Development and Use of Distributions of Pesticide Concentrations in Drinking Water for FQPA Exposure Assessments: A Consultation
(Revised February 11, 2000)

Scientific Advisory Panel Consultation
March 3, 2000

Purpose.

The EPA Office of Pesticide Programs (OPP) is proposing to build on its existing approaches for estimating pesticide concentrations in drinking water as part of its assessment of dietary exposures to pesticides. The purpose of this consultation is to provide a progress report to and seek advice from the Scientific Advisory Panel (SAP) on the latest effort to further develop the methodology for drinking water assessments for Food Quality Protection Act (FQPA) aggregate exposure assessments.

Summary.

OPP is proceeding concurrently on several fronts to develop a variety of improved methods and tools capable of estimating the drinking water exposure component of the FQPA aggregate exposure assessment. The mixture of approaches adopted for use must be robust, scientifically defensible, and useable within the confines of the pesticide regulatory environment. This document describes the ongoing development of one of these approaches: the use of a suite of multi-site, regression-based methods to develop regional/national distributions of pesticide concentrations across very large numbers of drinking water utility intakes. The ultimate goal of this effort is to quantify exposure to pesticide in drinking water across as large a fraction of the population of the United States as is possible. The method is likely to include separate approaches for water drawn for drinking from larger rivers, from smaller streams, from shallow ground water and from reservoirs. Each approach is likely to present its own separate developmental challenges.

The Office is also proceeding with use of the Index Reservoir / Percent Cropped Area (PCA) concept, with evaluation of existing basin-scale hydrologic simulation models and with the collection of new monitoring data. Presentations have been made to the SAP and other scientific bodies on these approaches.

Organization of This Document

This paper is divided into two general sections. The first section describes work to date on development of these potential new regression-based methods and outlines plans for further development over the coming months. The second section describes the background and developmental history of the methods used to estimate drinking water exposure since the passage of FQPA in August 1996. This section also describes the evolution and use of other ongoing approaches.

Section I. Development of Regression-Based, Population-Weighted Distributions of Drinking Water Concentrations

This is an effort by the Office of Pesticide Programs (OPP) to move beyond conservative, single point estimates of exposure for FQPA drinking water assessments. The Agency envisions several potential advantages to this approach. First, it will give risk managers a more comprehensive and complete picture of the extent of the potential for drinking water exposure to a chemical or group of chemicals to the US population as a whole. Second, it will provide a probabilistic higher tier of assessment for those chemicals which fail to pass the conservative screen. Third, OPP believes that in order to combine a population-based drinking water exposure assessment with the distribution of pesticide residues on food items in a statistically rigorous manner, the water data should be developed with the same general distributional structure as that of the food. In this way, the Monte Carlo procedure currently in use for risk assessments for food stuffs could be extended, if desired, to the drinking water component for purposes of aggregate exposure and risk assessments.

If this new effort is successful, we envision three basic steps in developing national and/or regional, population-based distributions of pesticide residues in drinking water and aggregating them with distributions of pesticide residues in food. These steps include (1) development of distributions of pesticide drinking water concentration values across drinking water intake locations, (2) consideration of the impact of water treatment processes by water utilities, and (3) development of the methodologies to incorporate these residue estimates into appropriate strata for eventual incorporation into aggregate (food & water) exposure assessments.

This presentation to the SAP will outline initial ideas on steps 1 and 3, with the strongest emphasis on step 1. The details of how EPA will consider the effects of treatment (step 2) will be addressed in a proposed science policy on treatment and possibly in a future SAP meeting. The presentation on development of distributions of drinking water concentrations will describe an approach to analysis based on empirical analysis of pesticide monitoring data using regression based models that relate concentrations to pesticide use and watershed properties. The presentation on aggregating drinking water and food exposure assessments (Step 3) will focus on potential methods as well as possible obstacles.

OPP hopes to bring a methodology for developing and combining distributions of pesticide drinking water values into an aggregate FQPA exposure assessment to the SAP by September 2000.

Types of Drinking Water Concentration Distributions to Be Developed

Drinking water in the United States is derived from a variety of types of sources. Surface water sources of drinking water include large and small rivers and streams, natural lakes and man-made reservoirs. Ground water sources include deep and shallow wells and infiltration

galleries and springs. Due to the diverse nature of the sources, a variety of approaches will be necessary to adequately cover a significant proportion of the US population. Distributions will be developed for single chemicals as well as for multiple chemicals which have the same mode of action. The following briefly describes the methods investigated to date. Additional detailed information on several approaches is also found in attached appendices as indicated below.
Note: This paper discusses two distinct types of distributions. The first is a temporal distribution of concentration values at a single site over a period of a year or longer. The second is a spatial distribution of either peak or longer-term values across multiple sites.

Surface Water Approaches

Methods to develop distributions of pesticide concentrations at water utilities located on rivers are being developed using (1) **regression models** based on measured concentrations and nationally available predictor variables, and (2) the SPARROW (SPAtially Referenced Regression On Watershed Attributes) model. Detailed descriptions of both approaches are attached.

The regression models are further along in their development at this point in time than SPARROW and are designed to estimate annual mean concentrations and the complete frequency distribution of concentrations, including high percentiles for acute assessment. Regression models have been developed for major herbicides and analysis is in progress for extending the approach to other chemicals.

The SPARROW model is an alternative approach to estimating annual means and is based on regression methods and a mass-balance approach. Development of SPARROW for use in pesticide concentrations is in initial development using atrazine as the prototype chemical. Both the regression and SPARROW approaches to estimating the annual mean are being developed simultaneously to evaluate the pros and cons of these different methods.

Regression Models for Estimation of Pesticide Concentrations in Surface Water

Regression models are being developed for estimating pesticide concentration distributions for streams using nationally available data on pesticide use and other drainage-basin characteristics. Regression models have been developed for stream concentrations of the herbicides alachlor, atrazine, cyanazine, metolachlor, and trifluralin. Regression equations were derived using measured concentrations of the four herbicides as the response variable and nationally available agricultural use data and physiographic basin characteristics as predictor variables. Concentration data for the herbicides are from 45 streams sampled as part of the U.S. Geological Survey's National Water-Quality Assessment (NAWQA) Program during 1993-95. Separate equations were developed for each of six percentiles (10^{th}, 25^{th}, 50^{th}, 75^{th}, 90^{th}, and 95^{th}) of the annual distribution of stream concentrations, and for the annual time-weighted mean concentration.

Results showed several interesting outcomes. Agricultural use intensity (active ingredient applied per unit basin area) was the most important predictor in all of the models. Several hydrologic variables and soil parameters also were useful in explaining the variability in

concentrations among the streams. Climatic variables and parameters related to agricultural management practices were generally not significant in any of the regression models.

Results were generally best for atrazine, with R^2 values ranging from .80 to .91 for models of the 5 percentiles and the annual mean concentration of atrazine among the 45 sites. Values of R^2 were somewhat lower for metolachlor (.55-.77) and cyanazine (.44-.75), and substantially lower for alachlor (.08-.59) and trifluralin (.17-.75), although estimation reliability is sometimes high even when R^2 value is low. For atrazine, metolachlor, and trifluralin nearly all predicted concentrations for individual streams were within a factor of 10 or less of the actual values for the model development data set, across all percentiles and for the annual mean concentration. For alachlor and cyanazine, predicted concentrations for the higher percentiles (90^{th} and 95^{th}) and for the annual mean were within a factor of 30 of the actual values.

The regression models appear to improve explanatory power compared to a single mean for all sites. Use of the national mean as the estimate for all sites results in a high proportion of very high or low estimates. Incorporation of only atrazine use intensity shows great improvement. Even further improvement is shown by use of the full regression model, which adds improved representation of the effects of natural hydrologic and soil properties that vary among basins and affect pesticide concentrations. (See 'Estimation of Pesticide Concentration Distributions in Streams from Available Data on Pesticide Use and Watershed Characteristics').

The SPARROW Model. The United States Geological Survey (USGS) has recently developed SPARROW as a national water-quality model to assess watershed contamination in the conterminous United States. This model is being widely used for nutrient assessment. The SPARROW method uses spatially referenced regressions of contaminant transport on watershed attributes to support regional water-quality assessment goals, including descriptions of spatial and temporal patterns in water quality and identification of the factors and processes that influence those conditions. The method is designed to reduce the problems of data interpretation caused by sparse sampling, network bias, and basin heterogeneity.

The regression equation relates measured transport rates in streams to spatially referenced descriptors of pollution sources and land-surface and stream-channel characteristics. Spatial referencing of land-based and water-based variables is accomplished via superposition of a set of contiguous land-surface polygons on a digitized network of stream reaches that define surface water flow paths for the region of interest.

Water-quality measurements are obtained from monitoring stations located in a subset of the stream reaches. Water-quality predictors in the model are developed as a function of both reach and land-surface attributes and include quantities describing contaminant sources as well as factors associated with rates of material transport through the watershed (such as soil permeability and stream velocity). Predictor formulae describe the transport of contaminant mass from specific sources to the downstream end of a specific reach. Loss of contaminant mass occurs during both overland and in-stream transport.

In calibrating the model, measured rates of contaminant transport are regressed on predicted transport rates at the locations of the monitoring stations, giving rise to a set of

estimated linear and nonlinear coefficients from the predictor formulae. Once calibrated, the model is used to estimate contaminant transport and concentration in all stream reaches. A variety of regional characterizations of water-quality conditions are then possible based on statistical summarization of reach-level estimates. The application of bootstrap techniques allows estimation of the uncertainty of model coefficients and predictions.

SPARROW's digital framework (derived from EPA's river reach file RF-1) provides a nationally consistent method for segmenting large pollutant source areas. Although additional calibrations are required to account for targeted contaminants, the model can be used to address a variety of questions, including travel times, probabilities of exceedance of concentrations for contaminants at selected locations within the source-area watersheds, and relative contributions of different sources and sub-basins to contaminant concentrations near the locations of drinking water utility intakes.

Probability of exceedence of targeted contaminants at selected locations in the source area SPARROW was originally developed as a means to provide regional interpretations of water-quality monitoring data. The model relates measured transport rates in streams to spatially referenced descriptors of contamination sources and land-surface and stream-channel characteristics. Regression equations were developed for long-term mean annual transport of total phosphorus and total nitrogen. By using these equations, probability distributions for the exceedence of specified concentrations of targeted contaminants could be generated for selected locations in the watershed. (Probabilities here refer to annual mean concentrations; probabilities for short-term exceedence may differ greatly).

The current and planned capabilities of SPARROW include estimates of travel times useful for segmenting watersheds, probabilities of exceeding concentration thresholds for targeted contaminants near drinking water utility intakes and estimates of the "delivered" yield of targeted contaminants reaching these locations. The benefits of the model include its physically based approach, its ability to incorporate multiple contaminants by using an empirical methodology, and a nationally consistent method based on EPA's digital stream networks (RF-1).

The SPARROW model was originally designed with the capability to estimate nutrient concentrations at all drinking water facilities in the RF-1 database. The RF-1 includes the largest of the water bodies in the US and the largest of the drinking water treatment facilities located on them. It incorporates 567 drinking water intakes operated by 480 suppliers serving 60 million customers. SPARROW’s capabilities will be vastly increased with the completion of the RF-3 (National Hydrography Database - NHD). The NHD has data on smaller streams and rivers and will add up to 9,000 additional drinking water intake locations. When finalized it will include watershed boundary delineations, stream velocity and travel time data for 60,000 additional stream reaches. (See ‘Regional Interpretation of Water Quality Monitoring Data’ attached).

At present the application of SPARROW to pesticides is in initial development using atrazine as a prototype. It will be developed and evaluated in concert with regression approaches in the next several months.

Strengths and Weaknesses of the SPARROW Approach

The strength of the SPARROW method is its structure. The mass-balance approach facilitates the interpretation of model coefficients and provides a logical framework for including different predictor variables. This could prove useful in attempts to build multi-constituent models that depend on physical properties of the contaminants. For example, the chemical property of solubility is likely to be an important factor affecting the delivery of the chemical from land to the stream. Because the SPARROW structure distinguishes between land-to-water and in-stream delivery, solubility could be specified to affect only the land-to-water delivery component. The structural approach could also improve model fit. Our experience with nutrients suggests that recognition of in-stream decay reduced model mean-squared error by approximately 50 percent. Finally, the hydrologic structure incorporated in the SPARROW model provides a consistent framework for assessing the correlation of errors across neighboring stream segments.

The current version of SPARROW also displays weaknesses relative to the correlative regression model**.** Principal among these is the need to work in mass units rather than concentrations. This should improve once we develop a parallel flow model (by the end of this year) that is consistent with our model for generating pollutant loads. SPARROW also has the weakness that it produces flow-weighted rather than time-weighted concentration estimates. However, Gilliom and Larson have done comparisons showing that this distinction is not significant. A third weakness of the mass-balance approach used by SPARROW is that it is not readily adapted to estimate acute conditions. The problem here is that all areas within a basin do not experience acute conditions simultaneously, so there is no easy way of imposing the mass-balance restriction. Further developmental work will be needed to extend SPARROW to reliably estimate acute conditions.

The current version of SPARROW has low resolution relative to the other regression models (at least for the monitored basins). This is because the model is designed to accept monitoring data from larger basins on the RF1 network. However, the NAWQA data are generally collected in smaller basins for which the determination of pollutant use in SPARROW is rather crude. SPARROW is currently being redesigned to operate at a uniform 1-km scale

resolution so this problem should soon be solved. Work towards the 1-km model should be completed by the end of the fiscal year.

Regression Approaches for Development of Pesticide Concentration Distributions in Reservoirs

The regression methods provide a simple, flexible approach to estimating pesticide concentrations in unmeasured streams with relatively well characterized reliability.

Regression models have also been developed by Battaglin and Goolsby (USGS) for estimating the annual mean concentration of selected herbicides in Midwestern reservoirs. As for the national regression models for streams, a geographic information system (GIS) was used to manage and quantify characteristics on land use, agricultural chemical use, climatic conditions, topographic character, and soil type within the drainage basins. Multiple linear and logistic regression equations were developed to estimate annual mean herbicide concentrations in reservoir outflow as a function of these land use, hydrologic, and physical characteristics.

Results demonstrate a strong association between annual mean herbicide concentrations in reservoir outflow and the use of those herbicides within associated drainage basins. In many cases, models that use cropland acreage or agricultural chemical expenditure estimates work nearly as well as models using the harder to come by herbicide use estimates. (See 'Using GIS and Regression to Estimate Annual Herbicide Concentrations in Outflow from Reservoirs in the Midwestern USA, 1992-1993).

The USGS is in the process of evaluating the comparability of the stream and reservoir regression models, the consistency of predictor variables with improved information, and the optimal combination of the two approaches for drinking water intakes.

Groundwater Approaches

Regression approaches are also being developed and tested for development of distributions of pesticide concentrations in groundwater. Generally, compared to surface water, much less of the variance in ground water concentrations is accounted for by potential predictor variables, such as use intensity and soil properties. However, concentrations are generally much lower in groundwater compared to surface water. Even estimates with relatively low reliability may be adequate.

Toxic Endpoints for Which Distributions of Exposure Values Are Required

Exposure to pesticide residues in any media may have two distinct human health impacts: acute and chronic. An acute toxicity end point results generally from a short term, high exposure event to a toxicant, and the effects can be observed immediately (e.g., vomiting) or they could develop over time (e.g., subtle developmental changes). A chronic toxicity endpoint can result from long-term, lower exposure to toxicants, and the effects develop over an extended duration (e.g., cancer or chronic liver disease). Distributions of short-term peak exposure values are

needed for acute toxicity endpoint risk assessments, and distributions of long-term average concentrations are required for chronic non-cancer and cancer endpoint risk assessments for humans.

Projected Sequence of Additional Tasks for Develop of Distributions.

The first priority in the next few months is verification and testing of the regression models and SPARROW using independent monitoring data for drinking water intakes. This will lay the foundation for expanding the methods to additional pesticides and for determining the optimal combined application of regression models and SPARROW.

The following additional short-term steps are envisioned in the next six months. First, the team will work on development of a distribution of peak concentration values for one or more organophosphate (OP) insecticides at the drinking water intake locations found in the RF1 database using regression methods. Second, the team will attempt to develop distributions of concentration values for one or more organophosphate insecticides in shallow groundwater based on USGS regression equations. The team will investigate cumulative exposure assessment (multi-chemical) for the OP's investigated. The team will encourage further development of the portions of the RF3 (NHD) necessary for continued development of SPARROW and the other regression approaches.

Medium term goals (six - twelve months) will depend partially on successful completion of the short-term approaches and may need be modified based on experience in this work Medium term work envisioned includes completion of the ReachFile 3 project - national hydrography database (NHD) and inclusion of additional drinking water intake locations found there and development of predictive capability for distributions of long-term average and peak concentration values for chemicals with little or no monitoring data. This phase will involve using pesticide use, chemical environmental fate and watershed hydrography data. Also envisioned is beginning development of capability to produce distributions of long-term average and peak concentration values for chemicals in reservoirs based on Battaglin-Goolsby regression work. The team will also continue to investigate possible approaches to cumulative drinking water exposure assessment for chemicals with a common mode of action (e.g. the OPs).

Long-term (beyond one year) goals include expanded use of the NHD database for SPARROW and the other regression approaches and finalization of development of capability to produce distributions of long-term average and peak concentration values for chemicals in reservoirs based on Battaglin-Goolsby regression work.

Consideration of the Impact of Treatment Processes

(Treatment will be covered in a science policy paper, and possibly at a future Scientific Advisory Panel presentation later in the year.)

Development of Aggregate Distribution for Pesticide Residues in Drinking Water Together With Residues in Food

Even if this development effort completely successful, it is not envisioned that this tool would be used for every chemical undergoing either the registration or re-registration process. Due to time and manpower requirements, a single, screening level assessment using a conservative scenario and assumptions will still be used for the first tier assessments. If estimated exposure at this screening level assessment using a conservative scenario and assumptions does not "trip" risk triggers, the Agency would conclude that the potential risk was low and not invest in the more complex and time consuming assessment.

Therefore methods will be required both for combining distributions of pesticide residues in food with a single conservative index reservoir concentration value, and for combining of distributions of pesticide residues in food with population-weighted national or regional distributions of pesticide residues in drinking water. The latter would be used for chemical cases where EPA believes that the severity and magnitude of the potential risk posed warrant the use of this approach and the incorporation of model-based distributions of residue estimates into the quantitative human health risk assessment.

Section II. Background and Developmental History.

With the passage of the Food Quality Protection Act (FQPA) in August 1996, Congress directed EPA to consider “all anticipated dietary exposures and all other exposures for which there is reliable information” in determining whether pesticide residues in food are safe. Because water is also a major component of dietary intake and a number of pesticides have been found in groundwater and surface water throughout the United States, drinking water should be considered an “anticipated dietary exposure” for certain pesticides. The picture emerging from available federal, state and local water monitoring efforts is complex. Typically a mix of pesticides are detected in water at low levels with seasonal pulses of higher concentrations. Of the major sources of monitoring data that OPP routinely uses – the United States Geological Survey’s (USGS) National Water Quality Assessment Program (NAWQA), Toxic Substances Hydrology Program (TSHP), and National Stream Quality Accounting Network (NASQAN), and the EPA’s National Pesticide survey – a majority of the streams (up to 95 percent) and half of the wells near agricultural and urban areas contain detectable levels of at least one, and often two or more, pesticides. Most groundwater aquifers and half of the streams investigated by these programs are direct sources of drinking water.

Prior to FQPA, OPP’s strategy for managing pesticides which had the potential to contaminate water was to emphasize prevention – requiring mitigation measures such as geographic restrictions on pesticide use (to protect groundwater) and “buffer zones” near water bodies where pesticide use is prohibited (to protect surface water). Only since FQPA has OPP routinely begun to consider exposure to pesticides in drinking water in its dietary risk assessments to decide on acceptable levels of pesticide residues on food (i.e., setting tolerances). (See US

EPA. 1999. Estimating the drinking water component of a dietary exposure assessment).

Evolution of OPP's FQPA Drinking Water Exposure Assessment Methods for Pesticides

During the first year after the enactment of FQPA in August 1996, work was undertaken on developing a more science-based policy for estimating exposure to pesticides in drinking water and for collecting and interpreting available monitoring data. Through this period, an interim approach was used which assumed that up to 10% of what it considered acceptable exposure to a pesticide could occur via the drinking water route (PRN 97-1). Therefore, OPP reserved 10% of the "risk cup" for drinking water related risks and allowed food residues and other routes of exposure to take no more than 90% of the "acceptable" risk. This 10% value for drinking water was a default assumption that OPP knew was likely to overestimate actual exposure in many cases, while potentially underestimating actual exposures in some others. This assumption was used until adoption of a new policy in November of 1997.

At that time, the following new but still interim process for addressing drinking water exposures was formally adopted:

1. OPP scientists review all available laboratory and field data submitted by the registrant to determine whether a particular pesticide will easily move to groundwater or surface water, will degrade quickly or persist, and will form toxic breakdown products as it degrades.
2. OPP uses pesticide-specific data from these studies in mathematical screening models to estimate pesticide concentrations in water in pesticide use areas. Peer reviews of these models generally supported OPP's view that modeled concentrations are high-end estimates of potential pesticide concentrations in drinking water derived from the upland regions of major watersheds.
3. OPP compares the screening estimates to human health-based "drinking water levels of comparison" (DWLOC), which are derived after first considering all food-related and residential exposures for which EPA has reliable information. This comparison determines whether OPP clears the pesticide from a drinking water perspective or attempts to refine its estimates of pesticide concentrations in drinking water to reflect more representative and realistic conditions. In some cases, the DWLOC may be very low – not because the pesticide is particularly toxic, but because contributions from food-related uses and other pathways of exposure are so great that very little or no room is left in the "risk cup" to allow for any exposure via drinking water. Alternatively, some pesticides (particularly newer pesticides) may have a very high DWLOC solely because they have very few food uses or other uses which result in exposure, leaving a lot of room in the "risk cup."
4. If the model estimates of pesticide concentration in drinking water exceed the DWLOC, OPP attempts to refine its estimate by gathering available monitoring data for analysis.
5. If monitoring data are not available or are not sufficient for purposes of refining the screening level estimates, OPP makes a risk management decision as to the need for groundwater and/or surface water monitoring and/or risk mitigation. Generally, OPP does not base significant risk management action (e.g., revocation or denial of a tolerance) on screening model estimates.
6. If monitoring data are available and reliable, OPP scientists analyze the data and consult

with risk managers as to how the data fit specific risk endpoints being addressed in the human health risk assessment. Appropriate short-term (for acute effects) and/or longer-term average (for chronic effects or cancer) drinking water concentrations are selected. OPP generally does not select the highest reported value from monitoring data; rather, OPP considers the distribution of reported values, compares them to model estimates, and selects value(s) from the high end of the distribution. The values from monitoring data used in the human health risk assessment are usually less than the model estimates but, in a few cases, may be greater than that predicted by OPP's screening models.

7. Estimates of pesticide concentrations in drinking water, derived from monitoring data, are combined with estimates of water consumption to estimate human exposure via drinking water. This estimate of exposure is then added to estimates of food and residential exposure to complete the aggregate exposure assessment.
8. Although rarely sufficient to do so, the monitoring data may be used to produce a regional-based picture of the distribution of measurements.

Use of Hydrologic Simulation Models

OPP is using a tiered system of modeling based upon a process first developed by OPP for use in ecological exposure assessments and is based largely on models developed by EPA. For surface water, prior to January 2000, the GENEEC model was used as a first tier screen and the linked PRZM and EXAMS models were used as a second tier assessment for chemicals that failed to pass the screening tier. Both of these tiers used a field pond scenario. Since January 2000, the FIRST model is being used as a first tier screen and the linked PRZM and EXAMS models are being used as a second tier assessment for chemicals that failed to pass the screening tier. Both of these tiers use the 'index reservoir' scenario. For groundwater, the SCI-GROW model continues to be used as a first tier screen. There are no second tier models in use for ground water assessment. More information on the two tier system for surface water modeling will be provided later in this document.

If the modeled estimates of pesticide concentration in the conservative 'index' drinking water reservoir do not exceed the DWLOC, then OPP concludes that the pesticide was not expected to pose an unacceptable risk via exposure to drinking water and no further evaluation is necessary. However, if model estimates do exceed the DWLOC, OPP gathers available water monitoring data and uses it to characterize the anticipated human exposure to the pesticide via drinking water. By the time a pesticide reaches this stage of OPP's review, OPP scientists are operating under the assumption that the pesticide has some potential to reach surface water and/or groundwater and that it has some potential to be present at levels of concern to human health. At this time in the assessment, it would be very beneficial to have the capacity to predict a distribution of concentration values across as large a number of sites as possible to better quantify the potential extent of the risk

Use of Field Measured Monitoring Data

Typical sources of monitoring data include USGS's NAWQA, NASQAN, and Toxic

Substances Hydrology programs (USGS, 1998), EPA Office of Water's STORET database (US EPA OW, 1998), OPP's Pesticides in Groundwater Data Base (US EPA OPP, 1992), and the National Pesticide Survey (US EPA, 1990). OPP may also seek additional water monitoring data from open literature or state agencies. OPP scientists gather and review as much information as is readily available on how the samples were collected and analyzed, where and when they were collected, and the circumstances surrounding their collection to determine whether existing monitoring data are reliable and relevant. A current monitoring program is underway in conjunction with the USGS for drinking water reservoirs and an extensive stream monitoring program is being planned for early 2001.

The availability of adequate temporal and spatial monitoring data can reduce much of the uncertainty associated with models, and can provide a more accurate estimate of the distribution of drinking water concentrations in areas of use. In a few cases, EPA will have "considerable" water monitoring data available for a particular pesticide, including small-scale prospective groundwater monitoring studies and monitoring data from state, local and federal programs. Nevertheless, even when such data are available, they may have been collected in a manner that limits the usefulness for estimating the distribution of drinking water concentrations in areas of use. Therefore, EPA must exercise considerable judgement concerning the best use and interpretation of these data, and how to interpret exposures and risk estimates calculated from them. This is particularly true when trying to characterize exposures from a region where there may be more than one source of water monitoring data.

In evaluating, characterizing and interpreting water monitoring data, OPP scientists attempt to collect as much information as is readily available on the design of the studies. That is, OPP scientists try to determine how the samples were collected and analyzed, why they were collected and where they were collected. To complete the FQPA assessment, OPP scientists review the reliability and validity of the monitoring data and present the range of values reported, the highest values reported, various return frequencies (e.g., 1 in 10 year concentration) the 95th percentile value, and the mean and median values. If OPP has adequate data to produce a regional "picture" of the distribution of reported values, this is completed as well.

Because of the level of variability and uncertainty associated with existing monitoring data, OPP's selection of a value or values to be incorporated into the human health risk assessment can be very difficult. Sometimes valid reported values vary from one region to another by several orders of magnitude. Often the detection limits in the available studies may vary by several orders of magnitude making the data difficult if not impossible to combine into a coherent picture of the existing conditions. In the vast majority of cases, the samples are not collected at sites of drinking water facilities reducing there value for drinking water analysis. Without having specific information on the history of the use of the pesticide in the sampled area, it is very difficult to fully understand the reasons for these differences. In many cases, the number of "non-detects" greatly exceeds the number of measurements above the limits of detection. While non-detects may result when a pesticide is not likely to move to and persist in water, they may also result when the pesticide is not used in the watershed. EPA often lacks data to verify that reported "non-detects" were in actual areas of use and, thus, has difficulty concluding that the pesticide, when used, is not in fact reaching water frequently enough to be of concern.

Despite the challenge of analyzing and interpreting these data, OPP has felt it was appropriate to choose a value or values from valid monitoring data to make decisions in the human health risk assessment. Values have been chosen from valid monitoring data even when the data were limited in time or location. Generally, this was done because model-based estimates suggest that DWLOCs may be exceeded. To assume that drinking water exposure is "zero" in the human health risk assessment simply because available, valid monitoring data are highly variable (making it difficult to select a number or numbers) appears counter to OPP's objective to use the best science available in its decisions to ensure protection of human health. As OPP has gained experience in reviewing and incorporating monitoring data into making tolerance decisions, it has generally chosen "reasonable high end" monitoring values for use in the human health risk assessment. That is, OPP has selected a value on the "high end" of the range rather than the highest measured value.

Mathematical models allow OPP to rapidly screen pesticides to determine whether the Agency can confidently conclude they are unlikely to occur in drinking water at levels that will result in exceedances of the RfD (when combined with food and residential exposure) or whether the Agency needs more information on them to complete an assessment. While available monitoring data to evaluate the accuracy of these models are scarce, EPA believes that model-based predictions for single, high exposure- sites generally overestimate the concentration of pesticides in most drinking water sources due to a combination of factors: (1) the bodies of water modeled are generally farther up in the watershed than the drinking water intakes (and, thus, the pesticide is less diluted than it would be downstream); (2) the estimates do not include the effects of any dilution or treatment that may occur in many, but not all, distribution systems; and (3) the existing models assume the entire watershed is cropped. Hence, for some pesticides, drinking water exposure may appear to contribute to an exposure that would represent an unacceptable dietary risk (alone or in combination with food) even though actual risks to most people would in fact be lower. Reliable and representative data on measured pesticide residues in drinking water are a valuable "real world" assessment tool when available. However, because pesticide concentrations vary greatly in location (some drinking water sources are more vulnerable than others) and time (both seasonally and year-to-year), most existing monitoring data provide little more than a piece of a complex puzzle.

Use of Monitored Values in Raw Intake Water versus Value in Treated Water

Another issue is that much monitoring data is from water that has been treated in some way by a public drinking water facility. The effectiveness of treatment processes is extremely variable from site to site as well as from sample time to sample time within the same treatment facility. This data, therefore, has little or no value for predictive purposes, for extrapolation to other sites or in developing modeled estimates. There is no way to separate the agricultural/hydrologic impacts from the treatment impacts.

Use of the 'Index Reservoir' and 'Percent Cropped Area' in Surface Water Modeling Scenarios

In July, 1998, OPP presented to the FIFRA SAP a proposed "index" reservoir scenario to replace the "field pond" scenario used at that time in its screening models to estimate pesticide concentrations in drinking water derived from surface water. The concept behind use of a model of an "index" reservoir to screen pesticides is that the chosen reservoir – and its associated characteristics – would become the standard set of conditions by which EPA would judge the potential of a pesticide to contaminate drinking water derived from surface water. The "index" reservoir would be selected from a group of reservoirs that provide drinking water to communities throughout the country. EPA would pick a particular reservoir that has characteristics associated with a higher potential for pesticide contamination of surface water and use those real world characteristics in its mathematical screening model. Because the "index" reservoir models real world characteristics, it is likely to produce more realistic estimates of pesticide concentrations in surface water. Because the "index" reservoir has characteristics that are associated with a higher potential for pesticide contamination of surface water, the model is likely to be protective of other drinking water sources which are less vulnerable to contamination.

Out of an initial list of about 20 possible reservoirs, OPP selected Shipman City Lake in Shipman, Illinois, for use as its "index" reservoir in its screening assessments. This reservoir was selected because it was representative of a number of reservoirs in the central Midwest that are known to be vulnerable to pesticide contamination. These reservoirs tend to be small and shallow with small watersheds, and frequently have Safe Drinking Water Act (SDWA) compliance problems with atrazine, a herbicide widely used on corn grown in these watersheds. Shipman City Lake is 13 acres in area, 9 feet deep, and has a watershed area of 427 acres. Its ratio of drainage area to capacity (volume of water in the lake) is approximately 12. As a comparison, the "field pond" currently used has a ratio of 5. As such it is more conservative than the field pond scenario which was used until January 2000.

Percent Cropped Area

OPP has implemented the percent cropped area approach for five major crops and their joint occurrences since January 2000 and continues investigations for minor crops. OPP has developed the necessary data bases and Geographical Information System (GIS) tools to enable it to consider the percentage of the area around an index reservoir that is cropped (i.e., the "percent cropped area" or "PCA") and, thus potentially treated with a pesticide when it uses its model to predict pesticide levels in a drinking water reservoir. Before January 2000, OPP assumed that the entire area surrounding a body of water was planted with a crop and treated with the pesticide being evaluated. This approach generally resulted in an overestimate of the amount of pesticide leaving the field and running off into surface water and, therefore, an overestimate of pesticide concentrations in surface water used as drinking water.

OPP used the PCA in the initial index reservoir scenario using Shipman City Lake (July 1998 FIFRA SAP) and found that the resulting modeled concentrations for atrazine were in good agreement with available monitoring data. However, several substantial uncertainties in the analysis warranted further evaluation and development before a percent cropped area was implemented. The PCA was taken from one county included within the Shipman City Lake

Watershed. The FIFRA SAP recommended that percent cropped areas be developed on a watershed rather than a county basis.

OPP presented its plan for implementing the percent cropped area (PCA) as a refinement to the FQPA drinking water assessment process to the FIFRA Scientific Advisory Panel (SAP) in May 1999. The SAP agreed with the concept of the PCA as an "appropriate and reasonable" adjustment for major-use crops while still providing a protective (i.e., "highly vulnerable") assessment. It observed that the PCA "provides a technically defensible approach to reduce estimates of acute and chronic pesticide exposures to levels similar to those found in monitoring data." However, the SAP also identified several limitations to the approach, which have been outlined in Section II.E.2. [SAP Report No. 99-03C, May 27, 1999; available via the public docket].

Using 1992 Agricultural Census data, OPP ranked counties by PCA (since the data are reported on a county basis). For each crop, OPP used GIS tools to select the small watershed (the 8-digit Hydrologic Unit Code was the basis for evaluation) which has the highest PCA. PCAs were derived on a watershed basis in response to recommendations from the December 1997 SAP. The May 1999 SAP expressed concern that the Agency would be unable to validate PCAs for minor crops and recommended that EPA consider requesting low-cost, targeted monitoring data to evaluate pesticide contamination from use on minor crops [SAP Report No. 99-03C, May 27, 1999]. The May 1999 SAP also recommended that, for multiple crop use, the Agency could derive PCAs based on the maximum combined acreage of crops in a watershed. If pesticide application rate and timing vary from crop to crop, an aggregate pesticide concentration estimate could be made by separately simulating each crop in the watershed and then summing the individual model estimates.

OPP has implemented the "index" reservoir and percent crop area factors for the major-use crops presented to the May 1999 SAP in its Tier 2 (PRZM/EXAMS) surface water screening models since January 2000. OPP is working on developing a Tier 1 index drinking water reservoir model, similar to that of GENEEC. Based on recommendations from the July 1998 SAP, PCAs will not be used with the Tier 1 model. The method for deriving watershed-based percent cropped area (PCA) correction factors will be converted into guidance for developing PCAs for major crops and cropping combinations through early 2000.

3. The Use of Watershed-scale Models

OPP completed and presented to the FIFRA SAP in July 1998 its preliminary evaluation of seven watershed-scale surface water models. Further efforts to evaluate these models against actual monitoring data are ongoing. This model evaluation effort is expected to provide an understanding of the relative accuracy of each of these models. OPP expects that one or more of these watershed-scale models will ultimately be used to produce more refined estimates of pesticide concentrations in drinking water. EPA is aware of the difficulties in developing and evaluating a watershed-scale model and is investing considerable effort in this area in FY2000.

The Use of Watershed-scale Models

EPA is also in the process of evaluating a variety of watershed-scale models which more accurately captures basin-area processes and could be more appropriate for drinking water assessments. OPP completed and presented to the FIFRA SAP in July 1998 its preliminary evaluation of seven watershed-scale surface water models. Further efforts are ongoing to conduct preliminary model validation of watershed-scale models for the White River watershed in Indiana. This model validation effort is expected to provide some preliminary understanding of the relative accuracy of each of these models. OPP expects that one or more of these watershed-scale models will ultimately be used to produce more refined estimates of pesticide concentrations in drinking water for those cases where an unreasonable risk is estimated by the use of a screening level estimate. Whether this would be an additional tier or replace the existing field-scale surface water models will depend on the simplicity and data/resource demands of the watershed model(s).

OPP is soliciting comments on the availability of watershed-scale models and the potential viability of such models as screening tools for drinking water exposure assessments for pesticides.

Groundwater Screening Model Approach

OPP will continue to use SCI-GROW as an initial screening tool to determine the potential of a pesticide to contaminate ground water sources of drinking water at concentrations high enough to indicate a potential for risk. On the basis of recommendations of the FIFRA SAP in December 1997 and the experience of OPP in using SCI-GROW as an initial screen for drinking water assessments, OPP will systematically evaluate SCI-GROW against additional groundwater monitoring data and other models. Included in the evaluation will be an assessment of the potential limitations in the predictive capacity of SCI-GROW. For instance, are there certain classes of chemicals or certain environmental fate parameters for which SCI-GROW is not well suited? This evaluation is expected to run parallel to the development of a tier 2 screening model for groundwater. Depending on the outcome of the assessment, some changes in OPP's approach to the initial screening tier for groundwater may occur.

OPP is evaluating models and developing a procedure for a second tier assessment of pesticides in ground water. The Agency has evaluated approximately 50 candidate models and has selected 6 models for detailed evaluation. OPP plans to use data from existing prospective ground water monitoring studies to evaluate the ability of the models to predict pesticide concentrations in ground water. To date, OPP has completed a preliminary evaluation with one data set. A similar evaluation with data sets from at least two other pesticides representing other crops, pesticide groups, use patterns and areas of the country is underway. OPP intends to develop a set of model scenarios similar to those used with PRZM/EXAMS to maximize efficient use of these models.

OPP's Use of Regression Models for Exposure Assessment

Hydrologic simulation models used by OPP for exposure assessment are mostly physically based models that represent the agricultural landscape, climate and pesticide use by measurable properties of the soil, the weather and the chemical. The SCI-GROW tier 1 groundwater

screening model is the only regression model currently in use by OPP for exposure assessment in a regulatory context. The Agency in 1997 also investigated the properties of a surface water regression model called Surface Water M I (SWMI) which was developed by pesticide industry under the sponsorship of the American Crop Protection Association (ACPA).
SWMI was based on several intensively monitored watersheds in Ohio and had many attractive properties. It was not adopted for regular use in favor of the index reservoir. However, the expanded regression analysis of USGS, based on more extensive monitoring data and more comprehensive analysis of potential predictor variables, is causing this early conclusion to be revisited.

Development of Aggregate Exposure Methodology.

Aggregate exposure is defined to encompass multiple potential sources of exposure to pesticides and includes exposure from pesticide residues in food, in drinking water and in the home. Levels of residues in food items have been routinely monitored and reported for a number of years for conducting human health risk assessments. During this period of collecting and analyzing pesticide food residue data, procedures have been developed which attempt to quantify on a statistical, probabilistic basis the exposure received by any person consuming food in the United States. In order to account for regionality of food consumption habits, the country is divided into four quadrants for analysis. A Monte Carlo procedure is then used to select from the measured distributions so as to represent potential exposure to the entire US population.

Questions For the Panel

At the request of the risk managers, EFED is seeking to improve its current approach to factoring drinking water exposure into tolerance decision making by developing a new interim approach which would allow it to produce sufficiently reliable estimates of pesticide concentrations in drinking water such that these estimates could be used in quantitative human health risk assessment. At this stage, the Agency envisions using this new approach in a limited number of cases; cases where EPA believes that the severity and magnitude of the potential risk posed warrant the use of this tool and the incorporation of model-based residue distribution estimates into the quantitative human health risk assessment.

1) The Food Quality Protection Act (FQPA) requires the Agency to consider "all anticipated dietary exposures and all other exposures for which there is reliable information" in development of an aggregate exposure assessment. For FQPA exposure assessments in food, the Agency now develops population-based regional distributions of pesticide residues in the diet. Are we correct in our assumption that population-based regional (or national) distributions are also the most appropriate representation of pesticide residues (concentrations) in drinking water for incorporation into aggregate and cumulative risk assessment as defined by FQPA?

2) We are exploring the use of regression models and the SPARROW model developed in large part by the US Geological Survey for development of distributions of pesticide concentrations at drinking water facility intake locations. This is likely to include a nested set of methods for water drawn for drinking from larger rivers, from smaller streams, from shallow ground water and from

reservoirs. Does the SAP believe that these approaches are sufficiently rigorous and promising at this time to warrant further developmental efforts?

3) FQPA requires the Agency to address "major identifiable subgroups of consumers" who might be impacted more adversely than the population at large. How could EPA use this method of developing regional and national distributions of concentrations across hundreds or thousands of sites to identify such subgroups and estimate their exposures?

4) Some pesticides (e.g. the OP's) present more of an acute than a chronic health risk. The Agency currently estimates acute pesticide risk based upon a maximum annual daily exposure value (99.7th percentile each year). Regression approaches can predict distributions of concentration values at various exceedence percentiles, but the potential error of the estimation increases at the highest percentile. Are the regression approaches for shorter-term (95th percentile) maximum annual concentration values likely to produce values that are appropriate for acute risk assessment? Or, should we build the approach for estimating the 99.7 percentile and accept the greater uncertainty? Are there additional approaches which the panel could recommend?

5) The ability to estimate distributions of atrazine using the regression approaches including SPARROW is due partially to the availability of extensive monitoring data for the chemical in both surface and ground water. Although good monitoring data sets are available for some other pesticides, OPP will also be required to conduct drinking water exposure assessments for pesticides for which there is little or no field data. A method will be needed to estimate distributions of concentration values for those chemicals for which there is insufficient monitoring data to use a normal regression approach but which have failed the screening level exposure assessment using a single, conservative, high exposure site. a)Would the panel support an effort to build a level of predictive capability into the regression approaches presented, based upon adding pesticide use and important environmental fate properties as additional regression variables? b) Would it be appropriate to use national or regional distributions of atrazine concentration data adjusted for use area and environmental fate properties as a conservative benchmark for evaluating other compounds in a regulatory setting. c) Does the panel have other suggestions for developing distributions of pesticide concentrations in drinking water?

VI. BIBLIOGRAPHY

ILSI. 1998. *Assessment of Methods to Estimate Pesticide Concentrations in Drinking Water Sources*. Report of a workgroup on Aggregate Exposure Assessment, International Life Science Institute, Washington, DC.

SAP. 1997. *Estimating Drinking Water Exposure as a Component of the Dietary Risk Assessment.* Report of FIFRA Scientific Advisory Panel, December 10-11, 1997, Crystal City, VA.

SAP. 1998. *Proposed Methods for Basin-scale Estimation of Pesticide Concentrations in*

Flowing Water and Reservoirs for Tolerance Reassessment, Report of FIFRA Scientific Advisory Panel, July 29, 1998, Crystal City, VA.

US EPA. 1990. National Pesticide Survey.

US EPA OPP. 1992. *Pesticides in Ground Water Database – A Compilation of Monitoring Studies: 1971-1991 National Summary*. EPA 734-12-92-001. US EPA Office of Pesticide Programs, Washington, DC.

US EPA OW. 1998. U.S. EPA Office of Water Storage and Retrieval Database (STORET). <http://www.epa.gov/owowwtr1/STORET/overview.html>

USGS. 1998. The National Water Quality Assessment (NAWQA) Program, National Stream Quality Accounting Network (NASQAN), and Toxic Substances Hydrology Program can be reached through the U.S. Geological Survey's main web page at <http://usgs.gov/>.

US EPA. 1999. Estimating the drinking water component of a dietary exposure assessment. < http://www.epa.gov/fedrgstr/EPA-PEST/1999/November/Day-10/6044.pdf >.