Creating New Scenarios for Use in Pesticide Surface Water Exposure Assessments

U.S. Environmental Protection Agency
Office of Pesticide Programs

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1. Executive Summary

OPP developed methods to select realistic input parameters for field scenarios used in the Pesticide in Water Calculator (PWC), which is OPP's main tool to estimate aquatic concentrations of pesticides. While PWC estimates aquatic concentrations for both surface water and groundwater, this effort focuses on field scenarios used for estimating surface-water concentrations. These input parameters (or field scenarios) are spatially comprehensive such that the PWC output can reflect aquatic concentrations across the landscape. The field scenarios are ranked here by the concentrations they produce. These rankings may facilitate policy makers' decisions on selecting the appropriate level of scenario vulnerability. OPP performed preliminary analyses of the scenarios by running the PWC and using the output concentration endpoints of acute, chronic, and cancer concentrations as ranking criteria. Additionally, since chemicals are transported in solution by runoff and sorbed to eroded soil, OPP used organic carbon sorption coefficients of 10, 1000, and 10000 mL/g which should allow capture of both mechanisms of transport in PWC simulations. Preliminary results suggest that the difference between a 90th percentile scenario and a 50th percentile scenario is usually less than a factor of 2, regardless of the endpoint or the dominant transport mechanism (i.e., runoff or erosion).

2. Introduction

2.1. Regulatory Context

Pesticides are regulated in the United States under both the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) and the Federal Food, Drug and Cosmetics Act (FFDCA). Through these statutes, the United States Environmental Protection Agency Office of Pesticide Programs (OPP) must determine that aggregate exposure to the pesticide residues is safe, i.e., that "there is a reasonable certainty of no harm" from aggregate exposure to the pesticide, before issuing a tolerance.

OPP's Environmental Fate and Effects Division's (EFED) scientists are responsible for conducting Drinking Water Assessments (DWA), which include an analysis of the potential for and magnitude of pesticide occurrence in both surface water and groundwater sources. OPP estimates Drinking Water Concentrations (EDWCs) in surface waters that supply Community Surface Water (CWS) intakes and compares them to benchmark values called Drinking Water Level of Comparison (DWLOC) to determine if pesticide concentrations have the potential to cause adverse effects to human health (USEPA OPP, 2019a, p. 13). EFED employs a robust, tiered DWA process that is designed to efficiently screen out pesticides that do not pose a potential risk to human health from those requiring more highly refined analyses to better understand potential risks (*e.g.*, in terms of when and where there may be concerns). Lower tier assessments are intended to be conservative so that the assessor can confidently screen out chemicals that represent a low risk. Higher tiers successively incorporate refinements that draw on more focused chemical, spatial, temporal, and agronomic information, including consideration of available monitoring data to inform risk management decisions. For additional information on OPP's tiered approach to DWAs, including a detailed description of individual tiers, see the *Draft Framework for Conducting Pesticide Drinking Water Assessments for Surface Water* (USEPA OPP, 2019a).

2.2. Purpose Statement

OPP estimates pesticide exposure concentrations for DWA primarily using the Pesticide in Water Calculator (PWC). The PWC requires specification of environmental conditions, or scenarios, that include both water body and field (or watershed) components, in order to calculate surface water concentrations. This effort focuses on the field scenario components. Currently, OPP uses scenarios it developed largely using best professional judgement. With recent advances in automation and improvements in data quality, OPP is proposing a step toward improving the field scenario-development process. OPP's goal for this current effort is to build new scenarios for surface water risk assessments that better reflect environmental characteristics and to facilitate policy maker's decision on selecting the appropriate level of scenario vulnerability.

2.3. Document Organization

- **Section 3 (Overview of OPP Surface Water Modeling)** provides an overview of the OPP model used to calculate surface water concentrations and gives background on previous scenario developments.
- **Section 4 (Methods)** details the methods for creating the new scenarios.
- **Section 5 (Preliminary Results)** gives preliminary results and indicates how the new scenarios will compare with OPP's previous scenarios.
- **Section 6 (Summary)** summarizes the methods and preliminary results and discusses potential impact to risk assessments.

3. Overview of OPP Surface Water Modeling

Surface waters potentially impacted by pesticides are widespread across the U.S, and efficient assessment requires the assistance of models which simplify the task. To this end, the OPP uses a simplified conceptualization of the pesticide use area as depicted in Figure 1. In this conceptualization, runoff and erosion move the pesticide from an agricultural field into an adjacent water body where it mixes with the water column and sediment. A computer model called the *Pesticide in Water Calculator* (PWC) performs the necessary calculations (Young, 2019), taking into consideration the chemical properties of the pesticide along with the characteristics of the soil, weather, hydrology, and agricultural management conditions. Ultimately, the PWC estimates the pesticide concentrations in the waterbody that OPP uses for regulatory decisions.

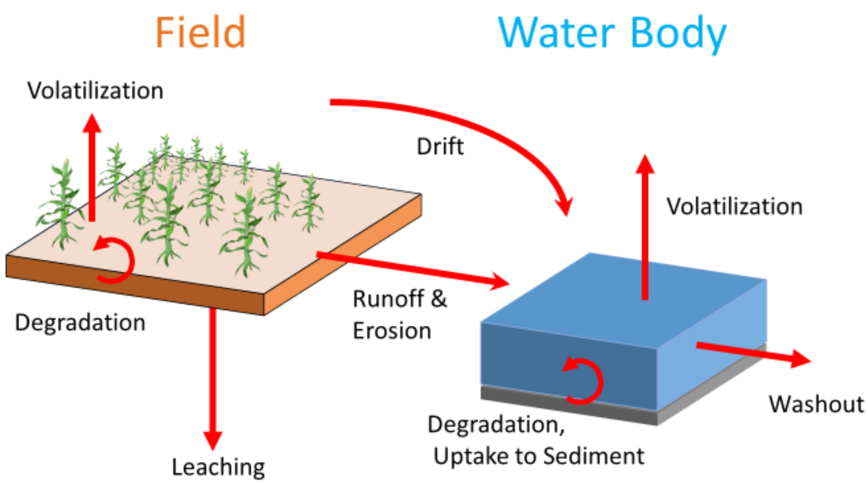

Figure 1. The conceptual model for calculating waterbody concentrations of pesticides due to runoff and erosion from an adjacent field. (Drift is also a transport mechanism, but OPP calculates drift independently of the PWC and is independent of location or scenario.)

The PWC requires inputs for pesticide properties (e.g., degradation rate, application rate) and inputs for the environmental properties (field and waterbody characteristics). The set of PWC inputs that characterize the field (e.g., soil organic matter, runoff characteristics, crop/land cover, rainfall amounts) and waterbody (surface area, depth, benthic carbon) makes up a *scenario*, while the subset of parameters that describe only the field properties is a *field scenario*. In this current effort, OPP is only addressing improvements to field scenarios, while improvements to water body characterization and watershed-size characterization are being addressed in a concurrent project (USEPA OPP, 2015).

3.1. Scenario Background

For surface water exposure assessments, OPP currently has 125 field scenarios developed over the previous two decades using guidance (USEPA OPP, 2007), professional judgment, and the best available data at the time. In developing these scenarios, OPP's goal was to produce reasonably conservative scenarios, or those with higher-than-average runoff, erosion, and chemical transport. In the past, OPP sometimes referred to these protective scenarios as "90th percentile" scenarios, but the actual percentile was unknown, and the scale upon which percentile comparisons were made also remained undefined (i.e., 90th percentile of what?). With acknowledgement of this uncertainty, OPP subsequently characterized these scenarios simply as "high-end."

4. Methods

OPP proposes the following steps to develop scenarios for use with the PWC in a reproducible manner. In a preliminary effort, OPP has followed these steps to develop example scenarios for corn and wheat in order to evaluate the method's performance.

Methods Step 1: Generate combinations of soil, land-cover, and weather

OPP generated combinations of soil, land cover, and weather using GIS data. To accomplish this, OPP applied a new guidance *Estimating Field and Watershed Parameters Used in USEPA's Office of Pesticide Programs Aquatic Exposure Models – The Pesticide Water Calculator (PWC)/Pesticide Root Zone Model (PRZM) and Spatial Aquatic Model (SAM)* hereafter referred to as *USEPA OPP (2019b)*. This guidance specifies parameters that are representative of the area of interest. The previous OPP guidance specified parameters with an upward bias with regard to pesticide transport. The details of the computerized methods used for finding and consolidating these parameters sets are given in *Methods for Automated Field-Scenario Generation for Use in the Pesticide Water Calculator and the Spatial Aquatic Model* (USEPA OPP, 2019c).

To build the parameters sets, OPP first obtained the following data layers:

- Soil map units from USDA's Soil Survey Geographic (SSURGO) database (USDA NRCS SSS, 2018)
- the latest five years of land cover/crop groups from the USDA's Cropland Data Layer (CDL) (USDA NASS, 2014-2018)
- meteorological data generated from the National Oceanic and Atmospheric Administration (NOAA) data for the years 1961 to 2014 (Fry et al, 2016)

OPP then combined these layers as shown in Figure 2. The three data sets are on the left of the figure; the resulting combination of the overlay is on the right of the figure. Each color on the right represents a combination of parameters that are identical. In this example, there are 7 different parameter combinations (7 different colors), and each of these combinations has a different pixel count (as seen by the different sizes of the colors).

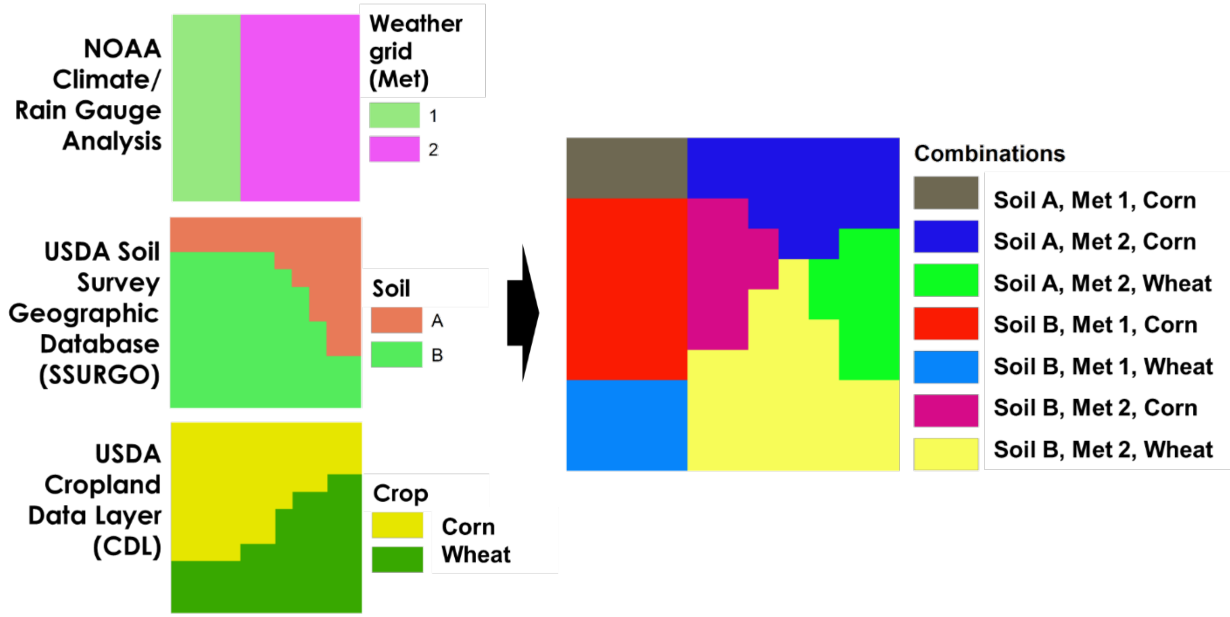

Figure 2. Systematic creation of field scenarios. Scenario are built from the overlap of spatial data layers – weather grids (NOAA), soils (SSURGO), and land cover (CDL).

Methods Step 2: Create tables of input parameters

With the overlays from Step 1, OPP created a *Field Scenario Input Table* as depicted in Figure 3 (Note: partial table shown with sample values). OPP first created a scenario ID (on the left of figure) that identified the pixel location and parameters (soil, weather, crop) from Step 1. OPP combined the parameters from each data set (middle of figure) into the Field Input Table (on the right figure). The Input Table is used later as an input to the PWC in Step 5.

Field Scenarios

ScenarioID	Soil	Met	Land Use
sAw1luCorn	A	1	Corn
sAw2luCorn	A	2	Corn
sAw1luWheat	A	2	Wheat
sBw1luCorn	B	1	Corn
sBw1luWheat	B	1	Wheat
sBw2luCorn	B	2	Corn
sBw2luWheat	B	2	Wheat
…	…	…	…

Parameters

Soil	Water _max	Water _min
A	0.3	0.2
B	0.4	0.1
…	…	…

Met	ireg
1	4
2	3
…	…

Soil	Land Use	curve_number
A	Corn	64
A	Wheat	60
B	Corn	74
B	Wheat	72

Field Scenario Input Table

ScenarioID	Water _max	Water _min	Ireg	curve_number
sAw1luCorn	0.3	0.2	4	64
sAw2luCorn	0.3	0.2	3	64
sAw1luWheat	0.3	0.2	4	60
sBw1luCorn	0.4	0.1	4	74
sBw1luWheat	0.4	0.1	4	72
sBw2lucorn	0.4	0.1	3	74
sBw2luWheat	0.4	0.1	3	72
…	…	…	…	…

Figure 3. Process to create parameters for field scenarios. Note: Partial table shown with sample values. Parameters are defined in USEPA OPP (2019b)

Methods Step 3: Group Scenarios into HUCs and Crop

To facilitate PWC runs, OPP organized the Field Scenario Input Table by the USGS Hydrologic unit code 2 (HUC2); thus, each scenario table contained scenario data for only one HUC2 region. HUC2 regions divide the conterminous United States into 18 units based on topographic, hydrologic, and other relevant landscape characteristics, as shown in Figure 4. OPP used the National Hydrography Dataset (NHDplus, version 2) processing regions, which further subdivides Regions 3 (southeast US) and 10 (Missouri River), resulting in 21 regions (Figure 4). OPP also organized the Field Scenario Input Table by crop, and thus the scenario tables used for PWC batch runs (Step 5) contained parameters for only one crop (as well as for only one HUC2).

OPP plans to develop a full set of field input parameters for crops/crop groups representing the top 16 annual cultivated crops listed in Table 1. To test the methods on a more limited scale, OPP developed field scenarios only for corn and winter wheat in the examples that follow. Corn and wheat are good test examples because they are among the most cultivated crops in the U.S., and they occur in each of the HUC2 regions. When the methods are fully implemented after review and revisions, OPP plans to develop scenarios for the other relevant crops in Table 1and for other important crops such as vegetables, orchards, vineyards, and perennial legume and grass pasture/hay/forage crops.

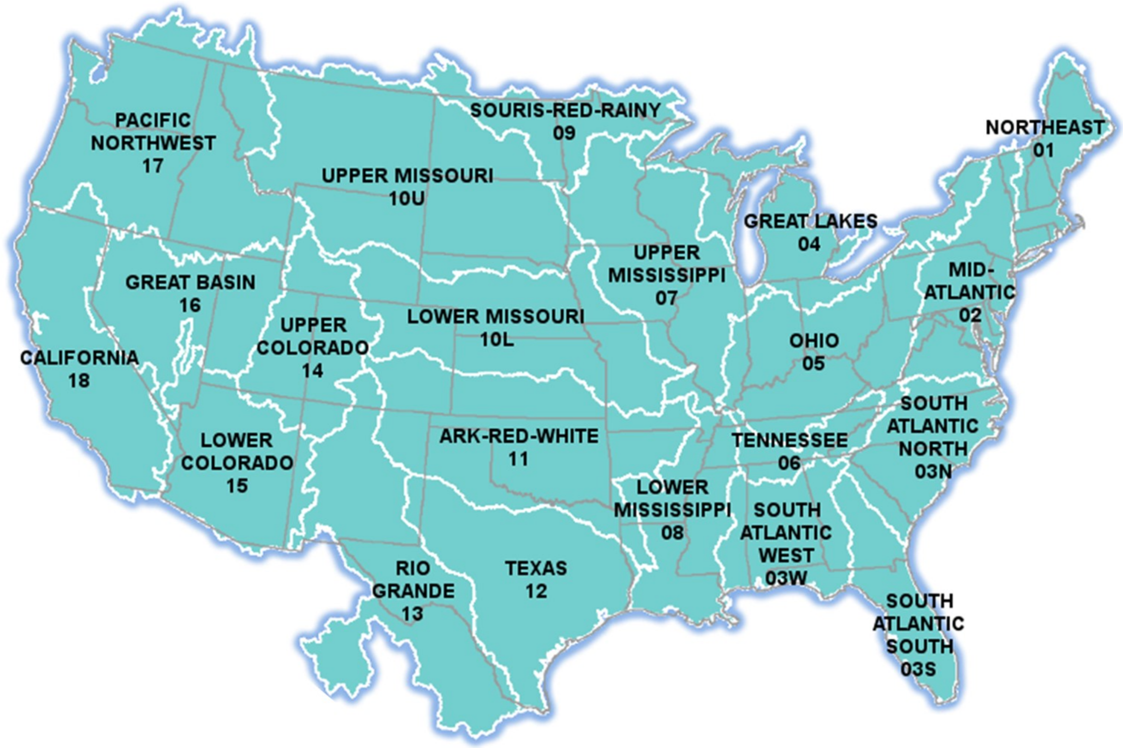

Figure 4. HUC2 Processing Regions for the National Hydrography Dataset (NHDplus, version 2) used for scenario selections.

Table 1. Top 16 major crops listed in order of acreage in the U.S.

Rank	Crop	2012 Census of Ag Acres	Major Crop/Crop Groups
1	Corn	94,609,673	Corn
2	Soybeans	76,104,780	Soybeans
3	Winter Wheat	34,723,361	Wheat
4	Spring Wheat	12,177,715	Wheat
5	Cotton	9,384,080	Cotton
6	Sorghum	5,628,744	Other Grains
7	Barley	3,283,905	Other Grains
8	Rice	2,693,759	Rice
9	Durum Wheat	2,139,150	Wheat
10	Sunflower	1,877,145	Row Crops
11	Canola	1,736,409	Row Crops
12	Dry Beans	1,642,797	Vegetables
13	Peanuts	1,621,631	Row Crops
14	Sugar Beets	1,249,481	Row Crops
15	Potatoes	1,168,199	Vegetables
16	Oats	1,078,698	Other Grains

Methods Step 4: Subsample Scenarios

Using this methodology, the number of scenarios OPP generated for corn and wheat for each HUC2 was quite large (USEPA OPP, 2019c), on the order of 100,000 within a HUC2 region in most cases. With PWC simulation times of about 10 to 20 scenarios per minute, the total run time for the full scenario set for an entire region would be too long for practical purposes. Therefore, OPP took random samples of 25% or a minimum of 1,000 random samples, whichever was greater, from the full Field Scenario Input Table sets generated within each HUC2 region from Step 3. For those regions with less than 1,000 scenarios, OPP processed the full set of field scenarios.

Methods Step 5: Select Chemical Parameters for PWC Simulations

OPP, through years of experience with the PWC, is aware that field parameters are not the only factor in determining the pesticide transport potential. Some chemical properties, most importantly the sorption coefficient and persistence (i.e., degradation rate), can have important effects on pesticide transport as described below, and thus the values used in modeling can have important implications on scenario results, as described below.

As modeled in the PWC, a pesticide is transported to surface waters in dissolved form by water runoff and in sorbed form by eroded solids. Depending on the chemical's sorption properties (typically characterized by K_{oc} or the organic-carbon-normalized sorption coefficient), the dominant means of transport will vary between these two mechanisms. Experience within OPP (and as shown later in Section 5: Preliminary Results) suggests that peak transport to surface water occurs somewhere between a K_{oc} of 500 and 1000 mL/g. This indicates that the pesticide concentration of a scenario is not monotonically dependent on the chemical's K_{oc}. Pesticide aquatic concentration may increase or decrease as K_{oc} increases. This is due to the tradeoffs with transport by the two processes of erosion and runoff. To address the effect of K_{oc}, OPP assessed scenarios using K_{oc} values of 10, 1000, and 10000 ml/g.

Although persistence of a chemical may also impact pesticide concentration, it is much less straightforward to evaluate. Effects of persistence will be heavily influenced by application timing because the date of pesticide application will determine whether the pesticide is on a crop canopy or in the soil and how long it will remain before rainfall moves the pesticide into another environmental compartment. This is an important aspect of pesticide risk assessments, but it is beyond the scope of this project. Instead, this current effort focuses on pesticide transport potential due to the physical processes of runoff and erosion regardless of application timing.

To decrease the effect of application timing on pesticide transport potential, OPP (1) used a chemical half-life that is relatively long, or persistent, (180 days) and (2) spread out the pesticide application over a long period (50 days, starting from emergence). Experience in OPP with PWC has shown that the EDWCs for any one scenario become insensitive to soil half-lives above 60 days. This is because the pesticide's typical residence time in the top few centimeters of the soil (where runoff and erosion occur) is on this order. Thus, for many scenarios, the pesticide will dissipate from the top soil by the time the next seasonal pesticide application occurs. For a few scenarios (mostly dry regions), the residence time may be quite a bit longer and thus the pesticide could accumulate in the top layer. A continuously increasing baseline pesticide mass (amount of pesticide accumulating in the soil) in the top soil could increase to levels where concentration variations due to year-to-year weather changes may become difficult to detect in the PWC output. Thus, OPP used the 180-day soil half-life to prevent excessive accumulation that may have occurred in some scenarios. OPP may explore optimizing this soil degradation value in the future to enhance the relevant response after OPP gains some experience with the initial phase of this work. The second action OPP took to decrease the effect of application timing was to evenly distribute the pesticide applications in our PWC simulations over a 50-day period within the growing season. Daily pesticide applications start on the planting date and end 50 days later. In this way, the variations caused by timing are damped, thereby increasing likelihood that concentration variations are due strictly to runoff and erosion variations.

Methods Step 6. Perform PWC Runs

In this preliminary work, OPP ran separate scenario batches for each of the three K_{oc} values (10, 1000, 10000 mL/g) for corn and wheat and each HUC2. Figure 5 shows a typical partial batch input file and output from the PWC. For this effort, OPP is interested in the outputs for acute, chronic, and cancer concentrations which are revealed in the bottom left of the PWC output page. The PWC records the acute (1-day), chronic (365-day), and cancer (overall, 53+ years) concentrations for each completed scenario in a text file (Young, 2019). When the batch run is complete, the text file contains a distribution of concentrations for use in the next step analysis.

Field Scenario Input Table

ScenarioID	Water _max	Water _min	Ireg	curve_number
sAw1luCorn	0.3	0.2	3	82
sAw2luCorn	0.3	0.2	3	82
sA3PLuCorn	0.2	0.1	3	77
sBw1luCorn	0.4	0.1	3	73
sBw2lucorn	0.4	0.1	3	73
...	...	...	...	...

PWC Output

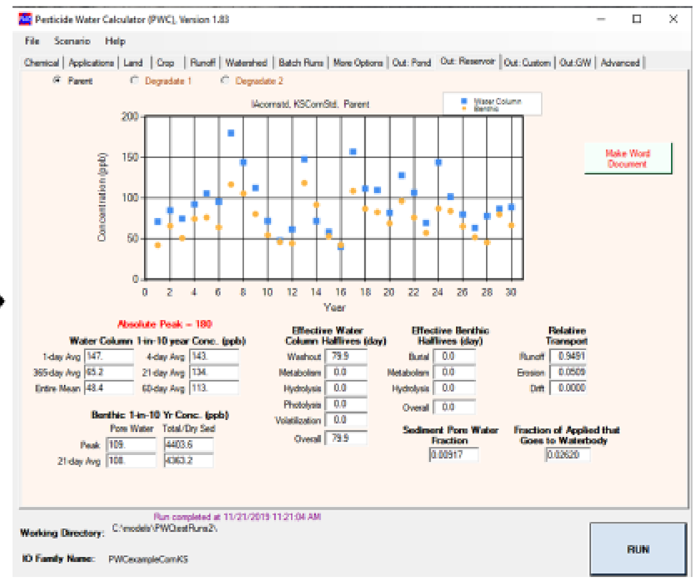

Figure 5. The batch input file and the output from the PWC (for one scenario) showing surface water concentrations for acute, chronic and cancer. ***Note: Partial table shown with sample values. Parameters are defined in USEPA OPP (2019b)***

Methods Step 7: Sort the scenarios from high to low concentrations

With the PWC output from Step 6, OPP sorted the scenarios by concentration. Details are described in USEPA OPP (2019c). As shown in Figure 6, this sorted list results in a plottable, cumulative distribution of scenarios.

Text file with Sorted Scenarios

Scenario ID	EDWC	Rank (%)
sAw1luCorn	50	99.9
sBw2luCorn	49	99.8
sAe1luCorn	40	98
sSk1luCorn	35	96
sTw1lgCorn	32	90
sAn1ljCorn	30	80
sAw1lhCorn	25	60
sAw1lyCorn	20	50
xAv2uhCorn	15	25
xAi2uhCorn	10	5
xAo2uhCorn	5	2

Graphical Distribution of Sorted Scenarios

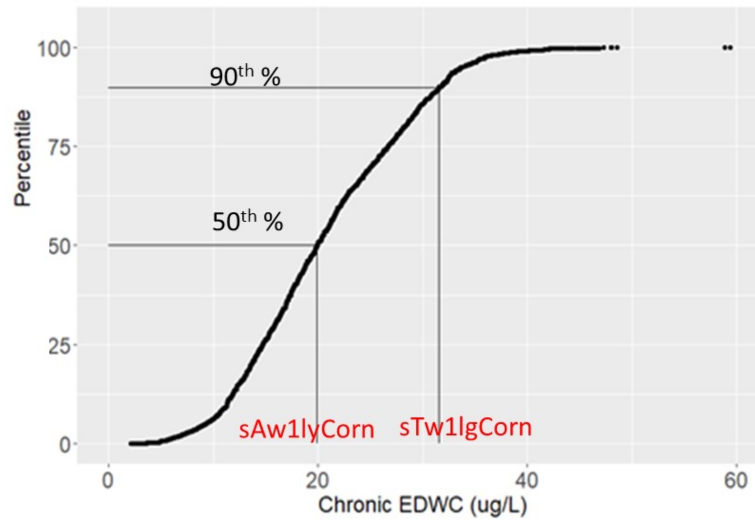

Figure 6. Sorting the scenarios by concentration and plotting them as a distribution. Hypothetical distribution showing the sorting of the original data and its graphical distribution. Also indicated are the positions of the 50th and 90th percentile scenarios. (Table is severely culled and truncated and shown for demonstration purposes only.)

5. Preliminary Results

5.1. Corn and Wheat Distributions

Figure 7 shows example distributions for corn and winter wheat for the chronic concentrations (in ug/L) from each scenario. Each x-axis concentration results from one scenario. In this regard, the absolute concentration values on the x axis are not determinative because they are dependent on the values that OPP chose for the application rate; OPP could have chosen any application rate for the simulations as long as the same rate was used in every simulation. This is because pesticide concentrations in the waterbody are proportional to the amount of pesticide application rate. The estimated concentrations are important only for determining the relative order of the scenarios.

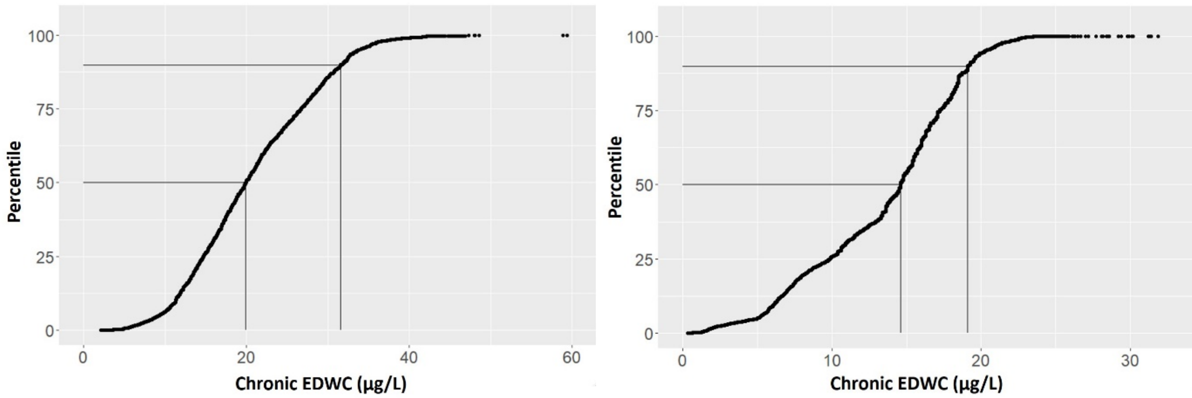

Figure 7. Distribution of chronic concentrations for Region 7 for corn and wheat, respectively, with K_{oc} of 10 mL/g.

5.2. Sensitivity of the Scenario Distributions

To explore the sensitivity of the results (as indicated by the slope of the curves), OPP calculated the ratio of the 90th percentile EDWC ($EDWC_{90}$) to the 50th percentile EDWC ($EDWC_{50}$) for the HUC2 regions for corn, as shown in Table 2. This ratio ($EDWC_{90}/EDWC_{50}$) has a practical meaning to a risk assessment as it represents how much the EDWCs could vary between scenarios. In other words, the primary purpose of these 90/50 ratios is to give risk assessors a quick idea of how much the EDWCs would vary if they chose a 90th percentile scenario instead of a 50th percentile scenario.

Table 2. Ratios of the 90th EDWC to the 50th EDWC for Corn in all cases examined

HUC2	K_{oc} (mL/g)	Acute 90th: 50th EDWC	Chronic 90th: 50th EDWC	Cancer 90th: 50th EDWC
r01	10	2.04	1.64	1.73
	1000	1.35	1.25	1.21
	10000	1.19	1.20	1.20
r02	10	2.47	1.90	2.20
	1000	1.56	1.29	1.35
	10000	1.45	1.51	1.51
r03N	10	2.39	1.75	2.02
	1000	1.60	1.33	1.35
	10000	1.48	1.38	1.38
r03S	10	2.71	1.87	1.97
	1000	1.70	1.37	1.64
	10000	1.47	1.29	1.27
r03W	10	2.89	2.26	2.58
	1000	1.64	1.34	1.38
	10000	1.50	1.54	1.46
r04	10	1.72	1.54	1.61
	1000	1.54	1.39	1.42
	10000	1.38	1.31	1.40
r05	10	1.60	1.54	1.63
	1000	1.42	1.29	1.34

HUC2	K_{oc} (mL/g)	Acute 90th: 50th EDWC	Chronic 90th: 50th EDWC	Cancer 90th: 50th EDWC
	10000	1.34	1.18	1.20
r06	10	2.11	1.59	1.79
	1000	1.78	1.40	1.44
	10000	1.46	1.48	1.60
r07	10	1.55	1.59	1.62
	1000	1.31	1.20	1.20
	10000	1.53	1.51	1.52
r08	10	1.89	1.69	1.84
	1000	1.40	1.25	1.35
	10000	1.36	1.23	1.22
r09	10	1.41	1.41	1.35
	1000	1.22	1.19	1.16
	10000	1.37	1.33	1.38
r10L	10	1.43	1.39	1.40
	1000	1.26	1.33	1.38
	10000	1.25	1.29	1.29
r10U	10	1.45	1.39	1.37
	1000	1.27	1.23	1.21
	10000	1.50	1.55	1.59
r11	10	1.86	1.59	1.47
	1000	1.29	1.52	1.53
	10000	1.28	1.30	1.25
r12	10	1.82	1.63	1.73
	1000	1.31	1.34	1.37
	10000	1.31	1.50	1.37
r13	10	1.81	1.67	1.83
	1000	1.55	1.53	1.55
	10000	2.03	1.58	1.93
r14	10	2.97	2.80	2.50
	1000	1.92	1.89	1.66
	10000	2.50	2.41	2.54
r15	10	2.79	2.83	3.05
	1000	1.36	1.36	1.36
	10000	1.65	1.58	1.57
r16	10	3.58	3.19	2.80
	1000	1.56	1.59	1.52
	10000	1.46	1.48	1.51
r17	10	3.91	3.86	4.30
	1000	1.58	1.65	1.81
	10000	2.53	2.77	2.98
r18	10	2.16	1.97	2.23
	1000	1.40	1.37	1.38
	10000	1.68	1.69	1.78

As a general trend, 90:50 ratios were higher and more variable for a K_{oc} of 10 mL/g across all regions and all exposure endpoints (acute, chronic, and cancer concentrations). The reason for the variation is not clear, but it could imply that runoff is more variable than erosion (since low-K_{oc} chemical are transported by runoff and high-K_{oc} chemicals are transported by erosion).

Generally, the higher K_{oc} classes (i.e., 1000 and 10000 mL/g) produced lower ratio values. HUC2 Region 17 consistently returns higher ratios across K_{oc} classes and exposure endpoints than most other regions. Further, Region 17 returns 90th percentile EDWC values for the 10 mL/g Koc class that are approximately 4 times greater than those estimated at the 50th percentile for all exposure endpoints, suggesting this region has greater variation in scenario characteristics.

5.3. Scenario Differences for Acute, Chronic and Cancer

Another consideration is whether there will be a need for separate scenarios to address acute, chronic and cancer assessments, or if scenarios for a single exposure endpoint would suffice. OPP performed an initial assessment of this with the results given in Table 3. In this example, OPP used the 90th percentile EDWC as the target scenario ranking. The first row gives the scenario with the closest ranking to the 90th percentile acute value; its corresponding ranking for chronic and cancer is slightly lower at 89th and 85th percentile, respectively. In a similar way, row 2 provides information for the scenario with the closest ranking to the 90th percentile chronic value and row 3 for the cancer value. The table demonstrates that the values are within 10% of each other regardless of the exposure endpoint. It is possible that such differences may not be determinative for risk assessments. This may ultimately reduce the number of necessary scenarios, but OPP needs to explore this further.

Table 3. Consideration for separate Acute, Chronic and Cancer Scenarios, for Region 7, K_{oc} = 10 mL/g

Target	Scenario	Acute Percentile	Chronic Percentile	Cancer Percentile
Acute	539W21130LC1	90	89	85
Chronic	542W22075LC1	95	90	99
Cancer	402164W20187LC1	96	90	90

5.4. Comparison with current scenarios

OPP currently has 13 field scenarios representing corn across the U.S. As previously mentioned, OPP constructed these using best professional judgement to produce “high-end” scenarios for a variety of assessment types (aquatic species, human health, cumulative risk assessments, etc.), but their actual vulnerability is unknown. OPP can use the same ranking scheme that we used for the new scenarios to obtain a quantitative ranking for the old scenarios. In this way, OPP can better assess the impact that the new scenarios would have on a risk assessment by comparing the old and new ranks.

For the comparison, OPP ran new and existing scenarios in the same HUC2 region with identical chemical inputs. OPP then compared the existing and new scenario concentrations for acute (1-day), chronic (1-year), and cancer endpoints. The rankings appear in Table 4.

Results show that the concentration for the existing PA corn scenario (first row) would rank as a 98.5th percentile scenario with the new ranking system (for acute concentrations and a K_{oc} of 10 mL/g). The PA corn scenario would rank higher than a 99.9th percentile scenario for acute concentrations and a chemical with a K_{oc} of 10000 mL/g. Further investigation is required, but these initial findings indicate the existing scenarios may in fact be "high-end scenarios" according to the new proposed ranking criteria.

At the low K_{oc} (10 mL/g), acute concentrations for 10 of the 13 existing PWC scenarios fell above the 95th percentile rankings for their specific regions. Only one scenario – Iowa Corn – fell below the 90th percentile ranking. For chronic and cancer, 7 of the 13 existing scenarios fell above the 95th percentile rankings for their specific regions. The percentile rankings for the existing scenarios ranged from the 69th to >99.9th percentile for chronic concentrations and from the 60th to >99.9th percentile for cancer concentrations. At the intermediate K_{oc} (1000 mL/g), the existing scenarios showed a wider range in percentile rankings (from 57th to >99.9th percentile) for acute concentrations than at the other two K_{oc} classes. For longer-duration exposures, the existing scenario rankings fall within the 83rd to >99.9th percentile in regional rankings. At the highest K_{oc} (10,000 ml/g), the estimated concentrations from all the old scenarios were around the 97th percentile ranking within their respective regions.

Table 4. Estimated percentile rankings for existing PWC scenarios by K_{oc}

		K_{oc} = 10 mL/g			K_{oc} = 1,000 mL/g			K_{oc} = 10,000 mL/g		
Current PWC Scenario	**NHD + Reg**	**Acute**	**Chron**	**Canc**	**Acute**	**Chron**	**Canc**	**Acute**	**Chron**	**Canc**
PA Corn	R02	98.5	96.2	94.1	99.2	>99.9	>99.9	>99.9	>99.9	>99.9
NC (east) Corn	R03N	95.6	97.7	99.2	99.3	>99.9	>99.9	>99.9	>99.9	>99.9
IN Corn	R05	90.0	68.7	82.1	99.7	96.7	96.8	>99.9	>99.9	>99.9
OH Corn	R05	>99.9	99.8	99.8	98.1	>99.9	>99.9	>99.9	>99.9	>99.9
IA Corn	R07	85.0	76.6	59.6	78.8	87.6	83.2	99.9	99.9	99.9
IL Corn	R07	99.2	76.2	84.0	93.1	98.9	>99.9	>99.9	99.9	>99.9
MN Corn	R07	99.3	84.5	95.5	98.5	>99.9	99.9	99.5	99.7	99.2
MS Corn	R08	99.9	99.7	99.0	57.9	>99.9	>99.9	>99.9	>99.9	>99.9
ND Corn	R09	97.9	93.5	99.1	96.7	93.4	96.9	99.4	99.2	99.4
KS Corn	R10L	>99.9	98.4	99.5	>99.9	88.9	>99.9	99.9	>99.9	>99.9
NE Corn	R10L	99.0	73.7	91.5	99.9	92.0	90.9	>99.9	>99.9	>99.9
TX (south) Corn	R12	>99.9	>99.9	>99.9	>99.9	99.8	99.4	96.8	>99.9	>99.9
TX Corn	R12	93.2	99.7	76.6	57.0	92.7	94.7	>99.9	>99.9	>99.9

6. Summary

OPP developed methods to create a comprehensive set of new PWC scenarios and quantitatively ranked them by their resulting surface water concentrations (EDWCs). Importantly, and unlike previous OPP scenario-creation efforts, these new scenarios comprise parameters that are biased neither up nor down and are consistent and transparent. OPP then ranked these scenarios according to their resultant surface water concentrations.

A scenario's ranking depends not only on the environmental properties captured in the field scenario but also on the chemical applied (namely the K_{oc} value) as well as the endpoint desired (acute, chronic, cancer). The PWC's dual mechanisms of transport, in which runoff and erosion compete to carry dissolved and sorbed pesticide, causes a scenario's rank to be dependent on chemical sorption. Rank dependence on endpoint is likely due in part to application timing issues and weather variations, although this is not fully understood. OPP intends to explore these issues further after review of additional results.

Using this new approach, OPP developed scenario distributions for corn and wheat. These demonstrate that corn and wheat have similar scenario distributions with a relatively small range in EDWCs within percentile ranks in the central region of the distribution. Preliminary review indicates that EDWCs at the 90th percentile are rarely greater than 2 times the 50th percentile value for any K_{oc} or endpoint examined for corn and wheat. The relatively small difference in concentration change for a relatively large change in rank (percentile) means that EDWCs estimated from the PWC in any one HUC2 region will generally vary within a factor of 2 or less in most cases regardless of the percentile rank of the scenario.

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