DA/VC ratios for small, permanent surface waters (e.g., wetlands, pools, ponds) should be considered?

b.) Please describe the merits or limitations to the approaches and assumptions evaluated for using the U.S. Department of Agriculture's (1997) guidelines to derive field size, surface water volume, and surface area input values for specific crop scenarios? What, if any, additional approaches and assumptions should be considered?

c.) A default minimum depth was set as 0.01 m. What minimum depth would the SAP recommend as a criterion to evaluate the biological relevancy of the scenario?

d.) Simulations with the PRZM/VVWM were performed using both the crop-specific surface water area and volume and the historic standard values (DA/VC = 1.5 acres/acre-ft) to characterize effect on exposure outputs for a relatively arid growing region (DA/VC = 50 acres/acre-ft) and a wetter climate (DA/VC = 1 acre/acre-ft) for both a short-lived and a long-lived pesticide. In addition, the effect on volume in the surface water body was characterized for all crop-specific scenarios. Please discuss what, if any, additional crop scenario/pesticide evaluations should be performed to further characterize the impact to exposure outputs, and/or to volume.

e.) What are the advantages or disadvantages to characterizing exposure for small, perennial surface waters at the edge of treated fields using the method selected for setting crop scenario-specific DA/VC ratio, depth, surface area and volume input values? What adjustments or changes to the method does the SAP recommend, and what are their advantages and disadvantages?

f.) Please describe the weaknesses and strengths of using simulated exposure concentrations from these crop scenario-specific water bodies as a surrogate for a low-order stream at the edge of a field, for a temporary pool or pond, and for a small tidal creek or estuary.

g.) Simulations with PRZM/EXAMS, a fixed volume surface water model, will be performed using both the crop-specific DA/VC approach and the historic standard values to characterize effect on exposure outputs for relatively arid growing regions (DA/VC = 50 and 80) and a wetter climate (DA/VC = 1) for both a short-lived and a long-lived pesticide. Please discuss what, if any, additional crop scenario/pesticide evaluations should be performed to further characterize the impact to exposure outputs in a fixed volume situation.

h.) Please discuss sources or approaches for national or regional DA/VC ratios and associated water depth and size information for temporary pool and pond aquatic-life resources.

4. Curve Number. The SAP 2001 recommended that additional characterizations of variability should be given to those parameters in the exposure model that have a major impact on exposure concentrations. The curve number is perhaps the most influential parameter in PRZM, and it has been interpreted in recent literature as a random variable. PRZM currently treats the curve number as a function of soil moisture, although recent literature suggests that the curve number may more appropriately be interpreted as a random variable.

a.) Please discuss the pros and cons of assuming strict dependence of curve number on calculated soil moisture versus treatment as a random variable unrelated to soil moisture as a means of characterizing runoff variability. Please identify and discuss alternative methods.

b.) Since the curve number was not designed for use in continuous modeling, what problems may arise when the curve number is used in this manner? Could a probabilistic interpretation address some of these issues? If so, how?

c.) What is the impact on interpretation of probabilistic-simulated exposure values when the curve number is used as a random variable and autocorrelation of temporally-varying physical properties that may impact runoff is ignored?

d.) A lognormal distribution is being investigated to characterize variability in certain curve number parameters. Is it reasonable to assume such a distribution has stationary properties (constant mean and variance) for all rain events (e.g., large and small)? Please provide rationale.

e.) Monte Carlo modeling is being investigated as a method of integrating the potential variability of curve numbers into exposure modeling.
Can the SAP recommend other methods available to incorporate variable and uncertain curve numbers into a continuous runoff model? Please discuss the pros and cons of these methods versus Monte Carlo.

SUMMARY OF PANEL DISCUSSION AND RECOMMENDATIONS

The FIFRA SAP reviewed the Agency Document and made suggestions for the Aquatic (Level II) model. Additional related issues are also noted. Below is a summary of the Panel's findings and recommendations.

1. The Panel commended the Agency for the initiative of developing a methodology and tool for refining the Level II aquatic probabilistic ecological assessments for pesticides. The Varying Volume Water Model (VVWM) with daily varying input parameters is an important advance over the constant volume EXAMS model using monthly averaged data. The degree of complexity included in the conceptualization of the field-pond system is appropriate for Level II analysis. The temporal variations in water level and volume and the resultant pesticide concentrations appear to be reasonably predicted. The model captures the important hydrological and pesticide fate processes and appears to give reasonable and realistic predictions and refined estimates of exposure. However, implementation of the hydrology and fate processes varies regionally.

2. Verification procedures to ensure that the VVWM code correctly replicates the corresponding code in EXAMS have been well thought out. The Panel noted, however, that it would be useful to know what QA/QC procedures were previously undertaken to ensure that the EXAMS code is correct.

3. Additional sensitivity analyses are needed. Given the large number of input parameters for the VVWM model, formal sensitivity analyses to identify those variables that most influence the results are needed. Such analyses should consider the relative influence of the standardized inputs.

4. There was general agreement that a regional approach was needed for defining DA/VC and pond depths. The watershed size chosen by EPA of 0.1 to 1.0 km^2 falls into the most vulnerable watersheds for pesticide contamination. Sources for regionally characterizing types of ponds and their locations in the landscape were identified.

5. The merits of including subsurface flow for Level II risk assessment models were discussed. The most immediate effect of the presence of groundwater is dampening the fluctuations in pond water elevations. Neglecting ground water pesticide inputs was appropriately conservative for Level II analysis, with the possible exception of cases where tile drainage lines play a significant role in watershed transport.

6. Additional modeling scenarios for running the Level II risk assessment should be considered. For a comprehensive evaluation to determine which of the many

variables are important, the use of appropriate experimental designs (e.g. Kleijnen 2004) is recommended.

7. The Agency is commended for attempting an innovative solution to the difficult problem of simulating runoff. It is possible to spend considerable time and energy on a detailed infiltration model based on physical principles. While such a model might be appropriate for Level III or IV assessments, it is not clear that such a model is needed at Level II.

8. Panel members felt that EPA should consider modifying the code to include physical relationships (CN linkage to important physical parameter(s)) and probabilistic aspects. The Panel proposed an alternate probabilistic approach that will aid in fusing physical and probabilistic issues.

9. Independent of which approach is used, the final model should be tested under a wide range of conditions (different catchments sizes, size and intensity of rain events, etc.) in order to adequately account (if possible) for the unexplained sources of variability. The final code itself should be well documented and published.

PANEL DELIBERATIONS AND RESPONSE TO CHARGE

The specific issues addressed by the Panel are keyed to the Agency's background documents, references, and the Agency's charge questions.

Charge

1. <u>Varying Volume Water Model</u> (VVWM). For aquatic risk assessments, OPP currently uses a water body fate model that has a fixed volume and does not consider hydrologic inputs and outputs. The SAP 2001 suggested that adding volume variations and overflow to the Level II fate model would improve the characterization of the water body and improve estimates of aquatic pesticide concentrations.

In response, a new model has been developed that allows volume variations and overflow in the water body. The new model also allows for meteorologically dependent parameters, such as temperature and wind speed, to vary on a daily basis, rather than a monthly basis, to better capture temporal variability. In addition, the model was constructed to improve runtime because of the potential use in Monte Carlo simulations.

a.) Please discuss the new model's capability to capture the most salient processes influencing the variations in water body volume, and also discuss the modification allowing daily variations in meteorological dependent variables.

Response

The Panel agreed that the VVWM with daily varying input parameters is an important advance over the constant volume EXAMS model using monthly averaged data. The degree of complexity included in the conceptualization of the field-pond system is appropriate for Level II analysis. The temporal variations in water level and volume and the resultant pesticide concentrations appear to be reasonably predicted. The model captures the important hydrological and pesticide fate processes and appears to give reasonable and realistic predictions and refined estimates of exposure. However, implementation of the hydrology and fate processes varies regionally. Whether the model captures the most salient processes depends on the similarity between the conceptual model and the real system. Special attention should be paid to the simplifying assumptions when the model is used for any real world applications.

The Panel had several comments on the model structure and suggested possible refinements. These are presented for the following areas:

<u>Pond Inflow</u>

In the VVWM, surface runoff is considered as the primary water and pesticide source for the surface water body adjacent to the field. The Panel is supportive of the daily time step calculations of surface runoff for the Level II model. Currently, the Agency uses the SCS curve number method (in PRZM) for runoff estimation. The curve number method is essentially an empirical, event-based approach. Thus, caution should be used when the curve number method is used for runoff simulation. Detailed comments are given in the response to question 4.

In arid regions, irrigation is the primary water source for growing crops. Incorporating irrigation is critical to pesticide fate, transport and risk assessment. Moreover, runoff of irrigation water provides inflow to the pond and maintains the water level whereas under rainfall-only conditions in arid regions the pond might evaporate completely. PRZM is capable of simulating irrigation. The Panel recommends that EPA include water addition by irrigation in the Level II model pesticide risk assessment.

<u>In-Pond Processes</u>

One of the most significant modifications from EXAMS to VVWM is the way that pesticide movement across the sediment-water interface is computed. The resulting ingenious analytical solution is ideally suited for running Monte Carlo simulations. However, the explanation given (in the March 4, 2004 document) as a mass transfer process between the littoral and benthic zones can be more realistically explained as a mixing process. Note that the term describing the rate of pesticide transfer between the two zones, $A \times D/\Delta x$ (pages 36-37 in chapter IV of the March 4, 2004 Document), has units of volume per time. This is exactly like a mixing term where, on a daily basis, a fraction of the volume of one compartment is added to the other and vice versa. For two water compartments, obviously, this is a turnover rate, where the same volume is transferred between the two compartments at each time interval, and this exchanged volume is then completely mixed into the new compartment. This would be similar for the mixing of sediments. The mixing of each phase (water into water, sediment into sediment) is likely driven by biological activity. Rather than view this as a diffusional flux requiring a characteristic length (as is true for the case of large, compartmentalized lakes), this should be viewed as a turnover rate. The question is, how frequently does the water in the first 5 cm of sediment 'turn over' to the littoral zone due to biological activity? Any water pumped out of the sediment (which includes excretion from worms) must be replaced with water from the littoral zone. The selection of 5 cm as the depth of the benthic layer is consistent with the biologically-active layer in sediments.

Pond Overflow

Overflow from the pond is an important addition to the new model and results in predictions of persistent pesticide concentrations in the pond water that are more realistic than those of the EXAMS model. It is also an important improvement for better prediction of downstream (spatial) effects. One concern is that the simulated exposure concentrations (especially for persistent pesticides) overly depend on the selection of the shape and volume of the surface water body. The Panel recommends that the Agency consider realistic regional variable pond depths and adjust the shape to more appropriate (simple) geometric forms. More details are given in the response to question 3.

Ground Water and Surface Water Interaction

The Panel unanimously agreed that the groundwater and surface water interaction is an important issue. In some regions, subsurface flow and its impact on pesticide exposure levels in the surface water body can be significant. Subsurface flow, especially from tile drainage lines, may contain high levels of pesticides and may result in inputs over longer periods of time. To enhance the capability of handling a wide range of real-world problems across the United States, the groundwater-surface water (GW-SW) interactions should be taken into account, even if only at a qualitative level. Indeed, considering the complexity of this issue (tremendous modeling efforts are required to characterize the dynamic interaction between surface and subsurface water systems), most of the Panel members recommended that this issue be addressed in the models at Levels III and IV.

The Panel suggested that, for conditions where groundwater determines the water table height, rather than assume that all excess volume above the design maximum goes to outflow at the end of each day, it would be preferable to assume that this excess volume decays to the design maximum through a simple first-order process with a half-life on the order of 3 days to 1 week.

b.) *Inputs of mass on a given day are assumed to occur instantaneously. Please discuss the advantages and disadvantages of this assumption with specific consideration for the trade off between runtime, accuracy and the consideration* *that input data are given as daily values. What, if any, additional approaches regarding modeling input mass would the SAP recommend? Please provide a discussion of the pros and cons as compared to the current method.*

Response

The model is computationally efficient because analytical solutions were found for the differential equations describing the processes in the pond. To obtain these analytical solutions, individual pond processes are assumed to be at steady state and mass inputs to the pond are instantaneous. Instead of instantaneous inputs, continuous daily varying steady state application could be used, but no significant differences are expected. The Panel endorsed the current Level II modeling approach involving daily instantaneous inputs, especially because instantaneous mass loadings likely are to be more conservative in the risk assessment.

In the VVWM, additions of the soil itself—originating from erosion from the field to the pond—are neglected. Pesticide masses adsorbed to the soil are distributed evenly and instantaneously to the littoral and benthic zone (50% each). The Panel would like to see additional justification for this assumption. Some Panel members suggested the need for sediment transport modeling in the water column, and interaction between the water column and the benthic layer by quantitatively simulating processes such as settling, resuspension, and sedimentation. Most Panel members did not think this is necessary for a Level II risk assessment model and that physically-based modeling of sediment transport should be considered only in Level III or IV risk assessment models.

c.) What additional model characterization or documentation is required to ensure clarity and transparency?

Response

While the Panel is impressed with the significant progress in modeling Level II exposure risk assessment, at the same time it acknowledges that further extensions can be made to the current VVWM. These are presented in the following areas:

Probabilistic distribution of input parameters

The VVWM can easily incorporate probabilistic variables, as is the case with other modules of the Level II aquatic model. EPA has indicated that probability distributions are being developed for key input parameters for future iterations of the VVWM. These distribution inputs would be a good improvement. It is important that this effort not be restricted to the curve number only; other input variables are equally important. To improve the computational efficiency in the Monte Carlo simulations, consideration should be given to moving PRZM to a faster platform.

Refinement of modeling processes

The modeling system involves simulations of both water flow and pesticide fate and transport in the crop field and the adjacent surface water body (pond). The final exposure levels of pesticides are affected by a number of physical and biochemical processes that may vary both spatially and temporally. For some processes such as photolysis and metabolism, separation into daytime and nighttime segments (i.e., 12-hour periods) could be important. Seasonal variations in solar intensity could be important too.

Other refinements mentioned were:

- pH-dependent hydrolysis for some chemicals.

- Pesticide mass-balance for the benthic zone. No toxicity is currently expressed in this layer; however, without reporting concentrations for this layer, the analysis is incomplete.

- Freezing effects. On the small permanent surface water body, ice formation is not simulated in VVWM. In PRZM, snow melt is included.

- Impervious field conditions. Impervious plastic (mulch) culture affects the rate of runoff, the amount of sediment scour, and the frequency with which runoff events occur, particularly for lower intensity rainfall events.

<u>Documentation</u>

Several Panel members expressed the need for documentation of model testing with field-observed data and documentation of sensitivity analyses. Details are given in the response to question 2 and in "Additional General Comments from the SAP."

Major assumptions should be listed in table form for clarity. Model application conditions and limitations should be described. For example, if the water depth is large, the assumption of complete mixing may not be applicable.

<u>Future Improvements</u>

For Levels III and IV, it would be useful to have the capability of modeling different types of water bodies (e.g., small, low-order perennial streams receiving multiple inputs from adjacent fields), as is often the case in the real world. It would also be useful to incorporate the influence of geometry and water quantity/quality interactions between groundwater and surface water.

Without simulating settling, sediments eroded from the crop field might be accumulated in the water column under certain conditions. Due to settling, contaminated sediments can be buried and are thus no longer available for the mass exchange between the two zones. Thus, settling and sedimentation can be very important for a standing surface water body. It is recommended that these processes be addressed in higher level models.

Summary

In summary, there are a number of processes and factors that should be considered or clarified. Considering data availability, however, the Panel agreed that some processes, such as GW-SW interactions, need to be considered quantitatively only at a higher level (Level III and IV), although these processes should be considered qualitatively when defining certain variables in the Level II model, such as minimum volume. The decision of which processes to consider further at Level II should include consideration of whether each makes the model more or less conservative. If ignoring a process will lead to underestimation of exposure, then the process should be considered at Level II.

2. Exposure Model Testing. The QA/QC testing of the aquatic Level II Version 2.0 exposure model demonstrated that the refined risk assessment shell is consistent with the Level II Version 1.0 shell (PE4) for launching PRZM and is compatible with all crop scenarios and meteorological files. The testing also showed that the dissipation algorithms in the VVWM are consistent with EXAMS and that the volume and overflow algorithms are correct. Evaluation of the VVWM showed the potential effect that a varying volume water body, using current standard field size and water body volume and surface area, can have on estimated environmental concentrations due to dilution, evaporation, and overflow.

a.) What additional testing, evaluation and/or sensitivity analysis can the SAP recommend to ensure that the aquatic Level II exposure model meets the Agency objectives of transparent processes, and clear, consistent and reasonable products suitable for risk characterization?

Response

Verification

The Panel agreed with the procedures used to ensure that the VVWM code correctly replicates the corresponding code in EXAMS. It appears to have been well thought out and indicates that the VVWM is operating correctly, as evidenced by the lack of differences in the output from EXAMS and VVWM for water concentrations. Whereas the side-by-side testing showed that water concentrations were consistent between EXAMS and the VVWM, no data were shown for sediment or pore-water concentrations predicted by EXAMS. The Panel received verbal confirmation from Agency staff that sediment and pore-water concentrations were replicated by the VVWM. The PE4 or RRA shell launched PRZM successfully. The few minor problems with various input parameters from the standard scenarios were identified and corrected, or necessary code modifications were made. The Panel noted, however, that while everything appears to function correctly, the procedures assume that the original code in EXAMS is correct. It would be useful to know what QA/QC procedures were previously undertaken to ensure that the EXAMS code is correct. In addition, while recognizing that the model is still in the development and testing phase, the Panel recommended that at some point the code should be disclosed and a code audit undertaken to ensure its integrity.

In response to a request from EPA staff for references on the statistical design of a sensitivity study, the following references are suggested as a starting point: Kleijnen, J. P. C. (1997 and 2004); Sacks, J., W.J. Welch, T.J. Mitchell, and H.P. Wynn (1989).

Sensitivity Analysis

Panel members agreed that additional sensitivity analyses are needed. Although a limited number of sensitivity analyses were presented, they were all "inward-looking" with respect to the variable volume water model. In this respect, the Agency was cautioned that the sensitivity analysis conducted to determine the influence of maximum pond depth (Dmax) on concentration indicated that variation in Dmax had a relatively minor effect on average daily concentration, particularly for high precipitation areas. However, the analyses only varied Dmax slightly (2.44 to 3.05 m in California, 1.83 to 2.13 m in Florida). Thus, pesticide concentrations could vary quite substantially between systems with widely varying maximum depths.

Given the large number of input parameters for the VVWM model, formal sensitivity analyses are needed to identify those variables that most influence the results. Such analyses should consider the relative influence of the inputs that are standardized (e.g. fraction of organic carbon, light attenuation factor, benthic dispersion coefficient, boundary layer thickness, O_2 exchange coefficient, etc.). Many of these standardized input values are based on empirical data, but the variability associated with them is not discussed and their effects on model outcomes appear to be unknown. The need for further examination of "standard" input values was referred to in the document as an area needing review but was not identified in the ongoing/future activities.

Specific suggestions were made regarding sensitivity analyses for several parameters in the model. These parameters included pH, biomass and total suspended solids (TSS). For example it was suggested that TSS could range from 10 to 20,000 mg/L. This is important for highly erodible soils such as Loess soils (which are found in western Tennessee and elsewhere) and would affect strongly-sorbed (high Koc) chemicals. At high TSS, the consequences of mass transport could be significant even for pesticides with low Koc values. Ultimately, the suspended solids load could be generated from the mass of soil identified in PRZM output (maybe at Level III?). The pH was identified in the document as a candidate parameter for further examination of its influence on model results. pH was identified by the SAP in 2001 as being a parameter that should be varied as it can have a direct influence on hydrolysis rates and on dissociation of certain compounds. While there may be merit in varying this on a scenario basis, there may also be merit in considering using a distribution or using a minimum/maximum/mean approach in those instances where hydrolysis or dissociation is affected by pH across the normal range found in aquatic systems. One possible approach would be to include this at Level II, but hold constant in Level I. This type of approach could be used for several other influential parameters.

In addition, sensitivity analyses for compound-specific parameters, i.e., physical and chemical properties and degradation rates, were suggested. This should include determining the influence of varying Kd/Koc on the output. Both the short-lived and persistent chemicals that were used for some of the QA/QC work had similar Koc values (487 vs. 422). Because this parameter can have a major effect on eventual partitioning and fate, particularly in the variable volume scenarios, there needs to be assurance that the partitioning is consistent between the two models.

Sensitivity analysis was also suggested to examine the influence of assumptions made with regard to dynamic processes in the model. It was noted that particulate surface- or humic acid-catalyzed hydrolysis was assumed not to occur. A simple analysis toggling this factor on or off could provide insight into its importance.

Additional evaluation of the approach for determining the appropriate DA/VC should be considered. According to the USDA (USDA 1997), the values for DA/VC can vary greatly in a local area when drainage areas have unique characteristics. USDA recommends reducing DA/VC values by as much as 25 percent for drainage areas having extreme runoff-producing characteristics and increasing them by 50 percent or more for low runoff-producing characteristics.

Risk Assessment

The Panel acknowledges that VVWM intended for use in a Level II assessment is still relatively conservative. It is suggested that the Agency consider conducting case studies to look at the effect of using the VVWM and using a regional scenario-based approach on risk assessment conclusions.

The receiving water body scenario has been derived from information on pond construction from USDA. However, an analysis to relate receiving water scenarios to vulnerable aquatic ecosystems is needed. This can be done by comparing hydrologic parameters (i.e., area, depth, and volume) of real ecosystems with the basic parameters of the pond characterizations derived from the USDA Handbook. A more difficult task will be to characterize the drainage area. There seems to be a paucity of data for these types of receiving environments. This could help to move away from the misconception that a farm pond is being simulated rather than a more relevant natural ecosystem such as a wetland.

From the perspective of the overall risk assessment process, the Agency may want to compare results from the VVWM regional scenarios with GENEEC for a range of chemicals to determine if there are some which result in higher concentrations from the VVWM. If there are, several options might be available, including dropping the use of

GENEEC in Level I, Tier I, and replacing this model with the peak values from PRZM/VVWM for the scenario which consistently results in the highest runoff concentrations.

Comparisons with Observed Data

Given the flexibility that VVWM now has, it would seem relatively easy to obtain existing pesticide monitoring data sets from edge-of-field ponds and compare these monitoring data results to VVWM model predictions derived from comparable site-specific scenarios. With this information, model performance could be determined. If possible, model performance should be estimated for a range of regions and crop scenarios to determine how well the model performs under different scenarios. Alternatively, evaluation of model performance could be conducted under controlled situations or in selected watersheds.

One Panel member noted that EPA already has data submitted by registrants which could be useful for both characterizing the receiving water body morphometry and for examining model performance. The Agency may want to evaluate data generated from farm pond studies and from constructed mesocosm and microcosm studies conducted by registrants for the EPA between the late 1970s and the mid-1990s. Pesticide registrants conducted these studies to satisfy data requirements for ecological effects rather than exposure. However, they may contain relevant information/data that would be useful to benchmark (ground truth) the models discussed. Farm pond studies should be available from the late 1970s to the late 1980s and mesocosm/microcosm studies from the 1980s through the 1990s. Farm pond studies were conducted with ponds (1 to 3 acres in surface area) with watersheds approximately 10 or more times larger. One Panel member was aware of farm pond studies submitted for a range of compounds, including synthetic pyrethrins, endosulfan and organophosphates. Parameters measured included (but were not limited to): meteorological conditions, pond morphometry (for farm ponds, depth, area) and chemical concentrations. Pesticide application in these types of studies was done according to typical label application practices for the crop and chemical combination. Edge-of field surface water runoff (%) values were also generated in these pond studies. Mesocosm and microcosm studies were conducted with a host of pyrethrins, organophosphates and herbicides. Constructed mesocosms were up to 0.25 acres in surface area and six feet deep, with similar parameter measurements as farm ponds. Meteorological conditions are likely available for some of the mesocosm studies conducted in the midwest, southwest and southeast parts of the U.S.

Although the model construct may not represent the reality of hydrologic and other physical/mechanistic processes, it is a tool to estimate environmental concentrations. It is important that the model and the associated scenarios reasonably represent the concentrations likely to occur in the environment and meet the needs of the conceptual model for a Level II assessment. Additional refinement of the model and scenarios will be necessary for Level III assessments.

b.) *Based on the evaluation performed using the VVWM under standard field (10 ha) and standard surface water scenario conditions (1 ha surface area, 20000 m3 volume), please discuss the advantages or disadvantages to characterizing risk by replacing a single standard with multiple, crop scenario-specific standards at Level II.*

Response

Advantages of Multiple Crop-Scenario Approach

- This approach can be used to better characterize risk on a regional basis, thereby allowing the Agency to focus its assessment efforts on the crops and/or areas where potential problems are identified.

- This approach recognizes that there are regional differences in water bodies and rainfall patterns and gives the Agency the ability to account for regional differences.

- If peak values from PRZM/VVWM are incorporated into Level I, then this information could identify which regions and/or crops might need additional refinement in a Level II assessment.

- The approach for Level II should be to have regional representations of ponds and surface water scenarios. Otherwise, the present approach is good. There are advantages in having a probabilistic statement that can be made over a wider aspect of sizes (and maybe shapes) of ponds. Shallow systems can also be biologically important for macroinvertebrates, amphibians, etc.

- There is potential for improved ability to evaluate model performance, because the VVWM model can be tailored to match scenarios for which monitoring data have been collected.

- The Agency should examine the effect on sediment/pore water concentrations for the different crop-scenarios using the VVWM.

Disadvantages of Multiple Crop-Scenario Approach

- The results of risk assessments may be more challenging to communicate to risk managers.

- A possible disadvantage is the potential for increased resource requirements. However, given the cost of the resources to be protected, it may be worth the time and effort.

3. <u>Field Drainage Area and Water Body Size Selection</u>. At Level II, the risk assessment approach is aimed at addressing the risk to aquatic species in high exposure, edge-of-field situations. The surrogate surface water used for Level II consists of a small, perennial surface water body at the edge of an agricultural field. This water body is capable of being supported by agricultural field runoff alone, and of supporting an aquatic community. Crop scenario-specific input values for field size, surface water volume, surface area, and depth were developed and systematically explored using three methods. The methods used readily available drainage area to volume capacity (DA/VC) ratios and associated water depth guidance for construction of small permanent surface waters of the continental U.S.

a.) The U.S. Department of Agriculture's (1997) DA/VC ratios and depth guidelines for construction of small permanent water supplies (e.g., irrigation, livestock, fish and wildlife) were used as the source of national and regional DA/VC ratios and associated water depths. What additional existing sources of national or regional DA/VC ratios for small, permanent surface waters (e.g., wetlands, pools, ponds) should be considered?

Response

There was general agreement that a regional approach was needed for defining DA/VC and pond depths. The watershed size chosen by EPA of 0.1 to 1.0 km^2 falls into the most vulnerable watersheds for pesticide contamination (Schulz, 2004). This is especially important for coastal wetlands where tidal range, width or expanse of wetlands in terms of buffer size, and groundwater considerations must be taken into account on a regional basis. Other important regional differences that need to be taken into account are the depths to groundwater.

The following sources can be used to obtain regional information for types of ponds and their location in the landscape:

- NOAA's Oil Spill Environmental Sensitivity Index (ESI) mapping which identifies the most vulnerable habitats based upon exposure duration (e.g. depositional sheltered habitats are most vulnerable and sensitive areas). The ESI maps also denote locations of bird rookeries, marine mammal haulouts, and sea turtle nesting areas. These maps are prepared regionally for coastal areas.

- Canada is in the process of developing a suitable receiving water scenario for pesticide ecological assessments using PRZM/EXAMS. However, not having a similar guidance as the USDA document, they took a somewhat different approach. They first identified the type of ecosystem of concern and then proceeded to characterize the surface area (SA), depth, volume and drainage area by examining available data. While not finalized, the results for SA, volume, depth, and DA/VC appear to fall within the ranges in the proposed scenario-specific parameters. The data to do this type of evaluation are limited. EPA has on-going activities, including a GIS-based approach that was suggested by several Panel members to determine the relevance of regional scenarios.

- Empirical information is available in several recent publications. Some of the information is from certain areas in Canada, but would be relevant for northern states (e.g., Hayashi & Vander Kamp, 2000; Price, 1993; Brooks & Hayashi, 2002; Wiens 2002).

- Information can be obtained by contacting other government agencies (USGS) or groups such as Ducks Unlimited that may have pertinent unpublished information.

- Data are available from Agricultural Experiment Stations, such as the standard "farm pond" construction guides and recommendations. Local GIS surveys or data from actual use patterns are still desirable and should supersede the instructions in the manual.

b.) Please describe the merits or limitations to the approaches and assumptions evaluated for using the U.S. Department of Agriculture's (1997) guidelines to derive field size, surface water volume, and surface area input values for specific crop scenarios? What, if any, additional approaches and assumptions should be considered?

Response

The Panel discussed whether to include subsurface flow at Level II. The most immediate effect of the presence of groundwater is dampening the fluctuations in pond water elevations. In general, it was thought that neglecting ground water pesticide inputs was appropriately conservative for the Level II analysis, with the possible exception of cases where tile drainage lines play a significant role in watershed transport. The presence of groundwater can be obtained from regional maps. Alternatively, as suggested by one Panel member, high percolation rates predicted by PRZM output can possibly be used as a "red flag" for the presence of groundwater.

An alternative approach to developing scenarios is to use PRZM runoff volumes for a set drainage area—balanced by evaporation—to derive the sustainable volumes for permanent ponds in the various regions. There are a number of methods that might then be used to determine pond morphometry parameters such as surface area and depth. This approach assumes that the runoff estimates generated by PRZM are reasonable.

Additionally, the USDA guidance for pond construction indicates that, if known, runoff volumes for an area should be used rather than the generic values given. If available, EPA might want to consider taking advantage of these data. Limitations arise in arid areas where ponds either do not naturally exist or only periodically contain water and thus have no permanent aquatic resident species. In those cases, a more realistic scenario might be to model a small stream near the sprayed field.

Finally, the guidelines were developed for water supply purposes (construction of small permanent water supplies, such as irrigation) and not for "natural ponds". The depth was determined according to the handbook by the expected rate of infiltration. Because percolation from ponds is not included in the VVWM model, the pond depth can be smaller than what is proposed in the handbook.

c.) *A default minimum depth was set as 0.01 m. What minimum depth would the SAP recommend as a criterion to evaluate the biological relevancy of the scenario?*

Response

In general, the Panel was of the opinion that a minimum depth of 1 cm was too small, with the exception for coastal wetlands, where the shallow water depths proposed are extremely important for providing accurate exposure scenarios for wetland and estuarine habitats. In particular, the shallow coastal waters contain the most sensitive life-history stages of fish and shellfish, and are the point at which pesticides enter tidal creeks and bind to organically rich sediments.

In other cases, a depth of 15 to 30 cm seemed to be more appropriate for the Level II model. If the exposure simulation indicates that reduction to very low depths (e.g., 5 to 15 cm) is expected, it would be appropriate to redo the effects SSD such that species requiring larger water volumes (e.g., largemouth bass, pike) are removed from the analysis. In all cases, it is important to have a better identification of assessment endpoints for the Level II assessment.

As noted previously, in the current document several references are made to the littoral zone. In the background documentation, references to the "littoral zone" are in fact a reference to the water in the pond scenario, which is a misleading use of the term. From a limnological perspective the littoral zone or region is described as the interface area between the land of the drainage basin and open water of lakes. This zone includes both the water, sediments and associated biota in near shore areas and is important from an ecological perspective as an area with generally high biological activity when compared with pelagic (open water) and profundal (deeper bottom areas) regions. Currently, the assumption for Level I and II assessments is that pesticides entering water are instantaneously diluted into the entire water body. While this is likely suitable for a Level II assessment, it does not account for the mixing which would initially occur in the littoral zone of any receiving water. The consideration of such a mixing zone might be suitable for a Level III assessment.

d.) *Simulations with the PRZM/VVWM were performed using both the crop-specific surface water area and volume and the historic standard values (DA/VC = 1.5 acres/acre-ft) to characterize effect on exposure outputs for a relatively arid growing region (DA/VC = 50 acres/acre-ft) and a wetter climate (DA/VC = 1 acre/acre-ft) for both a short-lived and long-lived pesticide. In addition, the* *effect on volume in the surface water body was characterized for all crop-specific scenarios. Please discuss what, if any, additional crop scenario/pesticide evaluations should be performed to further characterize the impact to exposure outputs, and/or to volume.*

Response

The Panel suggested many additional scenarios that should be considered and are listed below. It was clear from the discussions that some of these scenarios would be more appropriate for a Level III assessment. In all cases, regional differences were considered important. In addition, the Panel felt that checking the model results with available pond pesticide data would be a good idea. In this regard, data collected on pesticide concentrations in ponds by Dr. Cobb in Texas might be useful for checking the models (see report: Refined (Level II) Terrestrial and Aquatic Models Probabilistic Ecological Assessments for Pesticides: Level II Terrestrial Model Session). The Panel had the following suggestions:

- Pesticides that include chemicals with a range of physical and/or chemical parameters from different major chemical classes should be further evaluated. In addition, subsequent evaluations might include new scenario-based parameters (such as timing of application) and include characterization of other application methods, particularly in-furrow or sub-surface applications.

- Eventually, the goal is to move from running specific scenarios to a more comprehensive evaluation in order to determine which variables are important. It is easy to run a scenario, but it is harder to pick those that are the most important for an assessment. In a situation with a need to determine which factor(s) among many factors actually drive the model, it is appropriate to use fractional factorial designs (Taguchi, 1986). Hicks and Turner (1999), Kleijnen (1997, 2004), and Schulz (2004) have developed experimental designs specifically for sensitivity analysis of simulation models like these. This is a much more appropriate approach in contrast to simply testing scenario after scenario as they come to mind. One of these designs could be applied to the model globally, or within a regionalized model.

- The regional approaches for predicting effects result in more realistic models that take into account differences in regional soil types, meteorological conditions and farming practices. EPA should consider regional factors such as plasti-culture and other farming and/or meteorological factors, which will result in larger volumes of runoff and more frequent connectivity between agricultural fields and surface waters.

- Type of irrigation (e.g. drip versus surface-applied) and time of application may be critical to environmental exposure outputs.

e.) *What are the advantages or disadvantages to characterizing exposure for small, perennial surface waters at the edge of treated fields using the method selected* *for setting crop scenario-specific DA/VC ratio, depth, surface area and volume input values? What adjustments or changes to the method does the SAP recommend, and what are their advantages and disadvantages?*

Response

The proposed approach represents a good first step and is appropriate for Level II risk assessments. The method seems reasonable. Advantages are that the method of calculating pesticide concentrations is transparent, easy to calculate, keeps field size in a reasonable range, and can take regional differences into account.

The Panel was impressed with the ability of the model to estimate overflow. This parameter can be used as a surrogate for estimating edge-of-field (within the pond) and downstream (overflow) effects. This allows EPA to focus on spatial effects and determining where the majority of risk will be. The model output clearly shows that for short-lived chemicals, there is little in the way of downstream effects, whereas for long-lived chemicals there could be a clear downstream effect. The disadvantage is that the edge-of-field contaminant losses are lumped and the distributed response is not known. However, distributed modeling is clearly a Level III or IV assessment process.

EPA is cautioned that in the USDA Handbook 590 guidance on constructing ponds, specific advice is offered on reducing DA/VC for high runoff soils: "To apply the information given in Figure 10 in USDA (1997) some adjustments may be necessary to meet local conditions. Modify the values in the figure for drainage areas other than normal. Reduce the values by as much 25% for drainage areas having extreme runoff producing characteristics. Increase them by as much by 50% or more for low runoff producing characteristics." With this in mind—and remembering that crop scenarios are currently chosen to represent a high runoff soil and high rainfall—some consideration needs to be given to the combination of DA/VC and the scenario. The model should be fine-tuned based on the results of any sensitivity analyses.

f.) *Please describe the weaknesses and strengths of using simulated exposure concentrations from these crop scenario-specific water bodies as a surrogate for a low-order stream at the edge of a field, for a temporary pool or pond, and for a small tidal creek or estuary.*

Response

The strength of the model is that it runs quickly and uses the available data to its best advantage. However, EPA is advised to more clearly define the endpoints of the assessment and their relation to the types of habitat. This in turn would help in determining the nature of the temporary habitat (e.g., amphibians, waterfowl, etc.).

Weaknesses listed by individual Panel members were:

- The fate parameters in estuarine areas are poorly characterized because all fate processes are determined in freshwater. Some information for older chemicals in salt water might exist in the open literature.

- Daily time steps are not appropriate for tidal creeks.

- To estimate exposure concentrations in low-order streams, it would be useful to consider linking the VVWM to models that predict mixing zones and downstream concentrations in streams following inputs from outfalls or other point sources (e.g., CORMIX, 7Q10).

- The modeled ponds have no littoral edge to them.

- The effect of surface area on evaporation rates and photolysis should be considered in more depth.

- Simulated exposure concentration with VVWM for a stagnant water body might not be representative for streams where advection is important.

g.) Simulations with PRZM/EXAMS, a fixed volume surface water model, will be performed using both the crop-specific DA/VC approach and the historic standard values to characterize effect on exposure outputs for relatively arid growing regions (DA/VC = 50 and 80) and a wetter climate (DA/VC = 1) for both a short-lived and long-lived pesticide. Please discuss what, if any, additional crop scenario/pesticide evaluations should be performed to further characterize the impact to exposure outputs in a fixed volume situation.

Response

Clarification was sought from EPA staff on the interpretation of the question. EPA clarified the statement by indicating that they are currently considering a Level I, Tier II assessment that would utilize the fixed volume receiving water body in PRZM/EXAMS using two DA/VC ratios (1 & 50), and then use a regional approach with PRZM/VVWM in Level II assessments. Because PRZM/EXAMS is already well characterized with respect to crop scenario inputs and pesticides, no further characterization is required. However, EPA may want to evaluate how this approach will impact the overall risk assessment process and, in particular, the movement from Level I to Level II.

In general the approach was considered good. In some cases, groundwater, plasti-culture and wet vs. dry weather scenarios (El Niño vs. La Niña scenarios) should be taken into account. EPA should also compare pesticides with differing Koc levels to test how sediment partitioning is affected by Koc.

h.) Please discuss sources or approaches for national or regional DA/VC ratios and associated water depth and size information for temporary pool and pond *aquatic-life resources.*

Response

In addition to government sources for data on the hydrometric dimensions for receiving waters (surface area, volume, depth, drainage area) other organizations may also have collected relevant information. For example, in Canada, Ducks Unlimited has compiled a database from Landsat imagery of 3,061,000 wetlands covering a total area of almost 11 million acres (4.4 million hectares). This covers about 90% of the prairie ecozone. This database was obtained from the Ducks Unlimited National Headquarters in Oak Hammond Marsh Conservation Centre, Stonewall, Manitoba (Wetland Habitat Inventory for Prairie Pothole Region of Canada). Summary data provided by Ducks Unlimited staff included distribution of surface area size for wetlands in the prairie region of Canada. Similar data may be available from this or other groups in the U.S.

In Canada data from Ducks Unlimited were used to develop one estimate of a typical drainage area for a 1-ha water body. While still under development, and not yet available for release, the approach used can be outlined. The database includes the area of water in each quarter section (160 acres) in the prairie ecozone derived from Landsat imagery. The database represented a compilation of Landsat scenes from 36 varied dates ranging from 1984 to 1995 and during the months April, May and June. Data were screened to eliminate those areas which might skew results (e.g. areas with incomplete data or which included major rivers). These data were analyzed by calculating the overall ratio between the area of the wetland and the total area (water and land). This ratio indicates the overall fraction of the surface area of the landscape that is occupied by wetlands. The inverse of this fraction is the mean catchment area, where catchment area is defined as the total watershed area. The mean drainage area is calculated by subtracting the mean wetland area from the mean catchment area.

The main advantage of this analysis is the very large size of the database that covers most of the Canadian prairie ecozone. The main disadvantage is the unknown degree of uncertainty introduced by the climatic and temporal variations in the data.

Texas A&M and the University of North Texas have high resolution (3 m) GIS maps of marshes along eastern Texas. We are sure that other state agencies are increasingly developing these.

An older, yet very influential, text by Hutchinson (1957) on Limnology contains descriptions on types of ponds and other water bodies, the importance of morphometry in determining biological activity, and changes in shape and its influence on biological dynamics.

Manuscripts by Schulz (2004) and Pennington et al. (2001) have information on the relationship between drainage area and pond size.

Other Information: Satellite Data: LIDAR Data and specifically the Beaufort County Special Area Management Plan in South Carolina is a good example.

4. Curve Number. The SAP 2001 recommended that additional characterizations of variability should be given to those parameters in the exposure model that have a major impact on exposure concentrations. The curve number is perhaps the most influential parameter in PRZM, and it has been interpreted in recent literature as a random variable. PRZM currently treats the curve number as a function of soil moisture, although recent literature suggests that the curve number may more appropriately be interpreted as a random variable.

General Comments

The Agency is commended for attempting an innovative solution to a difficult problem. It is possible to spend considerable time and energy on a detailed infiltration model based on physical principles. While such a model might be appropriate for a Level III or IV assessment, it is not clear that such a model is needed at Level II. The Panel generally supports the proposed curve number approach with the qualifications detailed in the response to the questions.

In order to better understand the limitation of the curve number approach, a short overview on its development is given here. The original form of the SCS equation as proposed by Mockus was

$$Q = \frac{(P - I_a)^2}{P - I_a + S} \quad \text{if} \quad P > I_a, \quad Q = 0 \quad \text{otherwise}$$

where S is the watershed storage and I_a is the initial abstraction or the amount of rainfall before runoff occurs (see also Eq 4.61 in the March 4, 2004 Document). In the SCS Handbook 4 a relationship was proposed between initial abstraction and S (Figure 1). Based on this data it was proposed that I_a=0.2S. As can be seen from Figure 1 this relationship between S and I_a is tentative at best. This should not be a surprise since S in the original theory of Mockus is a function of the amount of water that can be stored in the watershed after runoff has started. This S is a function of the depth of the soils in the watershed and should be only minimally dependent on the rainfall history. The initial abstraction, I_a, defined previously as the amount of rainfall before runoff starts, is thus mainly a function of the moisture content in the watershed and consequently the rainfall history. Thus S and I_a are fundamentally different parameters, each with their own distributions, and should not be related to each other. This is important when considering probabilistic approaches using the curve number equation to predict runoff.

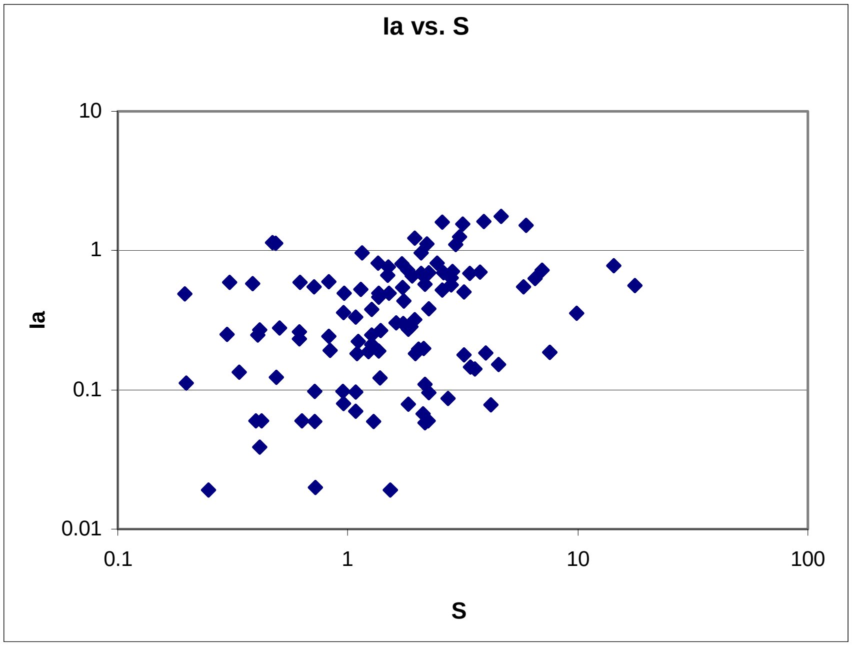

Figure 1: Plot of initial abstraction, Ia, and watershed storage S (both in inches). Redrawn from SCS Handbook 4.

a.) *Please discuss the pros and cons of assuming strict dependence of curve number on calculated soil moisture versus treatment as a random variable unrelated to soil moisture as a means of characterizing runoff variability. Please identify and discuss alternative methods.*

Response

Two methods are proposed for calculation of the runoff with the curve number (CN): Method 1, Physically-based deterministic CN method; and Method 2, Soil moisture independent probabilistic CN method.

<u>Deterministic Approach</u>

For the physically-based runoff model (Method 1) there are two prevailing theories for the runoff generation hydrologic process. The dependence of CN on moisture content depends on which runoff mechanism dominates. The first theory assumes that runoff begins when rainfall rates exceed infiltration capacities of soil. This theory is referred to as infiltration-excess, also called Hortonian flow, in honor of the related research by Robert Horton (1933, 1940). According to Hortonian flow theory, runoff amounts are directly controlled by characteristics that influence soil infiltration, such as land use and soil type. For watersheds where runoff is generated by infiltration excess, the dependence on moisture content is tentative.

Generally, high water content in the topsoil may indicate a higher runoff potential while dry soil tends to absorb more infiltrating water. However, no direct and definite relationship between water content and runoff exists. The second prevailing overland flow theory assumes most runoff is generated via direct precipitation onto or exfiltration from saturated areas in the landscape through a process termed saturation excess overland flow (e.g., Dunne and Black, 1970). The extent of these saturated areas can vary with season and depends on the moisture content, and can be predicted with the CN method (Steenhuis et al., 1995).

For watersheds where saturation excess overland flow dominates, a relationship between runoff amount and moisture content is expected. In watersheds where saturation excess overland flow is the main mechanism of producing runoff, the original SCS equation can well simulate the runoff pattern with a constant S value and with Ia calculated with a water balance (Thornthwaite Mather, 1955) for the shallowest soil in the watershed, which will produce the first runoff (Steenhuis et al., 1995; Lyon and Steenhuis, 2004). Figure 2 is an example from the Town Brook Watershed in the Catskills region of New York

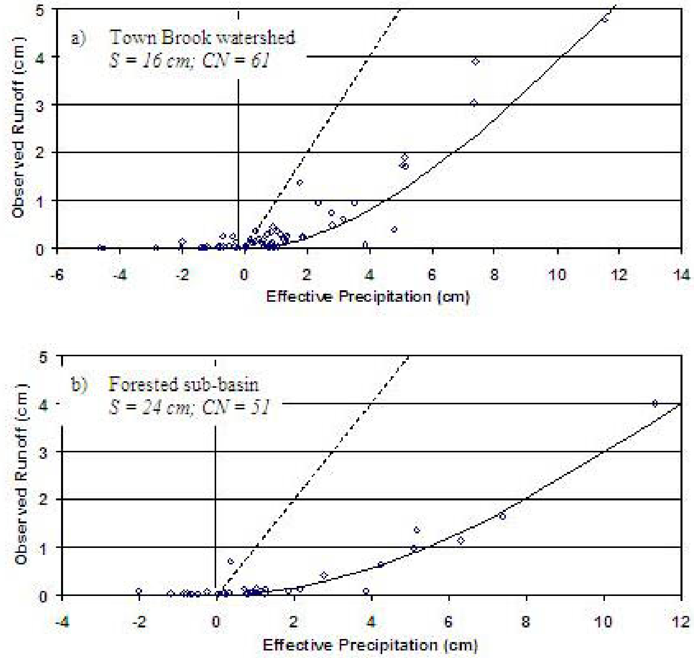

Figure 2: Prediction of Runoff for two watersheds in the Catkills Region of New York.

For the traditional curve number equation (i.e., with I_a=0.2S; See also Eq. 4-62 in the March 4, 2004 Document), it is assumed that CN_I, CN_{II}, CN_{III} represent the 10^{th}, 50^{th}, and 90^{th} percentile curve numbers, respectively. Statistically, this method is sound.

Physically, however, failure to use the available simulated soil moisture may miss some valuable information as indicated above. Note that the dependence of CN on moisture content occurs because it assumed that I_a =0.2 S. If we decouple the initial abstraction from S, then the CN should be independent of initial moisture content. Based on the above, further work is needed to evaluate the applicability of the presented log normal distribution with mean = -1.609 and standard deviation = 0.67 (note that the mean value is derived from $I_a/S = 0.2$).

Probabilistic Approach

Although incorporating variability by generating a random CN is a positive step, abandoning linkage among precipitation, infiltration, and runoff may cause other issues to become problematic.

There are several ways that these concerns could be addressed. A linear regression model is one straightforward alternative that could include both soil moisture dependence and variability. Analysis of the available data would quickly indicate the relative importance of the two. The physically-based components could be incorporated into the probabilistic code. One of the ways that EPA could consider changing the probabilistic approach is as follows:

CN_I and CN_{III} were early attempts to introduce variability into a deterministic model. The correlation between CN and antecedent rainfall is too weak to be useful. The Agency wants a model for runoff that is simple and interpretable, but still good enough for Level II risk assessments. The presented attempts to describe the unpredictability in runoff in terms of a random CN are unnecessarily convoluted and consequently confusing. We suggest that EPA apply the following approach instead of the current one.

In this approach, CN is considered to be a global property of a given terrain. Temporal and spatial variations in the soil are modeled by random variables. Pick CN (CN_{II}) according to the terrain from the standard table or, even better, derive *S* directly from watershed outflow data if available as this avoids having to assume anything about the relationship between CN and *S*. The model can then generate log-normal random variables X_1 and X_2 to give runoff Q by the following formulas:

$$S = \frac{1000}{CN} - 10$$

$I_a = X_1 S$ or $I_a = X_1 \theta$

$$Q = \begin{cases} X_2 \dfrac{(P - I_a)^2}{P - I_a + S} & P > I_a \\ 0 & P \le I_a \end{cases}$$

where θ is a variable that indicates the moisture status in the watershed, calculated with a simple water balance procedure such as introduced by Thornthwaite & Mather (1955, 1957) or calculated directly with PRZM. If we assume that $I_a = 0.2S$ and that the value of Q is centered on the deterministic formula, we could take

$$X_1 \sim \text{lnorm}(\log(.2), \sigma_1)$$
$$X_2 \sim \text{lnorm}(\log(1), \sigma_2)$$

This leaves two unknown parameters, the lognormal standard deviations, which can be set to reasonable values, perhaps by matching quantiles. We already have an accepted value $\sigma_1 = 0.67$. Figure 3 presents some simulation results showing runoff for given rainfall, assuming $\sigma_1 = 1, \sigma_2 = 0.5$, and the results appear to be quite realistic.

Final Comment

It is important to realize that the approach in Chapter IV (March 4, 2004 Document) was applied/tested in a very limited manner (e.g., the example used was based on a single dataset from a very small catchment). The final code should be tested under a much wider range of conditions (different catchment sizes, duration and intensity of rain events, etc.) in order to adequately account (if possible) for the unexplained sources of variability.

Panel members concluded that EPA should consider modifying the code to include physical relationships (CN linkage to important physical parameter(s)) and probabilistic aspects. The Panel proposed an alternate probabilistic approach that will aid in fusing physical and probabilistic issues.

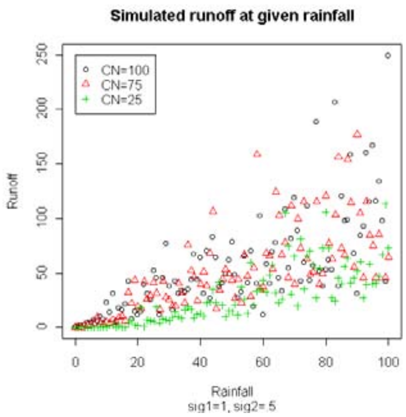

Figure 3: Probabilistic simulation of runoff

b.) *Since the curve number was not designed for use in continuous modeling, what problems may arise when the curve number is used in this manner? Could a probabilistic interpretation address some of these issues? If so, how?*

Response

The Panel expressed several concerns regarding this issue. The concern was high because, as stated in the EPA document, the CN is so important in predictions. The manner in which the program resets conditions at the beginning of each day was a major concern. The scale within which the CN approach was being used was seen as an issue to be addressed in the near future by EPA. The original CN application was for watersheds and annual extreme rain events; however, application here is for shorter temporal and smaller spatial scales.

Spatial and Temporal Scales

Spatial and temporal scales are important in addressing this issue. The choice of scale is important here because the different applications of the method differ markedly in their spatial and temporal scales. The original development of CNs in hydrological engineering was for a much larger spatial and temporal scale than the proposed farm field/daily application. Data collected on gauged watersheds are also at a large scale. Experimental runoff data (e.g., Wauchope et al., 1999) are collected on smaller spatial and temporal scales than the proposed application.

	Spatial scale	Temporal scale

Classic curve number	Watershed	Annual extreme rainfall event
Watershed data	Watershed	Rainfall event
EPA application	Farm field (10 ha)	Daily
Experimental data	Small plot	2 hours?

The Agency should carefully consider scale when it examines CN data. Changing scales usually changes variability, but the direction of the change is not obvious. Changing from an event time scale to a daily time scale adds a concern about autocorrelation discussed in the next question. A probabilistic interpretation does not address this concern. If anything, it hides the issue when estimates of variability from one scale are applied without change to other spatial or temporal scales. The Agency should evaluate whether the proposed standard deviation from very large-scale phenomena is appropriate for daily field-scale data.

When the Agency examines data, they should also consider the components of variability that might be present. Do the data represent variability among events on the same field? Variability among years on a single field? Variability among fields? All combinations are available and will not have the same population standard deviation.

Rainfall events of several days

A very important issue is how one defines a rainfall event. Rainfall events extending through two or more days would be treated in the code as separate (parameter values being independent). Especially in regions where saturation excess runoff is dominant, this leads to gross underprediction of runoff events. In the Northeastern US, for example, any rainfall event producing more than 15 cm of rainfall over several days will cause significant flooding. Currently, PRZM resets the CN at the beginning of each day. Making the CN probabilistic in such a case would ignore useful information from previous days. Because the CN is so important, it would seem that the consequences of this shortcoming should be explored more thoroughly. Would it be profitable to explore the addition of a subroutine that partially addresses this issue for such events? Relative to multiday events, on each rainfall event, the simulation could determine the number of days it will last and then modify the simulation for those days. The CN model was derived from event-scale information, yielding total runoff for the event. The proposed use is to apply the same model to daily precipitation to give daily runoff. An event-total runoff could be computed from the sum of the daily runoff events. At a minimum, the properties of the total daily runoff should be similar to the event runoff. The shape of the runoff distribution depends on the relationship between P and I_a. It is left skewed at low precipitation and right skewed at high precipitation (Figure 4).

The sum of the daily runoff will have a different distribution than the event-scale runoff. The annual total runoff is the sum of event runoffs or daily runoffs. The distribution of the annual total will also be different.

The I_a is commonly approximated as 0.2 S for event-scale data. Applying this value to daily data will underestimate the total runoff. When the model is applied to daily precipitation data, I_a values are subtracted from *each day's* precipitation in a multi-day rainfall event and will underestimate the runoff unless the same adjustment to I_a and S is made on subsequent days. Choosing and justifying such an adjustment will be difficult because of the lack of available data. One approach to evaluate the magnitude of the issue would use daily precipitation sequences. For each sequence, classify days into rainfall events. Some events may be single day; others may be multi-day. Compare event-level predictions to the sum of daily predictions. This approach could also be used to evaluate different methods to deal with autocorrelation.

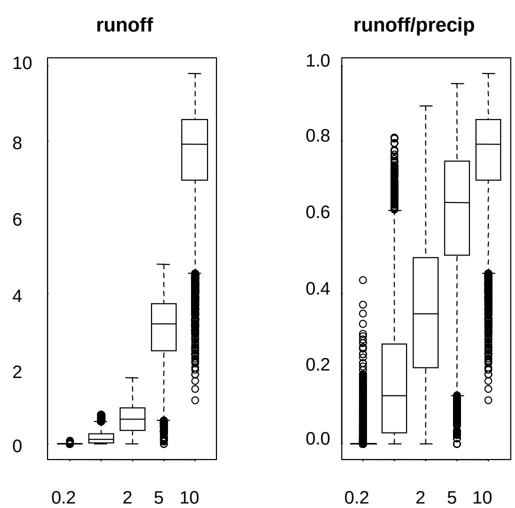

Figure 4: The shape of the runoff distribution depends on the relationship between P and Ia. It is left skewed at low precipitation and right skewed at high precipitation

c.) *What is the impact on interpretation of probabilistic-simulated exposure values when the curve number is used as a random variable and autocorrelation of temporally varying physical properties that may impact run off is ignored?*

Response

Autocorrelation between random variables influences the variance but not the mean. Regardless, the presence of autocorrelations could insert error in predictions from the probabilistic model. Several methods were identified by Panel members for coping with potential autocorrelation. They include permutation tests, including the autocorrelations in future versions of the probabilistic models (i.e., using correlation coefficients in Monte Carlo simulations), and running a crude sensitivity case study. These methods are discussed below.

A data set provided to the Panel indicated no apparent dependence of CN on rainfall in the previous 5 days, thus ignoring autocorrelation may have no significant impact most of the time. Potential impacts are difficult to determine heuristically. The effect of ignoring autocorrelation (interpreted as a subsequent event having higher runoff than would be calculated under the random model) would lead one to conclude that the pesticide concentration in the pond would be slightly overstated.

If no dependencies exist between CN and temporally-varying physical properties, the autocorrelation of the latter properties is of no concern. However, if such dependencies exist, they should be incorporated in future versions of the probabilistic models (e.g., use of correlation coefficients in Monte Carlo analysis). In the latter situation, CN would need to be reselected for each time step of the analysis.

As with any data that are autocorrelated, ignoring this relationship can reduce the confidence in statistical analyses. Because this particular situation is not one of statistical significance testing *per se*, autocorrelation may be less of a problem. There are a number of statistical approaches that could be used to handle spatially- or temporally-autocorrelated data including permutation tests. The latter can be used in situations where data are independent (default) or known to be autocorrelated. Permutation methods may also be appropriate because this form of testing is already incorporated as part of the refined Level II RA approach (e.g., Figure 4.1) and is being considered (in the form of Monte Carlo testing) as a method of integrating the potential variability of CN into exposure modeling (e.g., Question 4e).

d.) *A lognormal distribution is being investigated to characterize variability in certain curve number parameters. Is it reasonable to assume such a distribution has stationary properties (constant mean and variance) for all rain events (e.g., large and small)? Please provide rationale.*

Response

The Panel understands the context (Level II) within which the lognormal distribution was being proposed. Regardless, several group members recommended that more work is needed because there is little evidence suggesting that the distribution will remain stable. It seemed unlikely that one lognormal distribution would provide adequate predictions for all relevant scenarios. The distribution can change even within a rain event. Expansion in the near future to include these issues is recommended.

e.) *Monte Carlo modeling is being investigated as a method of integrating the potential variability of curve numbers into exposure modeling.*
Can the SAP recommend other methods available to incorporate variable and uncertain curve numbers into a continuous runoff model. Please discuss the pros and cons of these methods versus Monte Carlo.

Response

The general response is that Monte Carlo is the method of choice, but as detailed in specific Panel member comments, there are some computational issues that should be considered. This is in addition to what is presented above. Below, an important issue relative to how one does the Monte Carlo simulations is highlighted, providing a specific alternate approach.

Monte Carlo Simulations

There may be a more appropriate Monte Carlo method. The current method has three important characteristics: 1) A lognormal distribution of Ia/S, based on Hawkins et al. (1985); (2) It can be adapted to specific regions and crops by setting the median CN according to standard tables; and (3) The output is a CN to feed to PRZM. The approach proposed by EPA is to:

> Calculate the value of S for the tabular value of CN
> Generate values of I_a/S from a log normal distribution and multiply by S to get Ia
> Calculate Q from P, S, and I_a,
> Recompute the S_e that corresponds to that Q and P
> Convert S_e back to a curve number

This approach puts all the variability into I_a. The alternative is to put the variability into S, by treating S_e as a lognormal random variable, e.g. $\log S_e \sim N(\log S, s.d.)$ where s.d. is the same s.d. used to simulate I_a/S, e.g. the Hawkins value, 0.67. When the precipitation is high, this approach generates a similar CN distribution as the EPA approach. It does not do so for low precipitation, because of the truncation when $P < I_a$. The practical effect of the difference in distributions may be small. The largest differences between distributions occur for low precipitation and moderate CN. These are conditions with relatively small amounts of precipitation. The CN distributions are similar for conditions expected to produce large amounts of runoff: high precipitation and large CN.

An important advantage of this alternate method is easy explanation. The current Agency method is indirect and hard to follow. The alternative method has the advantage of clarity and transparency. In the alternative method, a tabular value is used to set the median of the distribution. The remaining attributes of the distribution (standard deviation and distributional form) come from Hawkins' (1985) model.

This alternative method is not the only possible one. There are two random quantities, I_a and S. If data were available, distributions could be constructed for both quantities.

The distribution of CNs should be compared to field data sets, even though there are few appropriate data sets. The upper portion of the distribution (e.g. CN > 90) should be given the most attention. Are the quantiles of the probabilistic distribution similar to the empirical quantiles in the field data? This comparison should be restricted to comparable events. Because the field data come from rainfall simulator experiments, the field data do not include an event unless there was runoff. Hence, the appropriate comparison is to the probabilistic distribution, truncated to omit the zero values. The comparison of Figure 4.31 (in chapter IV of the March 4, 2004 Document) suggests they are similar, but it is hard to compare the distributions in a plot like figure 4.31. A quantile-quantile plot provides an easier way to interpret comparison of distributions.

The Panel discussions included other approaches. Second-order Monte Carlo techniques are often used to separate uncertainty due to variability and uncertainty due to lack of knowledge. Probability bounds analysis can also be used to separate and estimate the relative importance these two sources of uncertainty. If assuming constant mean and variance is inappropriate for either theoretical reasons or because the sample size is low, then second-order Monte Carlo analysis or probability bounds analysis would be useful techniques to deal with this situation.

5. Additional General Comments from the SAP

At the conclusion of the Panel discussions on the questions, Panel members were given the opportunity to make additional comments. Comments were on subjects previously discussed and also on subjects not specifically included in the Panel discussions of questions.

Several Panel members have been involved with this process from its early days and recognized that a significant amount of work has already been done and that EPA has moved forward in its proposed risk assessment methods. The currently proposed approach is reasonable given the Panel's understanding of the Agency's goals for a Level II assessment. Given that deterministic assessments are currently used for decision making, some Panel members lauded EPA's desire to start implementation within the next 8 - 12 months.

While this is a good start, additional work will be necessary. EPA must move beyond the current conceptual model, which is suitable for agricultural uses of pesticides, and identify which other conceptual models should be developed for other use patterns. During the course of discussions, several use patterns/scenarios were identified, e.g., mosquito control, forestry, urban uses or receiving water scenarios other than a permanent water body such as temporary pools. A number of Panel members identified the need for a conceptual model that includes tile drainage as an input source to receiving waters.

Several Panel members noted that the topic for this SAP focused exclusively on estimation of exposure concentrations. Panel members had the following comments with respect to the characterization of toxicity and the use of toxicity data in risk assessment.

The species sensitivity distribution (SSD) approach currently being proposed in the Level II aquatic model relies on LC/EC50s derived by probit analysis. Probit analysis is appropriate for quantal endpoints, e.g., mortality, but for other types of endpoints, e.g., count or continuous variables, other types of models must be used. The Generalized Linear Model (GLiM) framework described by Kerr and Meador (1996) and Bailer and Oris (1997) is a useful framework for deriving concentration-response relationships for a variety of toxicity test endpoints, e.g., quantal, count and continuous endpoints. The framework involves using link functions to transform effects metrics, e.g., probit or logit link functions for quantal responses, log transformation for count and continuous variables, and assigning appropriate error distributions, e.g., binomial distribution for quantal responses, Poisson distribution for count variables, normal distribution for continuous variables. Linear regression can then be conducted on the transformed data to derive the concentration-response relationship. Thus, the framework can be used for all available types of response variables. By adding a quadratic term to the linear model, the framework can be adapted to incorporate simulations at low concentrations.

The use of lower percentiles, e.g., LC/EC10s, should be considered in deriving SSDs, given that the goal of Level II assessments is to err on the side of conservatism.

Newman et al., 2001, showed that formal hypothesis testing results in rejection of the lognormal distribution in more than half of 50 species sensitivity data sets assessed. Therefore, using a lognormal model for all SSD analyses may not be optimal, given that the lower part of the curve that is used for doing predictions will show the most difference among the models.

Other distributions can and are used; see other chapters in the book in which Newman et al. (2001) were published. Also there are bootstrap methods that can be used that avoid assumptions of any particular distribution such as presented in Grist et al. (2002).

Where peaks in ponds are short-lived, it may be inappropriate to rely on 96 h toxicity test endpoints. Shorter duration toxicity test endpoints should be used in these situations. Effects at different exposure durations can be matched to exposure peak durations through use of time-to-effect modeling. This assumes that toxicity results are available for multiple times during the test.

With respect to the topic of exposure duration, one Panel member provided the following publications and reports which provide detailed explanations of pulsed dose responses: Clark et al. (1986, 1987), Scott et al. (1989, 1992), and Moore et al. (1989).

For assessment of chronic effects, it was suggested that endpoints from chronic studies need to move from NOAELs (hypothesis testing study design) to regression-based endpoints. This is currently being done with endpoints for acute effects, for pesticides with sufficient data, (e.g., re-registration pesticides that are fairly persistent and have large aquatic toxicity data sets). Some noted that this would require a change to the existing protocols for these types of studies.

It may be appropriate to compare the model soil loss predictions with agricultural runoff (soil loss and runoff) and golf course runoff (reduced soil loss). Both have ponds and should provide interesting comparisons. Golf courses with ponds and a vegetative cover throughout. may experience a greatly reduced loss of sediment because of this vegetative cover.

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