
A national probabilistic characterization of local crop proximity and density for refining US screening level exposure estimates of pesticides in surface water arising from agricultural use

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Abstract

Rising world population and changing diets are increasing the need for efficient and effective food and fiber production. Pesticides are used across the US to control pests and improve food yield and quality, but these benefits are offset by their potential to reach and possibly impact aquatic or terrestrial ecosystems. Regulatory agencies rely on prospective exposure models that often start with conservative simplifying assumptions that are refined with additional information if needed. The USEPA ecological risk assessment framework for pesticides assumes, at screening level, that 100% of the area draining to a water body is cropped. However, at the grower's real-world scale, this simplifying assumption is generally not realistic and should be refined for higher tier assessment. The present study developed a US-wide spatially explicit analysis of crop density and proximity to surface waters to characterize the potential for pyrethroid insecticides to enter flowing surface waters. Reliable, transparent, and publicly available government spatial cropping and hydrology datasets were employed at the catchment-scale across the full extent of agricultural production in the US were used to generate fifteen novel crop-specific probabilistic distributions describing the extent and proximity of each crop to the flowing water body defining small catchments. These were used to refine estimated environmental concentrations using USEPA standard regulatory scenarios to evaluate the importance of considering agricultural landscapes when refining aquatic pesticide concentrations. Incorporating these real-world probabilities of crop occurrence and proximity showed that, while potential maximal aquatic exposure concentrations are unchanged, the probability of exceeding regulatory decision-making concentration endpoints is much lower than predicted by standard assumptions (e.g., 1.9 to ~50-fold reductions by crop for 90% of catchments). Additionally, we show that the relative ranking of crops by their aquatic pesticide exposure potential may change from that indicated when cropping density and proximity are considered.

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Abbreviations: Catchment Agronomic Distributional Analysis (CADA); Cropland Data Layer (CDL); Crop of Interest; (CoI); Estimated Environmental Concentration (EEC), Federal Insecticide, Fungicide and Rodenticide Act (FIFRA); Geographic Information Systems (GIS); Hydrologic Unit Code (HUC); Multiplier Factor (MF);, National Agricultural Statistics Service (NASS); National Hydrography Dataset Plus (NHD+); Percent Crop Area (PCA); Pesticide Root Zone Model (PRZM); Proximity Zone (PZ); United States (US); US Department of Agriculture (USDA);,US Environmental Protection Agency (USEPA); Vegetated Filter Strip (VFS).

Introduction

With a world population expected to reach over nine billion by 2050 [41], an increasing proportion of people rising out of poverty [70] and assuming a wider-ranging diet [16], the capability to increase agricultural output from the same land area while maintaining human and ecological safety and environmental quality is increasingly critical [9]. The US produces and exports more agricultural products than any other country in the world [9]. In order to maintain or improve on current yields, efficiency must be increased while competition and damage from pests needs to be minimized. For example, to manage pest pressures, many growers employ a suite of options for the control of insects, weeds, fungi, and other damaging pests via Integrated Pest Management programs that utilize a range of chemical, biological, mechanical, and agronomic technologies to protect crops [20].

Pyrethroids are a class of synthetic chemicals similar in mode of action to pyrethrins (sodium channel modulators, subgroup 3A) [22] that are naturally found in the flowers of pyrethrums (e.g., chrysanthemum). Pyrethroids effectively

control a wide variety of insects and are registered for use on an extensive range of agricultural crops across the US and worldwide. They are of critical importance for US agricultural production [52, 57] and have been used for more than 45 years to support food and fiber production in the US [1, 2]. In addition, pyrethroids are becoming even more important as some currently used insecticides are being restricted or removed from the market [55].

Countries around the world have implemented regulatory frameworks to ensure that new and existing active ingredients can be used safely. For example, the US Environmental Protection Agency (USEPA) is mandated by the Federal Insecticide, Fungicide and Rodenticide Act (FIFRA) to assess new, and periodically re-assess existing uses of pesticides to ensure there are no adverse ecological impacts because of pesticide usage described by the label. The ecological element of this risk assessment process utilizes a tiered approach that incorporates highly conservative assumptions at lower (or screening) levels with increasing realism (and complexity) being incorporated during refinement where needed. If an active ingredient passes the

lower, more conservative, screening, it is considered not to cause adverse ecological effects. Failing a screening tier necessitates additional problem formulation and data generation [52, 63] for evaluation in a refined assessment.

For pesticide aquatic exposure modeling, the USEPA utilizes a set of 125 well established crop-specific scenarios that provide crop- and location-specific weather, soil, and cropping data intended to estimate a “reasonable worst case” aquatic ecosystem exposure [45]. For aquatic exposure assessments, the weather and soil parameterization are based on actual data (e.g., 30 years of site-specific daily weather) for a particular scenario location, while the characterization of the area contributing runoff/erosion to the receiving water body is assumed to be 100% cropped with the crop of interest and 100% treated (with the maximum pesticide application rate and number of applications allowed on the label with the minimum application interval). While this “100% cropped” assumption may be suitable for screening, if we are to refine the problem formulation it should incorporate the real-world variability in cropping density and proximity.

Spatial methodologies have been used for over 20 years to characterize landscapes in order to investigate potential environmental pesticide exposure to soil and surface water from drift and runoff based on proximity, soils, weather and cropping in the US [18, 24, 69], Europe [10, 30, 32, 40] and elsewhere [33]. These methodologies utilize Geographic Information Systems (GIS) to spatially combine potential pesticide use

areas based on land use information (e.g., cropped fields) with locations of non-target environments such as nearby surface water or terrestrial locations. The resulting modeled or measured variability of exposure potential across a landscape allows regulatory screening scenarios to be placed into context opposite cropping and usage patterns across wider scales. These have varied from local [36, 67], to regional [15, 35], to global [12, 21] scales. The work presented in this study incorporates a national framework of cropping density and proximity to surface water with a novel method applied to standard USEPA exposure scenario approaches in the US FIFRA pesticide regulatory framework.

A well-established approach for refined pesticide exposure and effects assessment is known as Probabilistic Ecological Risk Assessment. This has been explored in programs such as ECOFRAM [53], EUPRA [17], and WEBFRAM [11]. Probabilistic risk assessment approaches for pesticide risk assessment have been demonstrated by Solomon (2000) and Verdonck (2002) [37, 66]. The underlying concept is that due to actual field variation in exposure potential, organism sensitivity, and ecosystem responses, there are no absolutes in risk assessment. Instead, the probability of exceeding a given concentration or level of effect can be estimated by understanding the distributions of observed values for key parameters in the assessment. In a probabilistic refinement of a risk assessment, the fixed conservative inputs in screening assessments may be replaced by a combination of distributions of inputs. In this study, we set out to measure nationwide or

regional distributions of cropping intensities around receiving waters that can be used to refine the screening level assumption that water bodies are 100% surrounded by a crop(s) of interest hereafter referred to as CoI.

Thus, the primary objective of the present study was to utilize available spatial data on crop location, surface water location, and contributing land area to characterize the variability (i.e., distribution) in cropped areas within proximity to surface water that may contribute pesticide loadings. This will allow us to understand the frequency at which 100% cropping of a CoI adjacent to a water body occurs. Then to estimate crop-specific probabilities of potential aquatic exposure as it relates to cropping density and proximity in the exposure models. Since nationally consistent and geographically specific data are publicly available from US government agencies for the entire country at high spatial resolution, detailed and accurate assessments are now feasible. For this study, we used the nationally available and annually updated Cropland Data Layer (CDL) from US Department of Agriculture [43] and the National Hydrography Dataset Plus (NHD+) from US Geologic Survey and USEPA [64] to develop national and regional scale spatially explicit analyses of crop density and proximity to surface waters. The NHD+ scale of the analyses is highly relevant for farm scale operations and the resulting data for each crop have been examined on a probability of occurrence basis to produce derived datasets characterizing US cropping patterns. The NHD+ dataset is already used extensively by US government agencies to address water quality questions (discussed in Methods and Materials section). The national

or regional distribution of cropping density (or Percent Crop Area, PCA) values for each crop was applied to the standard 30 years of modeled Estimated Environmental Concentrations (EECs) using a probabilistic approach to place the 100% cropping assumption into a real-world context for aquatic ecological risk assessment. This concept was discussed during the ECOFRAM process (53) and applied to landscape-level ecological risk assessment [18]. More recently, USEPA have applied PCA-based EEC refinements to drinking water assessments [48, 57], but it has not yet been acknowledged as a regulatory approach for ecological aquatic risk assessments.

It is important to point out that these crop-specific proximity data are novel and, to the best of our knowledge, reflect a unique resource that also has application in considering crop-specific interactions in riparian border areas, mitigating potential nutrient and sediment transport at the catchment (i.e., farming operation) scale, or integrated for use at progressively larger hydrologic scales. For example, the crop-specific catchment PCA data generated in this study were combined with spatial data on soils and weather and used in a national examination to place the USEPA scenarios into a national context of catchment-scale off-field transport of pyrethroid mass [35].

Methods and Materials

Spatial Unit of Analysis

NHD+ is a suite of geospatial products developed by the USEPA, the U.S. Geological Survey, and Horizon Systems Corporation that builds on and extends the capabilities of the National Hydrography

Dataset (NHD) by integrating the NHD with the National Elevation Dataset and the Watershed Boundary Dataset. To provide the greatest flexibility for the results of the current assessment, the NHD+ framework of hydrologically connected catchments were used as the base spatial unit. The entire set (or a subset) of catchments can be used as a population from which to generate distributions of relevant metrics. The NHD+ data are government defined and are being used for various regulatory frameworks. This includes WATERS [50], USEPA Clean Watersheds Needs Survey [48], National Pollutant Discharge Elimination System [46] the USEPA Office of Water 303(d) list of impaired waters [62], and perhaps most notably USEPA's StreamCat dataset which contains over 600 water quality, biological condition, and watershed integrity metrics linked to NHD+ catchments [19] NHD+ are also used in National Rivers and Streams Assessment [27] and the National Lakes Assessment [51] as part of the USEPA National Aquatic Resource Surveys program. See [EPA Website](#) for a comprehensive list of over 150 government and private applications utilizing the NHD+. NHD+ contains a realistic representation of hydrologic pathways and spatially referenced attributes useful for landscape modeling [5] including elevation derived catchments and flow paths developed via a robust method evaluation process [23].

Data in the NHD+ framework are highly detailed spatially, although some limitations do exist. For example, the flowlines and catchments are derived from a contiguous and nationally consistent elevation dataset. However, in areas of little

elevation variation the flow direction could not be determined for some flowlines, and hence catchments could not be defined. While these flowlines were retained in the NHD+ dataset they were embedded as part of a larger catchment defined by a flowline in which the flow direction could be determined. This often occurred for engineered irrigation and drainage networks however this was not always limited to these 'canal/ditch' features. Usage of flowline-specific attribute information (e.g., estimated flow rates, velocity, etc) should be used with consideration after consultation of the NHD+ documentation [63]. However, we did not use specific flowline/catchment attributes beyond the feature type (FTYPE and FCODE, see Table S5 in Supplemental Information) and based our analysis on the spatial delineation only.

We selected the NHD+ catchments as the spatial unit of landscape analysis. This selection was due to the large number of catchments (over 2.5 million), of which each has a single flowing water body (either stream/river feature types or canal/ditch features where flow direction could be determined), where the outflow at the catchment outlet reflects the direct runoff from the entire catchment. These data account for the entire US land area and comprise a range of very small units highly relevant to farming practices at the local scale. Based on the 2.2 million catchments containing cultivated cropland across the US in 2011 [4] 90% are 650 ha (~1600 acres) or smaller and 50% are smaller than 160 ha (395 acres). To provide context, the average farm size in 2019 across the US was approximately 180 ha (444 acres) with state-level averages

ranging from 22 ha (55 acres) to 980 ha (2417 acres) across the individual 50 states [44].

These NHD+ catchments, with a median size of 160 ha (395 acres), reflect the scale of many typical farming operations and show the drainage areas that deliver to headwater streams and larger flowing water bodies. See Table S1 in the Supplemental Information (SI) for more details on size distribution of the NHD+ catchments. This is an effective surrogate based on actual data for the standard USEPA local agriculture representation of a square 10-ha area delivering runoff and drift to a 1-ha square pond. While ponds and small flowing waters are different ecological settings, flowing waters have a special significance for several reasons. Firstly, they form a connected network that serves as a fundamental element of the hydrological cycle and drains most of the land in the US. Secondly, measurements made on cropping intensity in the areas surrounding streams include many ponds and their surrounds and cover such wide extents that they are equally relevant to understanding pond drainage areas as they are for stream drainage areas. Thirdly, small streams are at least as sensitive to impacts by anthropogenic chemicals as ponds [25, 34, 68] and chemicals entering streams may eventually be transported to many other locations and larger water bodies (i.e., ponds only drain small areas of the US and are independent units). Finally, our intent was to use well-accepted government datasets, and such spatial data defining the drainage area for static water bodies did not exist (as it did for flowing waters). Even if it did, the drainage area limited to ponds and static water bodies would represent only a subset of

the total agricultural area in production. The subset of 2.2 million agricultural catchments that contained cultivated cropland as defined by USDA NASS [4], contained all agricultural land in the US, and formed the pool of catchments for this analysis. This ensured that catchments with no agriculture were excluded from the analysis as this might have biased the findings toward low density agriculture catchments.

An efficient methodology to process the more than two million catchments and their stream reaches was needed to implement proximity zones nationally within a GIS. Therefore, the proximity processing was performed in a raster rather than vector GIS environment. The source NHD+ flowing water features, originally supplied as lines and polygons, were converted to a raster dataset with a 10m resolution. This resolution was chosen as a compromise between the level of spatial accuracy of the original lines and as an even divisor of the source 30m pixel resolution of the CDL (described in the next section). More details are provided in the SI.

Crop Type and Location

Crop location information was obtained from the national USDA National Agricultural Statistics Service (NASS) CDL products that consist of digital raster data layers of 30m pixels with specific crop type information suitable for use in a GIS [42]. These data are generally agreed to be the best available data on agricultural cropping location and are used for FIFRA ecological risk assessments [14, 58], the development of a spatial aquatic model (SAM) for pesticide assessments [49], pesticide drinking water

human health risk assessments [48, 59] and national-scale endangered species assessments for pesticides [56, 59, 65] The CDL contains over 50 crop classes in the output dataset. For this study, these were grouped into CoI that represent crops with high pyrethroid use [13] or high potential for pyrethroid aquatic exposure [7, 57]. The CoI are alfalfa, almond, citrus, corn, cotton, grass seed, lettuce, peanut, pecan, pepper, potato, soybean, sunflower, sweet corn, and wheat. CoI areas were analyzed for the latest five years (2008-2012) of data available in mid-2013 when this study commenced. A separate 5-year composite layer was also created for each CoI such that if any pixel was classified as that CoI during the five-year period, the composite layer would classify it as that CoI. In this way, the composite layer represents all areas that have ever been classified as a particular CoI during the five-year period. This ensures proper accounting for areas where crops are rotated or where the CDL has less accuracy for a single year [56]. This is comparable to the approach used by the USEPA to identify pesticide use sites (i.e., Use Data Layers) for endangered species assessments [60] although the crop years included in the 5-year composite differ. A detailed analysis of 2012 USDA Census of Agriculture [1] was used to confirm that the CDL from our selected states represented a nationally significant occurrence of CoI for our analysis (see Supplemental Information).

CDL data were resampled from 30m to 10m pixel resolution to conform to the resolution of the raster representation of NHD+ stream segments used in evaluating crop proximity (discussed in the next section). Resampling the data from one

resolution to another involves assigning a pixel value in the output grid (the new resolution of 10 meters) based on the closest (i.e., “nearest neighbor”) pixel from the input grid (30 meters). Exactly nine 10m output pixels are produced, each with the same value as the single 30m input pixel. Details of the CDL crop groups, evaluation of CDL and census crop acreage data, and spatial processing are supplied in the Supplemental Information.

Crop Proximity to Surface Water

Because the transport of pyrethroids to surface water by drift or runoff is heavily influenced by proximity, several “proximity zones” (PZs) were implemented for which further metrics were characterized. We made the working assumption that the application area in an NHD+ catchment that might potentially contribute a significant fraction of pyrethroid loading to a receiving water is the 200-m proximity zone adjacent to both sides of the stream. Pyrethroid loading contributed by crop farther than 200m was considered much less impactful related to pesticide loadings and our analysis attempted to emphasize the impact of the most critical runoff and drift delivery areas. These notional areas around each stream reach were further divided into smaller PZs defined to represent some of the application restrictions on pyrethroid labels and allowed more detailed analyses as needed. A 0-10m PZ approximates the 25ft (7.6m) label buffer drift setback distance for ground applications of pyrethroids, while a 10-50m PZ reflects the minimum 150ft (45.7m) label requirement for a drift setback distance for aerial applications of pyrethroids. The 50-

200m (164 to 656 ft) PZ includes the remaining land area included in this proximity analysis. To reduce complexity and align with the standard screening assumption that all pesticide applications are aerially applied when allowed by the label, the 10- 50m and 50- 200m PZs were combined into a single 10- 200m PZ for the detailed analyses reported in this paper. Additional details of proximity zone GIS processing are supplied in the Supplemental Information.

Resampled crop location data from the CDL (at 10m resolution) were combined with the PZs using an overlay operation characterizing each PZ according to the percentage of its area that is composed of each CoI (i.e., the PCA). Figure 1 illustrates the NHD+ catchment (red outline) and stream (blue) with 10- 200m PZ extent (blue shaded area) overlaid with the CoI (cotton in orange). This figure shows a typical size NHD headwater catchment (651 ha, 1600 acres) and by comparison with the distinct field boundaries, it provides a good visual representation for how the NHD+ catchment scale is relevant to understanding farm scale operations.

Baseline Scenarios Based on USEPA Screening Exposure Scenarios

USEPA has designed >100 “scenarios” for the Pesticide Root Zone Model (PRZM, Suarez 2005) that are intended to represent crop-specific

landscape conditions vulnerable to chemical transport to aquatic ecosystems due to runoff and erosion. These scenarios simulate a typical soil and slope associated with the CoI in a particular region, using locally appropriate cropping parameters (e.g., emergence, harvest, rooting depth, etc.), and a weather station most relevant to the soil/crop location. Using a single representative pyrethroid [14, 18] scenarios covering 15 CoIs were modeled at a field scale using daily weather data for 30 years. Off-field runoff/erosion transport was routed onto the label-mandated 10-ft vegetated filter strip (VFS) (which has since been increased to 15/25 ft [55] d modeled using VFSMOD [26]. Water, chemical and sediment coming out of the VFS entered into the receiving water body and the AGRO-2014 model [29] was used to generate daily aquatic EECs. Additionally, the AgDRIFT[®] model (version 2.1.1) [39] was used to estimate off-target spray drift deposition into the water body after applying specific label no-spray buffer distances for ground, airblast, or aerial applications. Standard USEPA screening scenarios do not include modeling of a VFS; therefore, while the presented modeling matches the standard USEPA scenario approaches in most other aspects (see Modified modeling approach section in the SI), we are differentiating resultant EECs using the term “baseline” within this paper. See further information on exposure modeling in the Supplemental Information.

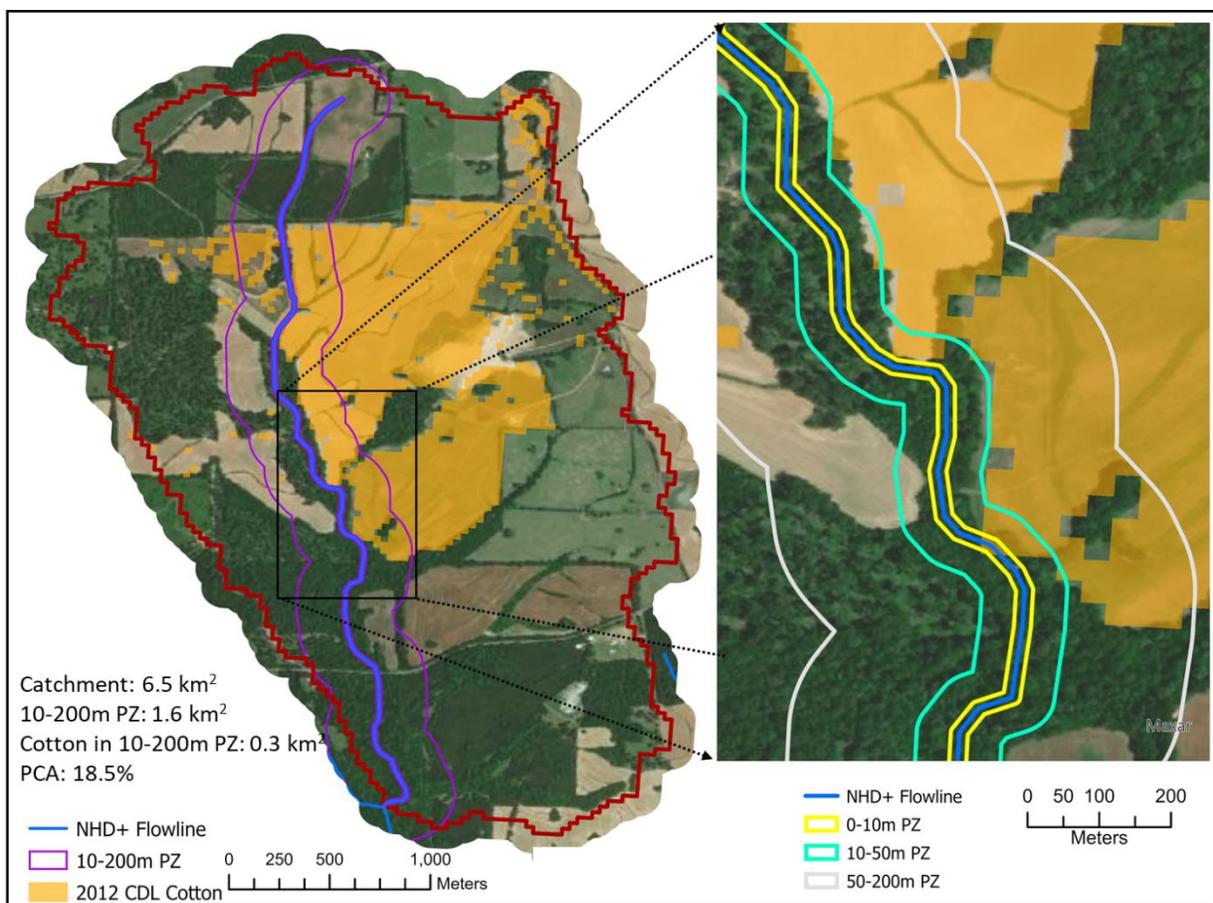


Figure 1. Example headwater catchment (outlined in red) showing NHD+ stream and 10-200m proximity zone (PZ) overlaid with 2012 CDL cotton (orange) to generate percent crop area (PCA). The inset also shows the three detailed PZs utilized for this study.

Catchment Agronomic Distributional Analysis (CADA)

In the present study, spatial analyses of cropping density and proximity were conducted with the resulting distributions used to provide probabilistic context for USEPA standard screening model assumptions. The selected CoIs comprised the vast majority of uses that are labeled for treatment by one or more pyrethroid active ingredients. Thus, the measured real-world crop occurrence data are highly relevant to

include in a probabilistic refinement of potential aquatic exposures.

From an exposure assessment perspective, an important driver of potential aquatic exposure is the cropping intensity in a watershed, quantified as PCA. Thus, the underlying assumption for this analysis is that the drift and runoff/erosion reaching the water body is proportional to the area cropped (i.e., PCA) since we assume all of the crop is treated. To simplify the analysis and remain congruent with the screening assumption that the 10-ha area delivers

runoff uniformly, we assumed that the distance from the stream reach was not a major variable (i.e., that transport is independent of the position of the crop in the catchment). However, it should be noted that the PCA data generated for the individual smaller PZs (i.e., 10-50m and 50-200m areas) would support this more sophisticated analysis. Thus, the crop specific PCA distributions provide a simple metric to characterize the landscapes where each CoI is grown.

In our Catchment Agronomic Distributional Analysis (CADA), we examined the effects of the real-world distribution of PCA values in the 10-200m PZ on runoff/erosion and drift entry on exposure modeling EECs in place of the 100% cropped assumption. These CADA analyses were conducted using relevant USEPA standard model scenarios to provide a combination of soil erodibility, slope, and weather data corresponding to each crop type examined.

The CADA calculations are based on the concept of estimating the range of exposures that might be expected if the USEPA model scenario was run many times to simulate the measured distribution of individual catchment PCAs. Because of the way that the USEPA scenario models behave, this conceptually means that the data from the baseline scenarios can be reused by simply multiplying the originally predicted EECs by the PCA fraction for every cropped catchment to create a distribution. This approach has been used by USEPA for pesticide drinking water risk

assessments where the entire area draining to a reservoir is not cropped [59].

To simplify this, we developed an approach that would divide the ranked distribution into “lumped” PCA groups. With crop-specific PCA distributions numbering tens or hundreds of thousands (Table 1), calculations using the entire set of catchments were not necessary, and a simplified sampling of the distribution was sufficient to describe the variability in the PCA data. To represent the complete PCA distributions in a reasonable number of calculations, each ranked crop distribution was divided into 10 non-uniform groups designed to provide optimum differentiation of the higher vulnerability catchments. To provide more granularity at the upper end of the PCA range where PCA is greatest, as a simplifying conservative assumption the catchments were divided into groups based on their PCA ranking in approximately geometric increments (0-25, 25.1-50, 50.1-75, 75.1-87.5, 87.6-90, 90.1-93, 93.1-96, 96.1-98, 98.1-99, 99.1-100%). The highest CoI catchment PCA value in a group was used to represent all catchments in that group to ensure that substantial conservatism was retained in the analysis (e.g., the 0-25% group was modeled using the PCA in the 25th percentile catchment, the 99.1-100% group using the PCA measured in the 100th percentile catchment).

The crop-specific baseline maximum annual EEC for each year of the analysis (n=30, Figure 2A) was multiplied by the maximum crop-specific PCA (as a fraction) for each group of PCAs (n=10, Figure 2B). This produced what are effectively 300

“simulated years” of annual EECs that reflect the range of crop-specific PCAs measured across the region or nationwide (Table 1). Each EEC/PCA combination has a probability of occurrence across the 300 “simulated years” that reflects both the likelihood of the year occurring (1 in 30) as well as the fraction of the PCA distribution that each PCA group represents (e.g., 1 in 100 for the 99.1-100% group or 25 in 100 for the 0-25% PCA group). The two probabilities must be combined to estimate the overall probability of occurrence of each of the 300 “simulated years” of annual EECs (Figure 2C); for example, an annual maximum EEC (1-in-30 years) in the 99.1 - 100th percentile PCA group (i.e., 1% probability of occurring) has an occurrence probability of 1/30 (3.3%) multiplied by 1/100 (1%) = 0.0003. Likewise, one of the 30 annual maxima EECs in the 0-25th percentile PCA group has an occurrence probability of 1/30 (3.3%) multiplied by 25/100 (25%) = 0.0083. The baseline EECs were ranked from high to low and each year rank baseline EEC was multiplied by 10 PCA values to compute 300 CADA EECs. The CADA EECs for the 300 simulated years were ranked from high to low and the cumulative occurrence probability of each CADA EEC was calculated and plotted (Figure 2C and Table S7 in Supplemental Information).

Assessing Influence of CADA PCA Results on Baseline Scenarios

To assess the influence of the CADA refinement on the baseline scenarios, we compared the 90th and 50th percentile EECs of the baseline model outputs with the corresponding 300 water-body-year CADA EEC 90th and 50th percentiles, respectively. The resulting multiplier factors (MF) report the factor by which each CADA EEC must be multiplied to match the corresponding baseline EEC and are calculated as:

$$\text{Multiplier Factor (MF)} = \frac{\text{Baseline 90th or 50th \%ile EEC}}{\text{90th or 50th \%ile CADA EEC}}$$

For example, an MF of 2 indicates that the CADA EEC incorporating PCA must be multiplied by a factor of 2 to equal the EEC from the baseline scenario.

Results

Crop specific spatial and temporal scope for each CoI

For each CoI (Table 1) provides the spatial scope of the assessment, the year(s) of CDL data used along with the number of acres, and the total number of NHD+ catchments modeled in the study. The total number of NHD+ catchments examined per crop ranged from 3,102 (vegetables/ground fruit in FL) to over 750,000 (corn in entire US). Thus, the number of catchments for even the CoI with the smallest sample size is still suitably large to support distributional analysis.

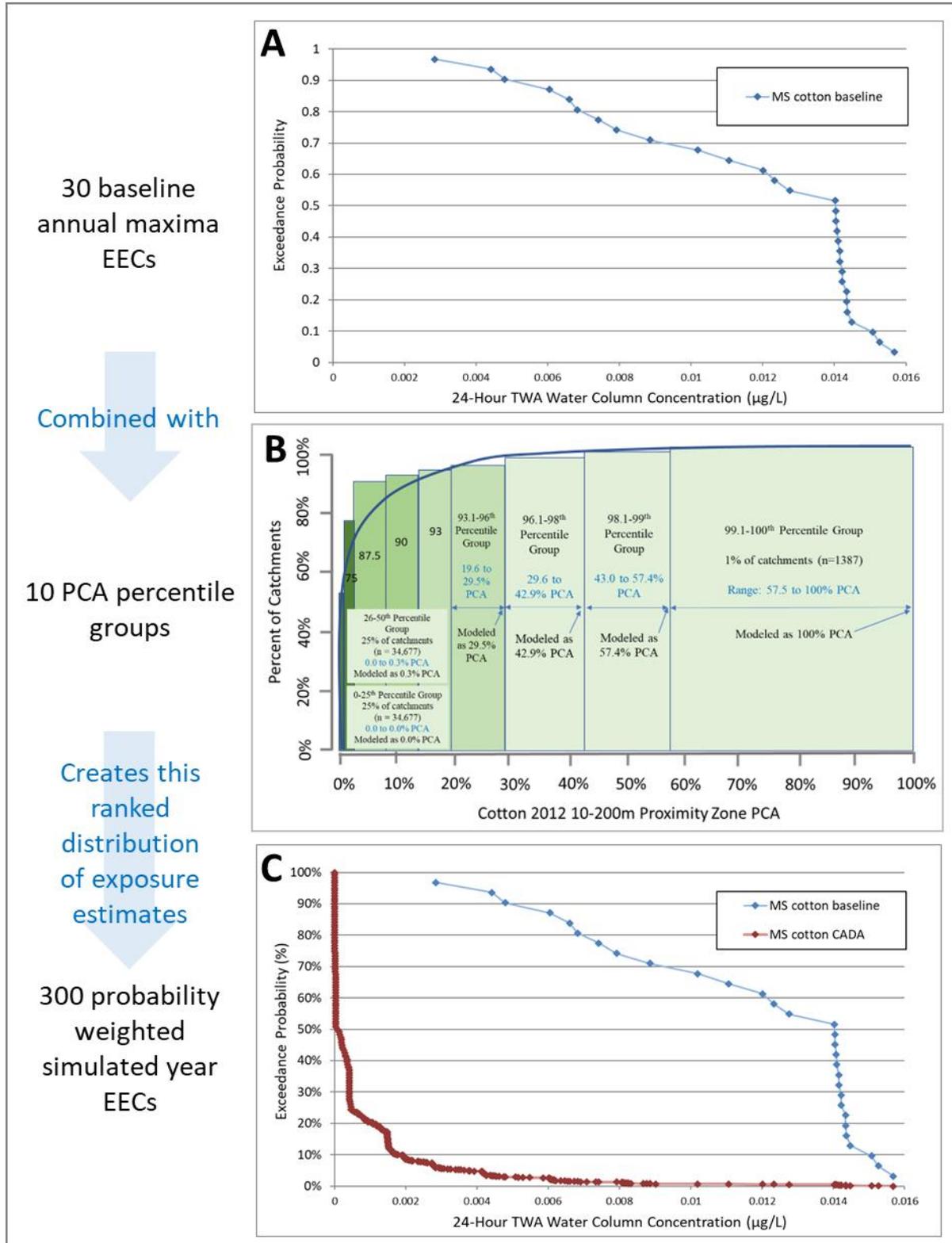


Figure 2. Schematic of the CADA approach combining 30 years of annual maxima EECs from baseline scenario modeling (A) with PCA distribution and probabilities (B) to create CADA distribution of 300 probability weighted simulated year EECs (C). For larger versions of (B) and (C), see Figures 3 and 4, respectively.

Representativeness of Spatial Extent for Each CoI

To verify that the spatial analysis using the CDL data (prior to estimating crop occurrence in the PZs) was producing reasonable estimates of cropped area for each CoI, the derived spatial data were compared with the 2012 USDA Census of Agriculture (USDA 2014) which is an official point of reference for agricultural statistics. Table 1 reports the CDL acres in the spatial extent of this analysis (e.g., national or state(s) as a percentage of the reported crop acres based on the 2012 Census of Agriculture). This number exceeds 100% if the data derived from the CDL exceeds the Census of Agriculture and, unsurprisingly, this was seen to occur more often when the 5-year composite CDL layer was used. The results showed that our selection of CDL analyses for 13 of the 15 CoIs accounted for 95% or more of the acres reported by USDA in the spatial extent analyzed, indicating that the approach was effective and realistic in addressing national or regional crop-specific risk assessment. The last two columns show data for individual CoI scenarios that are part of a larger CDL crop class (e.g., almonds as part of the tree nuts crop group). For these crops, the CoI percentage of the CDL crop class (based on USDA census) is reported,

along with the percentage of the individual CoI area covered by the spatial extent processed. For example, the CDL area contained in the 3,102 catchments in FL selected for processing represents 24% of the overall FL vegetables/ground fruit acres from the 2012 Census. However, peppers represent only 5.7% of the actual vegetables/ground fruit area in FL; therefore, the ~58,000 acres of CDL contained in those 3,102 catchments represent over 400% of the total FL pepper acres grown in 2012.

Percent Cropping in Proximity Zones (PZs)

As discussed previously, GIS processing produced datasets for the percentage of each CoI in the relevant catchments enumerated in Table 1 that occurred in PZs of 0-10, 10-50 and 50-200m to each side of the stream. This information is in the dataset but going forward the PZ data discussed herein simply refers to the combined percentage present in the 10-200m PZ. As an example of the data generated, Figure 3 illustrates the shape of the cumulative distribution of the entire set of NHD+ catchment 10-200m PZ PCAs for cotton (n=138,707), highlighting the location in the distribution of the 50th (0.3% PCA), 96th (29.5% PCA), 98th percentile (42.9% PCA), 99th (57.4% PCA) and 100th (100% PCA) catchments.

Table 1. Details of USDA cropping areas, numbers of NHD+ catchments, and fraction of the USDA Ag census crop areas accounted for in the analysis

Crop (USEPA Scenario)	Spatial Extent	Temporal Extent	CDL Crop Class	Catchments Modeled	CDL Acres of Crop in Spatial Extent	% of USDA Census Crop Class Area Covered ^b	% of USDA Crop Class that is CoI ^c	% of USDA Census Individual CoI Area Covered ^c
Alfalfa	National	2012	Alfalfa	465,650	16,165,805	97%		
Almond	CA	2012	Tree Nut	7,474	1,704,659	114%	63%	182%
Citrus	FL	2012	Citrus	7,490	976,906	181%		
Corn	National	2012	Corn	757,949	95,651,409	101%		
Cotton	National	2012	Cotton	138,707	13,451,958	143%		
Grass Seed	OR	2013 ^d	Sod/Grass Seed	3,693	4,201,222	998%		
Lettuce	CA	5-yr composite ^a	Veg/Ground Fruit	8,332	1,367,047	124%		
Peanut	GA, FL, AL	2012	Peanut	35,991	1,368,424	119%		
Pecan	GA, TX, NM	2012 (GA) and 5-yr composite ^a (TX, NM)	Tree Nut	41,339	585,389	152%	100%	152%
Pepper	FL	2012	Veg/Ground Fruit	3,102	57,657	24%	5.7%	421%
Potatoes	CO, ID, ME, WA, WI	2012	Veg/Ground Fruit	28,594	1,519,791	85%	39%	217%
Potatoes	ME	2012	Veg/Ground Fruit	7,801	123,434	110%	55%	202%
Soybean	National	2012	Soybean	658,633	75,243,102	99%		
Sunflower ^e	National	2012 (ND, SD) and 5-yr composite ^a (other states)	Sunflower	86,853	2,676,850	143%		
Sweet Corn	National	5-yr composite ^a	Sweet Corn	68,989	301,398	198%		
Wheat	National	2012	Wheat (spring, winter)	614,378	55,399,808	113%		

^a To account for higher than normal omission error in the CDL for some crops, the composite of all 5 years of CDL (2008-2012) was used for this analysis.

^b 2012 Census of Agriculture. (USDA 2014)

^c Column only included for scenarios that are part of a larger CDL crop class containing multiple crops

^d Grass Seed was added at a later time and 2013 was the latest available CDL at that time.

^e No EPA Sunflower scenario existed, so to cover this pyrethroid-important crop, this scenario generated based on the ND Corn scenario, see SI for details.

As discussed above, to turn these distributions of large numbers of catchment measurements into values that could efficiently be applied in a probabilistic analysis, each CoI distribution was expressed as 10 “groups” of PCA values. Table 2 reports the 10 geometric percentiles for the distributions of these PCA values for all CoIs. It may seem counter-intuitive that some crops have PCA values of 0.0 for the 25th percentile, but this is where at least 25% of the catchments contained the CoI but there was none within the 10-200m PZ. This table demonstrates that at the 96th percentile, the populations of catchments relevant to each CoI, have a wide range of PCA values (4.1-67.2%) while at the 90th percentile, the range has narrowed (1.3-44.4%). All but three of the CoIs have 99% of the catchments with

<75% PCA. However, the data also show that some catchments have 100% CoI in the 10-200m PZ for all but two CoIs (peanuts in GA, FL, and AL and vegetable/ground fruit [pepper] in FL) demonstrating that the USEPA screening scenario (i.e., an assumption of 100% PCA) does occur within the 10-200m PZ in NHD+ catchments, although very infrequently (<1% of catchments). One of the more striking findings is that for all CoIs in at least half of the catchments growing the CoI, its production acreage is less than 4% of the PZ area (50th percentile PCA values in Table 2). These data provide a snapshot of actual (measured) cropping practices at the NHD+ catchment scale and reveal highly skewed distributions of PCA.

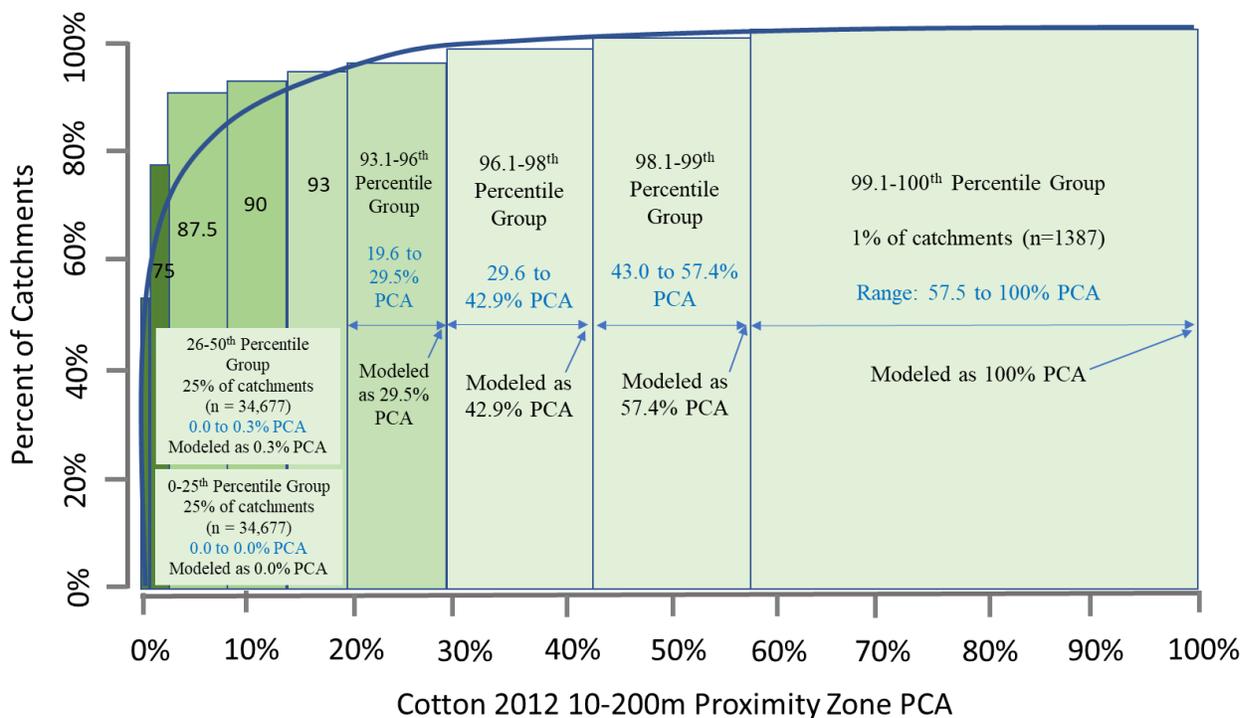


Figure 3. Cumulative distribution of cotton NHD+ catchment PCAs in 10-200m PZ showing the 10 PCA groups and PCA values used in the calculations in Table 1 to represent all catchments in the PCA group

Table 2 also indicates the magnitude of conservatism associated with the working assumption used in this paper of estimating the distribution of EECs by applying the maximum PCA in a PCA group to all the catchments in that group. For example, for cotton, we used the assumption that the PCA was 57.4% for all catchments in the 98-99% PCA group when Table 2 shows that the PCA ranged across this group from >42.9 to 57.4%. Similarly, for corn, the assumed PCA for all catchments in the 50-75% PCA group was 18.0% when the actual range was >2.7 to 18.0%.

The USEPA reported a set of PCA values based on 5,477 drinking water intakes using CDL as the cropping footprint. Results were reported for 18 Water Resource Regions (HUC-2s). Although only the maximum crop-specific PCA values were reported for

each crop and HUC-2 combination, it does show a geographic distribution of the maximal calculated PCA (Table 3-5, USEPA 2014). For example, the maximum PCAs for corn varied from 0% (HUC-2 16) to 68% (HUC-2 07) with a mean of 19% (SD 0.19). The USEPA data show considerable crop-specific geographic variability (at least in maximal PCA values). Our NHD+-based analysis also captures geographic variability, as well as reporting and utilizing the entire range of PCA values (25th percentile to maximum) when developing EECs (e.g., ranging from 0.1% to 100% PCA for corn). Our PCA range has higher maximum values than reported by EPA due to the smaller spatial unit of analysis (NHD+ catchment). Our method of applying the entire distribution of PCA values for a CoI provides a refined approach compared to single maximal values.

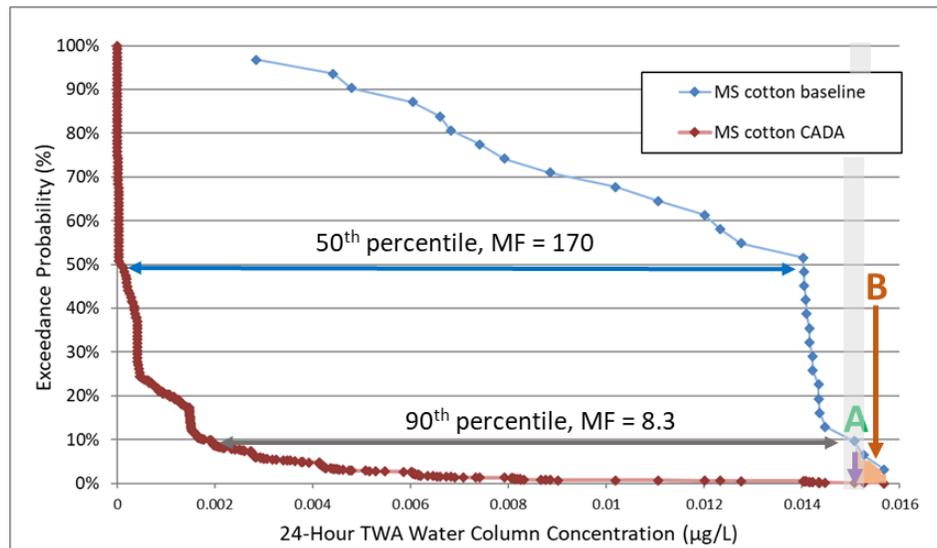


Figure 4. Results showing application of CADA (red points) to the distribution of 30 simulated annual maxima EECs for cotton from the baseline assessment (blue points) for water column with 50th and 90th percentile MFs illustrated (blue and grey horizontal lines, respectively). Vertical grey bar represents the single EEC that is selected for baseline scenario cases. Green arrow (A) shows the reduction in probability of exceeding the baseline EEC, and orange shaded area (B) illustrates concentrations greater than the baseline regulatory value may occur but with far lower probability.

Table 2. Selected percentiles of 10-200m PZ PCA distributions for individual CoIs

Crop of Interest (CoI)	Maximum PCA used to represent each percentile group 10-200m PZ PCA distribution for each CoI (%)									
	25	50	75	87.5	90	93	96	98	99	100
Alfalfa	0.1	0.5	2.8	7.6	9.6	13.3	20.0	29.9	40.8	100.0
Citrus	0.0	0.8	3.6	8.4	10.5	15.3	25.9	41.7	59.5	100.0
Corn	0.1	2.7	18.0	35.8	40.9	48.7	59.6	71.4	81.3	100.0
Cotton	0.0	0.3	2.9	10.5	13.7	19.5	29.5	42.9	57.4	100.0
Peanut	0.0	0.2	2.6	7.9	10.0	13.5	19.3	28.0	35.7	93.8
Soybean	0.2	3.4	17.8	33.0	37.5	44.2	54.2	66.2	77.3	100.0
Sunflower	0.0	0.0	0.4	2.0	3.2	5.8	12.3	22.8	34.1	100.0
Sweet corn	0.0	0.1	0.4	1.3	1.8	3.1	6.3	13.0	21.8	100.0
Almond	0.4	3.1	17.5	38.1	44.4	53.3	67.2	79.7	89.2	100.0
Pecan	0.0	0.2	1.0	2.6	3.3	4.6	7.2	12.3	19.5	100.0
Lettuce	0.1	0.9	4.8	14.4	18.7	25.4	38.9	55.5	67.9	100.0
Pepper	0.0	0.0	0.2	0.9	1.3	2.1	4.1	9.5	19.1	80.8
Potato ^a (ME)	0.0	0.1	0.9	5.1	7.8	12.6	21.5	33.7	44.1	100.0
Potato ^a (ID)	0.0	0.1	0.5	1.9	2.7	4.1	7.7	13.3	18.7	100.0
Wheat	0.0	0.4	5.4	17.3	22.0	29.7	42.0	56.2	69.0	100.0
Grass seed	0.1	3.7	18.9	33.8	36.8	43.4	51.7	61.7	69.9	100.0

^a see spatial extent details in Table 1.

CADA Analyses – Impact of PCAs on Baseline Exposure Assessments

Figure 4 illustrates the 24-hour water column concentration data from the baseline EEC distribution compared with the output from the CADA approach for the MS cotton scenario for a single representative pyrethroid [14]. The figure displays the distribution of 30 simulated annual maxima EECs from the baseline assessment based on the 100% cropped delivery area assumption (blue points) with the baseline EEC identified by point A (green). This presentation highlights the fact that the regulatory assumption is the 1-in-10 year value from 30 years of modeling and so there are exposures higher than this regulatory concentration endpoint. The red line shows the distribution of the CADA

simulated 300 water body yearly annual maxima obtained by applying the probability distribution of real-world PCAs. The purple arrow (at point A) shows the magnitude of reduction in probability of encountering the baseline EEC using the CADA approach. In this case 1-in-10 year (10% probability) is reduced to 0.067% probability. The horizontal grey arrow indicates the extent of the 1-in-10 year maximum EEC is reduction (i.e., the multiplication factor) by considering the impact of the crop-specific PCA on estimated aquatic exposures (in this case by a factor of 8.3). The orange shaded area identified by arrow B indicates that this probabilistic refinement does not negate the finding that concentrations greater than the 1-in-10 year baseline regulatory value may still occur. However, instead of exceedances

occurring in two years out of every 30 (6.7% probability), their likelihood of occurrence is greatly reduced (in this case to less than 0.1% probability). The impact of this probabilistic approach applies throughout the distributions. For example, the horizontal blue arrow shows the reduction magnitude of the 50 percentile (1-in-2 year) EEC (in this case by a factor of 170). Comparable results for 21-day TWA sediment concentrations are provided in the SI (Figure S5 in Supplemental Information).

Using the same approach, Table 2 reports the resulting MF values for the 90th and 50th percentile water body year EECs for a representative pyrethroid across the 15 CoIs and 18 USEPA scenarios. This table shows that 24-hour water column MFs for the 90th percentile range from 1.88 for CA almond (i.e., the CADA EEC must be multiplied by a factor of 1.88 to equal the standard CA almond scenario EEC) to almost 50 for FL pepper. As shown above, the influence of CADA on EECs is more pronounced for the 50th percentile EEC, with MF values ranging from 5.72 (CA almond) to over 500 (FL pepper). Differences were apparent for the same crop between spatial extents, where the IL corn 50th percentile MF is 22% greater than IN corn and MS cotton 50th percentile MF is 83% greater than TX cotton. Clearly the impact of the actual catchment cropping density is dependent upon both the crop and the national/regional/state scale as indicated by the shape of the distributions (Figure 3). Comparable results for 21-day TWA sediment MFs are provided in the SI (Figure S8 in Supplemental Information).

Discussion

This probabilistic analysis examined the impact of measured distributions of crop-specific cropping intensities on regulatory model outputs. These were compared to predicted potential exposures using the standard screening level default assumption that water bodies are surrounded by 100% of the treated CoI. The NHD+ catchments selected for this analysis are sufficiently numerous for all the CoI and regions examined to permit meaningful distributional analysis. These catchments are generally small, reflecting a range of areas highly representative of farm-scale operations. They are also defined by flowing water bodies that form part of the stream network draining the entire nation and are frequently used for other regulatory water quality evaluations. The study used GIS to intersect the NHD+ catchment data with best-available US government spatial data on cropping. The area of each CoI identified was successfully cross-checked against other government agricultural survey information. EPA's Spatial Aquatic Model (SAM, USEPA 2015d) (not yet released) also uses a drainage area as the unit of analysis (defined by a HUC-12) which, while somewhat larger than NHD+ catchments, utilizes a comparable approach to this study. CDL-based crop footprints were developed and summarized at the HUC-12 level for use in subsequent aquatic modeling using SAM.

Table 2. 24-hour water column Multiplier Factors (MFs) as a result of applying catchment based PCA distributions to standard baseline scenarios

	24-h Water Column	
	50th Percentile MF	90th Percentile MF
PA alfalfa	88	20
CA almond	5.7	1.9
FL citrus	28	6.6
IL corn	6.9	2.4
IN corn	5.6	2.2
MS cotton	170	8.3
TX cotton	93	7.6
OR grass seed	14	2.4
CA lettuce	21	4.1
NC peanut	108	10
GA pecan	461	31
FL pepper	564	49
ID potato	107	8.0
ME potato	426	37
MS soybean	8.1	2.7
ND sunflower	258	20
OR sweetcorn	251	34
ND wheat	24	18

For the resulting populations of NHD+ catchments that had evidence of cropping, each CoI ranged from approximately 3,000 to over 750,000 catchments. For each CoI, the GIS then generated distributions of PCAs in the stream proximity zones (10-200m) on either side of the stream reach. Due to the extensive sampling of relevant areas for each CoI in this study, the data are equally relevant to spatial distributions of crops around ponds and lakes. This is important since we have applied the catchment zonal cropping data to modeling conducted using the standard USEPA regulatory scenario

representing local agriculture transporting pesticide mass flux to a small farm pond. A numerical simplification was made to combine the measured PCA distributions with the regular regulatory model output distribution using groups of PCAs in place of individual values. However the inherent assumption of using the maximum measured value for each group showed that the output remained highly conservative. Other assumptions and potential sources of uncertainty are discussed in the Supplemental Information.

The catchment distributions indicated that for all crops 90% of the

catchments had a 10-200m PCA of 45% or less, while for six crops 90% of the catchments had a PZ PCA of less than 10%. Even at the 99th percentile (i.e., 99% of the catchments with CoI), all but two crops (almonds and corn) had less than 75% of the 10-200m PZ cropped. However, this analysis identified that the screening scenario of 100% cropped occurred at least once (but not for more than 1% of the catchments) for all but two crops (peanuts in GA, FL and AL and peppers in FL). The extensive variability of catchment PCAs across all crops highlights the diversity of real-world agriculture and since the associated variability can now be accurately quantified, it should be incorporated into probabilistic refined exposure estimation using distributions. We have demonstrated one probabilistic application of these PCA distributions with the USEPA standard scenarios. However, PCA data are not limited to pesticide exposure and could be used to examine other environmental transport issues associated with specific CoI within a probabilistic framework (e.g., nutrient or sediment loadings to surface water).

Scaling the influence of the PCA distributions as applied to pyrethroid modeling using the baseline scenarios, the resulting MFs show a range of reductions in estimated aquatic exposure which varied by CoI. The 90th percentile of maximum water body year EECs (the value used in the standard US regulatory screening approach equivalent to a 1-in-10 year event) for the water column was reduced by a minimum of 1.88 (CA almonds) to almost 50-fold (FL pepper), with larger reductions for the 50th

percentile water body year EECs (5 to over 500 factor reductions). The incorporation of the 10-200m PZ PCA distributions has a marked effect on the aquatic exposure predictions. Nevertheless, the results do not negate the fact that settings equivalent to the standard regulatory screening assumption do exist. The maximum concentrations are essentially the same in both the PCA-modified and standard distributions; however the estimated probability of these concentrations occurring is massively reduced. This indicates that the estimated 1-in-10 year maximum water-body year exposure in the output distribution (the regulatory endpoint used in standard screening assessments) is reduced by between a factor of ~2 and 49 depending upon crop and the size of the region considered. Because the magnitude of the reduction varies significantly by crop, an important finding is that the ranking of potential risk by CoI changes when the real world PCA distributions are considered. This is exemplified in Table 3 which shows the relative rankings of these CoIs using baseline inputs compared to those modified by the PCA distribution. The baseline ranking in this table relates only to our implementation (i.e., including VFS requirements) applied to pyrethroids and is not a general ranking for all chemicals. The table also shows the potential regulatory significance of conducting refined exposure assessments that examine sources of uncertainty such as cropping proximity and density. The refined assessment might focus attention on a different use pattern (i.e., application to a specific crop) as deserving more regulatory attention. Comparable results for 21-day

TWA sediment rankings are provided in the SI (Figure S9 in Supplemental Information).

Our analysis has examined the impact of crop PCA in the 10-200m zones around streams. However, this analysis also generated three intermediate PCA datasets covering the 0-10, 10-50 and 50-200m PZs². These datasets have other potential uses including assessing the risks and possible mitigation strategies for crop-specific nutrient or sediment transport to protect water quality.

In a full probabilistic risk refinement, many other input parameter distributions would have been considered at the same time to replace the conservative, single-point values assumed for screening assessments. For example, see the effect of wind speed, temperature, and humidity on drift loads [8] and wind direction relative to water body [18, 40]. The current study merely demonstrates the effect of one of the more important drivers of transport to aquatic systems. More detailed evaluations of potential sources of uncertainty have been developed [14].

Conclusions

The use of publicly available national-scale spatial data on hydrology and cropping allowed for an extensive analysis of crop-specific PCA distributions as a refinement for regulatory exposure modeling for pesticides. The large number of catchments and their representative size for local farming practices make NHD+ an ideal framework to examine national level

exposure. The temporally and spatially leveraged location data in the CDL for a wide range of crops provide a basis for examining crop occurrence and density associated with hydrologic, soil, or slope data. Combining crop information with surface water proximity at the catchment level produced measured crop PCA distributions for the areas most likely to lead to potential pesticide exposure to flowing waters.

The current work builds upon methodologies previously reported to characterize spatial proximity of cropped areas to aquatic or terrestrial areas of interest [6, 10, 18, 40, 68] by extending the spatial extent to a national scale. An innovative approach was used to refine baseline model output distributions (30 individual annual maxima) by probabilistically applying crop density adjacent to stream segments (the 10-200m PZs on either side) using measured distributions derived from GIS analyses. This resulted in a distribution of 300 water body year EECs. This analysis confirms that the refined output maxima match the baseline scenario EECs, however incorporating the measured adjacent PCA distributions contextualizes their probabilities of occurrence.

The study shows that for most crops only a small fraction of water bodies are surrounded by 100% of the CoI. This is in contrast to the default USEPA pesticide assessment screening-level conceptual model where this is assumed to occur for every waterbody. This dramatically reduces the

² These data were not specifically used in this work and are therefore not included in the SI. Contact corresponding author for data request.

probability of occurrence of higher predicted exposures. Consequently, when the PCA refinement is considered, the 1-in-10 year model output endpoint that the USEPA uses

as an aquatic level of concern [61] is reduced by a factor of between 1.9 and ~50 (depending upon crop).

Table 3. Ranking of crop scenarios for a representative pyrethroid showing 24-hour water column EECs (ranked from highest to lowest 90th percentile) comparing baseline approaches with results obtained by considering the impact of PCA in the 10-200m PZ (CADA).

Rank	24-hour Water Column	
	Baseline	CADA
1 (highest)	MS cotton	CA almond
2	TX cotton	IL corn
3	CA lettuce	IN corn
4	GA pecan	MS soybean
5	ND sunflower	CA lettuce
6	CA almond	OR grass seed
7	OR sweet corn	MS cotton
8	IL corn	TX cotton
9	FL pepper	ID potato
10	IN corn	NC peanut
11	NC peanut	ND sunflower
12	ID potato	ND wheat
13	ME potato	GA pecan
14	MS soybean	OR sweet corn
15	OR grass seed	ME potato
16	ND wheat	FL pepper
17	PA alfalfa	PA alfalfa
18 (lowest)	FL citrus	FL citrus

Importantly, the variability of crop-specific 1-in-10 year EEC reductions resulting from different crop-specific PCA distributions changes the ranking of the potential for different crops to contribute pesticide loadings to aquatic ecosystems. This indicates that crop-specific PCA data (currently not used in USEPA ecological assessments) are an important variable to consider when determining real-world priorities for pesticide mitigation strategies.

The crop-specific catchment PCA data generated as part of this study can potentially be used in other contexts including assessing the risks and possible mitigation strategies for crop-specific nutrient or sediment transport to protect water quality. The catchment cropping data generated as part of this study were also combined with spatial data on soils and weather and used in an examination to place the USEPA scenarios into a national context

of catchment-scale off-field transport of pyrethroid mass [31]. Alternatively, if other spatial datasets are combined (e.g., data layers classified by non-crop types like trees and brush), analyses similar to those used for cotton in Yazoo County, MS [18] could be conducted to understand the spatial arrangement of crops, non-crops, and water bodies and the resulting impacts on pesticide drift potential. Moreover, because these crop specific results use catchment boundaries from the NHD+ framework, these data and any associated findings can readily be associated with the hundreds of other catchment metrics (e.g., Streamcat) and NHD+ applications (See [EPA Website](#)) currently available.

Highlights

- A US-wide spatially explicit analysis of crop density and proximity to surface waters was developed to characterize the potential for pyrethroid insecticides to enter flowing waters
- Cropping and hydrology datasets were employed at the catchment-scale across the full extent of agricultural production in the US ranging from 3,000 to more than 750,000 catchments depending on the crop of interest
- Crop-specific probabilistic distributions describing the extent and proximity of each crop to the flowing water body were used to refine estimated environmental concentrations using USEPA standard regulatory scenarios

- Results showed that, while potential maximal aquatic exposure concentrations are unchanged, the probability of exceeding regulatory decision-making concentration endpoints is much lower than predicted by standard assumptions (e.g., 1.9 to ~50-fold reductions by crop for 90% of catchments)
- The relative ranking of crops by their aquatic pesticide exposure potential may change when cropping density and proximity are considered

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