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National characterization of pesticide runoff and erosion potential to put USEPA standard ecological scenarios in context for pyrethroids

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Abstract

Decision-making for pesticide registration by the US Environmental Protection Agency (USEPA) relies upon crop-specific scenarios in a tiered framework. These standard modeling scenarios are stated to represent "...sites expected to produce runoff greater than would be expected at 90% of the sites for a given crop/use." This study developed a novel approach to compare the pesticide runoff + erosion (Sum_{RE}) mass flux potential of a hydrophobic chemical using 36 of these ecological regulatory scenarios with national-scale distributions of modeled Sum_{RE} from over 750 000 USA-wide agricultural catchments to provide real-world context for the simulated transport predictions used for regulatory decision-making. For the standard scenarios and national scale modeling, "edge of field" Sum_{RE} mass flux was estimated using regulatory guidance for a hypothetical pyrethroid. The national-scale simulations were developed using publicly available soil, hydrography, and crop occurrence /regional timings databases. Relevant soil and crop combinations identified by spatial overlay along with weather data were used in a regulatory model to generate daily Sum_{RE} estimates, which were assigned to the catchments. The resulting average annual total Sum_{RE} mass fluxes were ranked to produce distributions to compare with the standard regulatory scenario outputs. These comparisons showed that Sum_{RE} flux from 25 of the 36 USEPA ecological regulatory crop-specific scenarios modeled ranked above the 99th percentile of pyrethroid runoff + erosion vulnerability from any catchment growing that crop; Sum_{RE} flux from six scenarios was more severe than any catchment. For 12 USEPA regulatory scenarios, the resulting eroded sediment corresponds to highly erodible land (HEL), which the US Department of Agriculture mandates should not be cropped without substantial additional erosion prevention controls for sustainability. Since the pesticide regulatory framework already incorporates many acknowledged assumptions to ensure it conservatively meets protection goals, these HEL observations suggest that the standard scenarios overestimate potential aquatic exposure and that the regulatory process is more protective than intended. *Integr Environ Assess Manag* 2023;19:175–190. © 2022 The Authors. *Integrated Environmental Assessment and Management* published by Wiley Periodicals LLC on behalf of Society of Environmental Toxicology & Chemistry (SETAC).

KEYWORDS: Risk assessment, runoff modeling, agricultural environment, erosion vulnerability, pyrethroid

INTRODUCTION

Before a pesticide may be used in the United States, it must be registered by the US Environmental Protection Agency (USEPA) under the Federal Insecticide, Fungicide,

and Rodenticide Act (FIFRA) and the Federal Food, Drug, and Cosmetics Act. To evaluate whether the pesticide has the potential to cause adverse effects to aquatic species, the USEPA has developed a tiered framework, which involves modeling pesticide aquatic exposure and comparing estimated exposures to the most sensitive ecotoxicity endpoints. The second tier of this framework uses the Pesticide Root Zone Model (PRZM) to simulate 30 continuous years of applications of a pesticide according to the proposed label to a 10-ha field that contributes runoff + erosion (Sum_{RE}) mass flux into a 1-ha by 2-m deep pond driven by daily precipitation data. Crop-specific Sum_{RE} mass flux estimates are generated using "standard scenarios," which combine a crop with a relevant soil and slope combination and specify a particular local weather station to generate 30 years of

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daily data. In the mid-1990s, there were 23 standard crop scenarios, but the number has since grown to over 120 scenarios located throughout the USA representing over 50 crops. For crops that are grown extensively across wide swaths of the USA, USEPA has defined multiple scenarios covering key states and ranges of soil and slopes—each using local weather data to ensure a good understanding of overall potential vulnerability is obtained.

According to USEPA (2004), “Classically defined, if all the sites where a particular crop could be grown in an area were placed on a distribution according to pesticide runoff, the high-end site (author’s note: by that they mean scenario) would represent a site where 90% or more of all sites would have less pesticide runoff but remain below the site that would yield the highest exposure.” This indicates crop scenarios are intended to represent an agricultural field that would produce pesticide runoff greater than would be expected at 90% of the sites for a given crop, use and growing region. Within the standard scenario Sum_{RE} modeling, there are also additional underlying assumptions to ensure the output is protective (Table S1).

The present study was designed to examine how the simulated Sum_{RE} mass flux outputs from these crop-specific ecological regulatory scenarios correspond to Sum_{RE} pesticide mass fluxes that might be expected to occur in real-world cropping systems at the catchment scale across the range of conditions where a given crop might be grown in the USA. The concept is that, while crops are often grown on a field-by-field basis, some fields can contain multiple crops; additionally, fields themselves often contain multiple soils. Moreover, streams typically receive runoff + erosion from multiple fields. Consequently, our approach examined runoff + erosion from soil and crop co-occurrences by catchment since the catchment defines the area, which delivers runoff and erosion to the corresponding stream reach (i.e., receiving waterbody) and, thence, to the hydrologic network covering the USA. Thus, these farm-scale catchments are the “real-world” areas that need to be understood to examine the potential for pesticide applications to a particular crop to lead to the off-target entry of runoff and erosion into USA waters. To ensure effective comparisons, Sum_{RE} pesticide mass flux leaving the field was used as the metric to avoid complications from considering how Sum_{RE} entry into a waterbody translates to water and associated sediment concentrations. The issue of pesticide drift was also disregarded in this analysis since the USEPA framework allocates drift directly (and additively) into the waterbody and is independent of the standard scenario selected to estimate runoff and erosion transport.

While the standard scenario reflects a 10-ha cropped field draining into a 1-ha pond, in the real world, flowing waters are likely to be of more concern since they form a connected system that drains most of the land in the USA and are a fundamental component of the hydrologic cycle. Streams are potentially the most ecologically sensitive category of flowing waters and consequently, we used the National Hydrography Dataset Plus (NHD+) framework of hydrologically connected

catchments as the base spatial unit for our national scale Sum_{RE} assessments (Winchell et al., 2018). This dataset accounts for the entire conterminous USA land area and is comprised of catchments with areas highly relevant to farming practices at the local scale and which deliver runoff and erosion into the stream network. These NHD+ data are government-defined and have been used as regulatory frameworks in many applications such as the USEPA Office of Water 303(d) list of impaired waters (USEPA, 2015). For more details, see the Supporting Information.

Another fundamental assumption underlying the present study was the use of a very strongly adsorbed molecule (i.e., a very strong affinity to bind to organic carbon, either dissolved or in sediment and soil particles) as the surrogate pesticide for the simulations (in this case, a pyrethroid). When modeled in PRZM, this effectively means that all the applied pesticide stays near the soil surface and does not move lower in the soil profile due to leaching. Therefore, it is available for transport to surface waters by successive postapplication rainfall events generating Sum_{RE} and this means that all the remaining parent chemical not degraded is available for transport from the field throughout the year and is a worst-case surrogate molecule for Sum_{RE} transport.

This study developed a novel approach to assess the real-world potential for off-target transport of a highly hydrophobic molecule after treating crops of interest (CoI) across soil and weather combinations and catchments across the USA. We examine the relevance of soil/slope/crop co-occurrences in delivery areas (catchments) that had been cropped at least one year in the previous five to specific crops within NHD+ catchments in comparison to the standard regulatory scenarios used for each crop in the early steps of an agrochemical risk assessment.

METHODS AND MATERIALS

In the pesticide registration process, the PRZM model is used in the aquatic risk assessment and it accounts for key processes of pesticide fate and transport from runoff and erosion from rainfall events. The PRZM model version 3.12 (Carousel et al., 2005), which is the model used when USEPA developed its standard scenarios, was used for this study. However, an updated version, PRZM5, has been developed and is currently used by USEPA (Young & Fry, 2020). These processes include factors such as the physicochemical and fate characteristics of the pesticide, the agronomic practices related to the production of the crop and the use of the pesticide as specified on the proposed label, the soil and hydrogeological conditions where the pesticide is used, as well as the climatological conditions at the time of and following its use. Table S1 documents the inherent assumptions underlying the standard regulatory modeling process and, except where discussed below, these assumptions were unchanged for both the standard crop scenarios and all national-scale soil and weather simulations. Importantly, these assumptions do not consider any best management practices (i.e., reduced tillage, contouring, vegetative filter strips, etc.) to reduce runoff or erosion that are increasingly

used by growers (either voluntarily or, in some cases, mandated on product labels).

Standard regulatory USEPA scenarios

The PRZM standard ecological crop scenarios for key Col (i.e., those with high pyrethroid use [GfK Kynetec, 2013] or high potential for pyrethroid aquatic exposure [Desmarteau et al., 2014; USEPA, 2016]) were run for the USEPA standard 30-year (1961–1990) period using local daily weather data associated with each specific scenario (USEPA, 2020a). Thirty-six USEPA standard crop scenarios were simulated with PRZM to represent the nine Cols, including alfalfa, almond, citrus, corn, sweet corn, cotton, pecans, soybeans, and spring wheat. The locations of the regulatory crop scenarios evaluated in the present study are shown in Figure 1. More details regarding these scenarios (weather station, soils, erosion factors, slope, curve number) are provided in Tables S2 and S3 (Col emergence, maturation, and harvest dates).

A single hypothetical pyrethroid representing the entire class of nine major synthetic pyrethroids was used for the simulations in this article since these compounds all share exceptionally high hydrophobic properties and similar

aerobic soil half-lives. Best professional judgment was used to derive typical combinations of physicochemical parameters, environmental fate behavior, and application use patterns designed to represent the range of pyrethroid product labels. This hypothetical molecule is referred to as “hypothrin” and represents a convenient and functional chemical for this assessment that applies to a number of synthetic pyrethroids as well as other highly adsorbed chemicals. As is typical of pyrethroids, hypothrin has a high soil K_{OC} coefficient (500 000 ml/g) with low solubility and is not volatile. The aerobic soil metabolism half-life is 66 days, and the foliar half-life is 5.3 days (Willis & McDowell, 1987). The application use patterns for each of the nine crops evaluated with hypothrin are provided in Table 1.

Each USEPA crop scenario was run with the standard 30 years of weather data (1961–1990) and postprocessed to calculate the total hypothrin mass from simulated daily Sum_{RE} mass flux for each year. Then the average annual total mass flux from 30 years was calculated and reported as kg/ha/year. This long-term average takes out the extremes in weather and is not as dependent on the application day selected for the PRZM simulation (application date in relation to rainfall date has been shown to be a key factor in

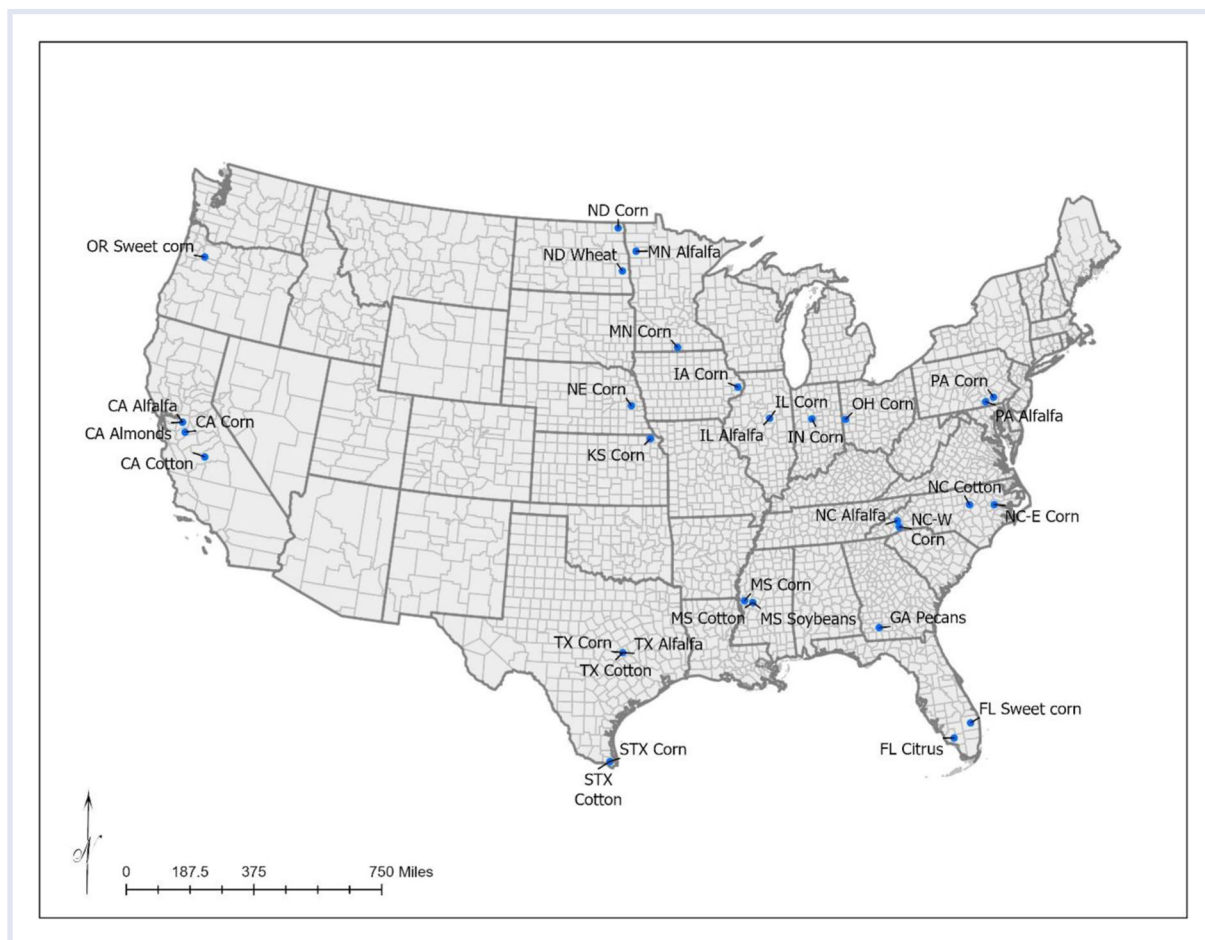


FIGURE 1 Locations of USEPA scenarios evaluated for the crops of interest (Col)

TABLE 1 Surrogate pyrethroid (hypothrin) application use pattern and modeling inputs for Cols analyzed

Crop of interest	Application rate (kg/ha)	Number of applications	Date of first application ^a	Application interval (days)
Alfalfa	0.034	5	10 days postemergence	5
Almond	0.112	4	May 15	7
Citrus	0.112	1	May 1	–
Corn	0.056	4	10 days postemergence	7
Cotton	0.056	6	10 days postemergence	5
Pecan	0.112	4	June 15	7
Soybean	0.056	4	10 days postemergence	7
Sweet corn	0.056	10	10 days postemergence	3
Wheat	0.043	2	10 days postemergence	3

Note: All applications were assumed to be aerial with 95% efficiency.

Abbreviation: Col, crop of interest.

^aCropping dates for standard scenarios are provided in Tables S3 and S6 for national and regional simulations.

off-site transport of Sum_{RE}). Thus, the 30-year average value is a good metric for evaluating Sum_{RE} mass flux into a waterbody (USEPA, 2020b).

National and regional hypothrin PRZM simulations

Soil and weather combinations and catchments where the Col was grown were used as the real-world units of analysis of Sum_{RE} mass flux to compare against the USEPA standard regulatory scenario for a given Col. To generate catchment-scale results, the Sum_{RE} mass flux of hypothrin (using the same environmental fate and application model inputs for the standard scenario runs) was estimated with PRZM for every soil in the USA identified as being cropped to each of the nine selected Cols over a five-year period (2008–2012).

The national agricultural landscape was characterized by utilizing publicly available spatial datasets on soils, crops, and their co-occurrence with appropriate local weather conditions throughout the USA. A brief description of the datasets and the parameterization of PRZM for the national simulations are provided in Table 2. One of the primary sources of data for this project was the national Soil Survey Geographic (SSURGO) database (Soil Survey Staff, 2009). The number of soils in the SSURGO database was reduced from the 673 658 unique soil and slope spatial identifiers in the SSURGO database to 377 566 soils once duplicates with respect to PRZM modeling variables (e.g., bulk density, organic matter, slope, etc.) were removed. For the national and regional modeling, all soils from SSURGO were modeled, including hydrologic soil groups (HSGs) A, B, C, and D (A = prone to leaching; D = prone to runoff and erosion). As seen in Table S2, the USEPA standard scenarios are predominantly prone to runoff and erosion (C and D soils). More details on the SSURGO data and additional data for the PRZM simulations, such as selected curve numbers (Table S4) and example derivation of erosion factors (Table S5), are provided in the Supporting Information. Full tables of planting and harvest dates used for each crop

are supplied in Table S6; cropping dates (emergence, maturation, harvest) were chosen for each crop following typical agricultural practices (USDA, 2000) based on the location (state in USA) of the soil/weather being modeled.

The weather stations were selected from the Solar and Meteorological Surface Observational Network (SAMSON) weather stations (NOAA, 1993) database since most of the stations have a 30-year continuous daily record suitable for modeling (referred to as 30 years for brevity) and these weather stations are used by USEPA for standard regulatory modeling. The assignment of SAMSON weather stations to SSURGO soil data is explained in the Supporting Information.

Crop location information for the nine Cols was obtained from the United States Department of Agriculture National Agricultural Statistics Service Cropland Data Layer (USDA NASS CDL) products for a period of five years from 2008 to 2012 (USDA-NASS, 2013). To ensure that the most representative collection of NHD+ catchments within a spatial extent was used for this analysis, the crop area from a five-year composite of crop location data (CDL) was used to generate the largest possible footprint of crop location to match with soils. These composite layers represent all areas that have been classified as a particular Col during the five-year period. A spatial overlay of soil and weather (SSURGO and SAMSON) and crop location (CDL) was performed to identify all soils on which each of the nine Cols were grown. For each Col, the number of soil/weather combinations, the number of catchments cropped to Col, and the total catchment area for catchments containing the Col is provided in Table 3. The table also shows the spatial extent of the analysis for each crop in terms of national (conterminous USA) or regional (e.g., FL for citrus) simulations.

Figure 2 shows a schematic of the preprocessor databases associated with running PRZM and then post-processing the daily outputs. A program was written to combine the information from the databases (soils data

TABLE 2 Datasets used in the national and regional analysis

Database	Version	Extent	Variables used	Reference
Soil Survey Geographic (SSURGO)	2009	28 000 000 spatial soil map unit polygons	Soil data: Component percent of map unit, land slope, hydrologic soil group, horizon depth, percent sand/silt/clay, bulk density, organic matter, Available water content, Universal Soil Loss Equation K factor	Soil Survey Staff (2009)
National Resource Inventory (NRI)	1997	15 Slope categories across the US	Computed 50 th percentile slope lengths for crops	USDA (1997)
Cropland Data Layer (CDL)	2008–2012	50 Cropland cover classes across the US	Crops: alfalfa, citrus, corn, cotton, soybean, sweet corn, tree nuts, and wheat	USDA-NASS (2013)
Solar and Meteorological Surface Observational Network (SAMSON)	1993	240 Weather stations across the US	Weather data from 1961 to 1990, including temperature, precipitation, evaporation, relative humidity, wind direction and speed, solar radiation, and sky cover	NOAA (1993)
Parameter-elevation Regression on Independent Slope Model (PRISM)	2008	Regional climate data	Used to validate the assigned SAMSON weather stations	Daly et al. (2008)
NHDPlus (NHD+, National Hydrography Dataset Plus)	2005	Hydrologically connected catchments across the US (>2.5 million)	Spatial unit of landscape or catchment	USEPA and USGS (2005)

Note: Further details on these databases are provided in the Supporting Information.

TABLE 3 Number of soil and weather combinations and catchment data per Col and spatial extent of analyses

Crop of interest	Spatial extent of analysis	Number of soil and weather combinations cropped to Col in spatial extent	Number of catchments cropped to Col in spatial extent	Total catchment area of catchments containing Col in spatial extent (km ²)
Alfalfa	National	242 607	465 650	2 272 342
Almond	CA, AZ	3343	7474	40 467
Citrus	FL	7008	7490	69 880
Corn	National	271 340	757 949	2 950 138
Cotton	National	57 719	138 707	762 884
Pecan	GA, NM, TX	9327	37 874	268 473
Soybean	National	229 110	658 633	2 272 197
Sweet corn	National	47 123	68 989	418 733
Spring wheat	ID, MN, MT, ND, OR, SD, UT, WA, WI, WY	93 246	92 455	566 000

Abbreviation: Col, crop of interest.

[properties and location], weather data, crop parameters, erosion parameters, and hypothrin properties, which included application data for each crop) into a single PRZM input file. Overlaying the soil and weather combinations with crop generated many unique soil/weather combinations for each Col ranging from 3343 for almonds in CA and AZ to 271–340 for corn nationally (Table 3) totaling almost 1 million soil/weather/crop combinations.

Once the PRZM simulations were complete, the daily output of hypothrin Sum_{RE} mass flux (kg/ha) was post-processed for each year. The average annual total Sum_{RE}

mass flux of hypothrin was computed to generate a unique PRZM output for each soil and weather and crop co-occurrence.

Implementation of soil and weather co-occurrence model output by Col

The annual average total Sum_{RE} mass flux results from all the simulations for a given Col, at the national (or regional) scale, were expressed as distributions for comparison with the standard scenario model outputs. For this analysis, the 30-year annual average total hypothrin Sum_{RE} mass flux for

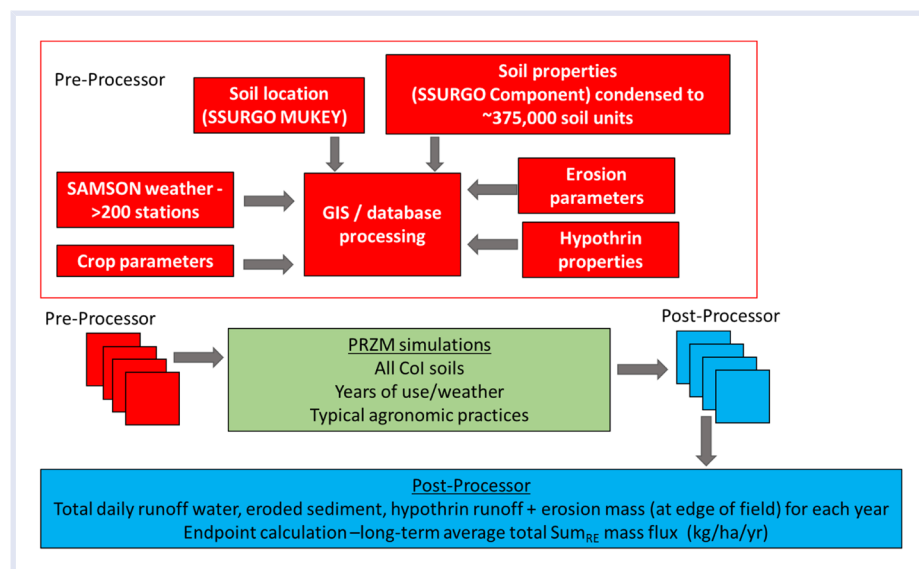


FIGURE 2 Schematic of the approach used to create and process PRZM model simulations for national and regional assessment. Col, crop of interest; MUKEY, mapunit key; PRZM, Pesticide Root Zone Model; SAMSON, Solar and Meteorological Surface Observational Network; SSURGO, Soil Survey Geographic

each Col was ranked from low to high. Each mass flux had a Col area associated with it from the soil and weather and crop simulation co-occurrence of crops grown from 2008 to 2012. The soil/weather/crop area was divided by the national/regional total soil/weather/crop area to compute an area-weighted national percentage represented by each soil/weather/crop combination. These area-weighted percentages were used to generate a cumulative distribution (see Table S7 for example). The annual average total Sum_{RE} mass flux (kg/ha/year) from the corresponding Col standard USEPA regulatory scenario was then plotted onto the same distribution for comparison. Table 4 summarizes the aggregation of PRZM Sum_{RE} mass flux output by Col for the soil/weather/crop approach utilized in the present study.

However, in the real world, the actual delivery of Sum_{RE} flux to the flowing waters of the nation depends on the extent to which each NHD+ catchment contains co-occurrence of soil and weather and crop and thus aggregation of the PRZM output to catchments was the next step in this investigation.

Catchment-level aggregation of soil and weather and crop model output

The average annual total PRZM edge-of-field hypothrin mass fluxes (kg/ha/year) from the sum of runoff and erosion were linked to the approximately 2.2 million catchments with agriculture in the conterminous USA to create a nationwide distributional ranking of the potential for nontarget mass loadings delivered into waterbodies from runoff and erosion sources. These estimates of predicted pyrethroid annual average total Sum_{RE} mass flux for each unique soil/weather/crop combination were distributed into a spatial framework that reflects real-world Sum_{RE} delivery areas relevant to farm-scale operations. The NHD+ framework of hydrologically connected catchments was used as the base spatial unit since this is now a standard base layer for many government hydrologic analyses and datasets, including USEPA's StreamCat dataset, which contains over 600 metrics of water quality, biological condition, and watershed integrity linked to NHD+ catchments (Hill et al., 2016).

TABLE 4 Aggregation of PRZM Sum_{RE} mass flux output for the two approaches

Soil and weather approach	Catchment approach
PRZM outputs	<ul style="list-style-type: none"> National/regional soil/weather PRZM model run outputs—total annual Sum_{RE} mass flux divided by the number of years for average annual Sum_{RE} mass flux. Standard EPA Tier II scenario PRZM outputs—total annual Sum_{RE} mass flux divided by 30 years for average annual Sum_{RE} mass flux.
Calculations	<ul style="list-style-type: none"> National/regional PRZM Sum_{RE} mass flux (kg/ha/year) soil/weather outputs are overlaid with Col to calculate the area (ha) associated with Sum_{RE} flux (kg/ha/year) for each soil/weather combination. Sum_{RE} mass flux by soil/weather is not adjusted by catchment area.
Distribution/ranking	<ul style="list-style-type: none"> National/regional PRZM Sum_{RE} mass flux (kg/ha/year) soil/weather outputs overlaid with each soil/weather for Col in the catchment to calculate a Sum_{RE} mass (kg/year). All Sum_{RE} masses computed within the catchment (different soils/same Col) are combined for a total mass (kg/year). Summed Sum_{RE} mass (kg/year) adjusted by dividing by total catchment area (ha) for Sum_{RE} mass flux (kg/ha/year) for each catchment. Multiple soils with the same Col within each catchment were considered in the analysis.
	<ul style="list-style-type: none"> All national/regional annual average total Sum_{RE} mass flux (kg/ha/year) for Col (along with soil/weather area [ha]) sorted from low to high. Calculated percentage of national/regional Col area represented by each individual soil/weather combination for that Col (i.e., soil/weather combinations with the larger area have a greater influence on the distribution). Cumulative distribution of national/regional Col cropped area at or below the annual Sum_{RE} mass flux for that Col. Generates distribution of the percentage of Col area associated with the environmental vulnerability (in terms of total annual pyrethroid Sum_{RE} mass flux leaving the field) of soil/weather combinations. Standard USEPA scenario annual average total Sum_{RE} mass flux (kg/ha/year) (single value) positioned on distribution for the Col to determine relative vulnerability compared to all soil/weather combinations for a given crop.

Abbreviations: Col, crop of interest; PRZM, Pesticide Root Zone Model; Sum_{RE}, pesticide runoff + erosion.

The NHD+ dataset includes approximately 2.2 million “agricultural” catchments in the conterminous USA that contain some portion of cultivated cropland as defined by USDA NASS (Boryan et al., 2012). These catchments account for the entire conterminous USA land area and comprise a range of areas highly relevant to farming practices at the local scale. These NHD+ catchments are typically small (90% of them are 650 ha [2.5 mi²] or less and 50% are smaller than 160 ha [0.62 mi²]). The approximate USA average farm size in 2019 was 180 ha (0.69 mi²) (USDA, 2020). These catchments, although derived from flowing water systems, serve as an effective real-world equivalent of the standard USEPA scenario representing local agriculture transporting mass flux to a small farm pond. This ensures capturing all the agricultural soils in the conterminous USA.

The PRZM postprocessed outputs (average total pyrethroid Sum_{RE} mass flux [kg/ha/year]) associated with the SSURGO soil database mapunit key (MUKEY) and component key (COKEY) attributes were linked to all the catchments, which contained those individual soils. The catchment hypothrin Sum_{RE} mass was calculated by multiplying the annual average total PRZM soil and weather and crop Sum_{RE} mass flux in kg/ha/year by % soil composition of that soil times the crop area (ha) of that soil in the catchment. This was performed for each soil that co-occurred with the Col within the catchment. The annual average total pyrethroid Sum_{RE} mass (kg/year) for that catchment was calculated as the summed Sum_{RE} masses from all Col cropped soils in the catchment. To remove any bias because of varying catchment sizes, the total Sum_{RE} mass for the catchment (kg/year) was divided by the total catchment area (ha) (including noncropped areas), resulting in a normalized catchment-level 30-year average total Sum_{RE} mass flux in kg/ha/year. Figure 3 shows an example of a single catchment containing all soils (not just predominant soils) with the Col (e.g., cotton), all of which were assumed to be treated with hypothrin. The figure also shows an example of the calculations summing Sum_{RE} mass flux for the catchment and normalizing it to kg/ha/year. The summed loads reflected the combination of Col (e.g., cotton) and each soil/weather in the catchment modeled.

Table 4 summarizes a comparison of the aggregation of PRZM Sum_{RE} mass flux output for the soil and weather approach and the catchment approach utilized in the present study. Additional details of the catchment-level aggregation approach are provided in the Supporting Information.

Implementation of national and regional hypothrin simulations

Table 3 shows the final number of catchments containing the Col for each crop on a national or regional scale ranging from approximately 7500 catchments for FL citrus and almond (CA and AZ) to over 750 000 catchments for corn nationally. As summarized in Table 4, the normalized 30-year average annual total mass fluxes for each Col were ranked from low to high and assigned an occurrence probability (plotting position). To account for the ranges of

catchment areas, the occurrence probability was weighted by catchment area (ha) so that larger catchments had a larger contribution to the probability than smaller catchments (see Table S7, for example). The catchment area weighting does not change the Sum_{RE} mass flux value; it only changes the probability of occurrence of that value. The resulting fluxes (assuming 100% treatment with hypothrin) were plotted for each Col to generate a crop-specific cumulative distribution of national or regional average annual total Sum_{RE} mass loading in kg/ha/year. The average annual total Sum_{RE} mass fluxes for the selected USEPA standard scenario(s) for each Col (recall that the USEPA standard scenarios assume 100% cropping in the 10-ha catchment) were then superimposed upon those distributions to assess their vulnerability relative to the full distribution of real-world catchment pyrethroid Sum_{RE} potentials for each individual Col. This places the regulatory scenarios into context in terms of real-world catchments characterized by actual Col cropping on distinct soils within the catchment using the nearest SAMSON weather station data.

RESULTS

Results from the present study provide two illuminating comparisons of the relative vulnerability of USEPA's standard PRZM modeling scenarios. In the first instance, the annual average Sum_{RE} fluxes (using local crop, soils, and weather data) from all the soil and weather combinations relevant to a particular Col across the whole USA are compared with the output from the standard PRZM scenario for that crop. Secondly, the Sum_{RE} outputs for soil/weather/crop co-occurrences aggregated to the regional or national NHD+ catchments are compared with the standard PRZM scenario outputs. Moreover, these crop-specific estimates of Sum_{RE} mass flux for a pyrethroid driven by local precipitation conditions both individually and when aggregated to a national or regional scale constitute entirely novel datasets. These data not only describe the estimated spatial Sum_{RE} mass flux potential of a highly adsorbed pesticide but also provide a relative measure of the likelihood of soil erosion potential by a crop because the vast majority of the pyrethroid mass transported from the field is bound to eroded soil particles.

Comparisons of soil and weather co-occurrence of model runoff + erosion with crop

Table 5 shows that there are regulatory scenarios that produce more Sum_{RE} mass flux than the 90th percentile from the total area cropped. Using cotton as an example, as shown in Figure 4A, three of the regulatory cotton scenarios (MS, NC, and TX) have more Sum_{RE} mass flux than ~95% of the total area cropped to cotton. Similarly, Table 5 indicates that most of the alfalfa standard scenarios are more erosive than ~92% of the USA national acres of alfalfa while the PA and IL alfalfa scenarios either exceed the 99.9 percentile or represent the worst-case soil/weather combination, respectively. However, there are some alfalfa regulatory scenarios with soils that

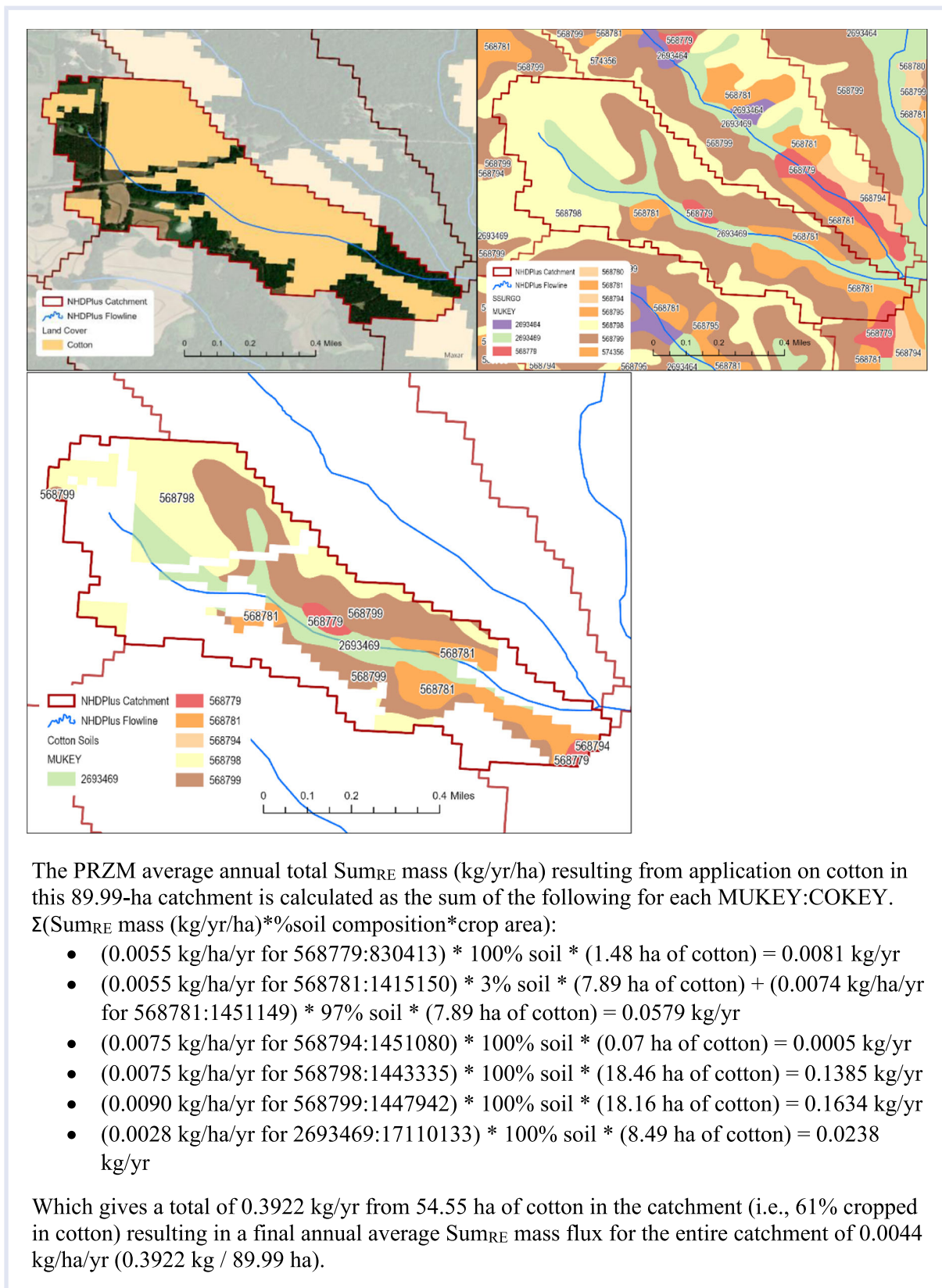


FIGURE 3 Example showing a catchment with the CDL cotton layer (upper left figure) and individual SSURGO polygons with soil MUKEY (upper right figure) with an overlay of only soil area over cotton (lower figure) described with an example Sum_{RE} mass flux calculation for this catchment. CDL, crop location data; MUKEY, mapunit key; SSURGO, Soil Survey Geographic

TABLE 5 Hypothrin Sum_{RE} mass flux (kg/ha/year) from USEPA standard scenarios compared with the national and regional ranked percentiles of annual average total Sum_{RE} mass flux in individual soils and every individual NHD+ catchment growing Col in the year(s) of analysis

USEPA Standard Scenario	Hypothrin average total for Standard Scenario Sum _{RE} mass flux (kg/ha/year)	Number of soil/weather combinations cropped to Col in spatial extent	Soil/weather combination ranking weighted by Col acres (%ile)	Number catchments with Col (spatial extent of analysis)	Ranking by total catchment area (%ile)	Number more severe than Standard Scenario for catchment
CA alfalfa wlrr	0.00011	242 607 (National)	97.3	465 650 (National)	>99.99	3
CA alfalfa nolrr ^a	0.00006		91.7		99.99	104
IL alfalfa	0.00033		100.0		100.0	0
MN alfalfa	0.00001		52.1		98.30	16 786
NC alfalfa	0.00007		95.0		>99.99	30
PA alfalfa	0.00027		99.9		100.0	0
TX alfalfa	0.00002		80.4		99.91	1094
CA almond wlrr	0.00022	3343 (CA, AZ)	98.1	7474 (CA, AZ)	99.99	13
CA almond nolrr ^a	0.00003		76.1		94.51	612
FL citrus	0.00065	7008 (FL)	90.2	7490 (FL)	99.99	3
CA corn	0.00020	271 340 (National)	3.3	757 949 (National)	64.93	322 714
IA corn	0.00290		65.9		99.75	5230
IL corn	0.00402		81.6		99.98	639
IN corn	0.00069		11.9		82.85	164 937
KS corn	0.00200		50.4		98.42	23 082
MN corn	0.00120		27.5		92.68	79 945
MS corn	0.00556		93.7		99.99	35
NC corn E	0.00331		72.3		99.90	2535
NC corn W	0.00170		44.1		97.17	37 024
ND corn	0.00062		10.7		81.15	179 930
NE corn	0.00166		42.8		96.92	39 705
OH corn	0.00352		75.6		99.94	1699
PA corn	0.00235		57.1		99.20	13 245
STX corn	0.00142		35.3		99.16	57 331
TX corn	0.00451		86.0		99.99	230
CA cotton nolrr	0.00005	57 719 (National)	1.3	138 707 (National)	63.97	63 056
CA cotton wlrr	0.00025		6.0		82.54	32 841
MS cotton	0.00692		96.0		99.99	8
NC cotton	0.00647		95.2		99.99	14
STX cotton	0.00279		59.9		99.76	1326

(Continued)

TABLE 5 (Continued)

USEPA Standard Scenario	Hypothesis average total for Standard Scenario Sum _{RE} mass flux (kg/ha/year)	Number of soil/weather combinations cropped to Col in spatial extent	Soil/weather combination ranking weighted by Col acres (%ile)	Number catchments with Col (spatial extent of analysis)	Ranking by total catchment area (%ile)	Number more severe than Standard Scenario for catchment
TX cotton	0.00619		94.8		99.99	21
GA pecan	0.00358	9327 (GA, TX, NM)	99.9	37 874 (GA, TX, NM)	100.0	0
MS soybean	0.00300	229 110 (National)	75.8	658 633 (National)	99.93	1638
FL sweet corn	0.00141	47 123 (National)	36.3	68 989 (National)	99.83	363
OR sweet corn	0.00320		56.7		99.99	43
ND wheat	0.00024	93 246 (ID, MN, MT, ND, OR, SD, UT, WA, WI, WY)	88.2	92 455 (ID, MN, MT, ND, OR, SD, UT, WA, WI, WY)	99.98	67

^aCA alfalfa and CA almond without irrigation are not a standard scenario; irrigation turned off for comparison. Abbreviations: Col, crop of interest; NHD+, National Hydrography Dataset Plus; nolrr, no irrigation; wlrr, with irrigation; SumRE, pesticide runoff + erosion.

are lower than the 90th percentile vulnerability for the Col (e.g., MN alfalfa is ranked 52.1% in Sum_{RE} vulnerability). Overall, 12 of the 36 USEPA standard scenarios, associated with six Cols, are more vulnerable than the 90th percentile. The scenarios that fall below the 90th percentile protection goal typically occur in regions with lower rainfall (i.e., less runoff and erosion). Figure S2 shows graphs for the other Cols.

These findings indicate that the annual average Sum_{RE} mass flux from a uniformly cropped 10-ha field of the Col estimated using the regulatory standard scenario is sometimes, but not in all cases, higher than the expected 90th percentile of the national distribution of soil and weather occurrences on a Col cumulative area basis. This has significant regulatory implications since USEPA regulates based on the standard scenario with the highest exposure concentration; by using this approach the USEPA assessment applies to the cropping area for the entire US. Thus, these regulations would often be well above the 90th percentile protection goal.

One key factor involved in the overestimation of runoff + erosion

Given the importance of these findings, the standard regulatory scenarios were reexamined in more detail with respect to erosion. Table 6 shows that, in 12 scenarios, the combinations of soil type and slope/length model inputs would produce 30-year average soil losses that considerably exceed the acceptable threshold erosion loss factor of 5 tons/acre (see Supporting Information for definition). Under real-world farming conditions, these would have been identified by the Natural Resources Conservation Service at the US Department of Agriculture as highly

erodible land (HEL) (USDA-FSA, 2014). In many states, USDA and other funding bodies have been providing support for more than a decade to encourage growers to invest in permanent or semipermanent engineering and landform management to reduce erosion and gully formation on HEL. Typical management practices include berms, grassed waterways, tile terraces, and so forth. These are generally installed on the fields most vulnerable to erosive loss and damage and therefore specifically target the areas of potential concern for pyrethroids transport via runoff and erosion. Therefore, the use of modeling results from the standard scenarios listed as HEL in Table 6 are unrepresentative of existing sustainable farming practices and should be used with caution, particularly when modeling strongly adsorbed chemicals.

Comparisons of catchment-aggregated model runoff + erosion

In the real world, the actual delivery of Sum_{RE} mass flux to flowing waterbodies depends on the extent to which each NHD+ catchment contains co-occurrence of soil and weather and crop, and thus, the PRZM output was aggregated to catchments as described above. Table 5 summarizes the pyrethroid average annual total Sum_{RE} mass flux for the NHD+ catchments containing each Col. The table reports the Sum_{RE} mass flux for each USEPA standard scenario, the number of catchments with modeling results, and the number of catchments that are more severe than the standard scenario.

For interpretation, the USEPA scenario can be considered analogous to a single catchment that is composed of a single soil (specified in the scenario) that is 100% cropped

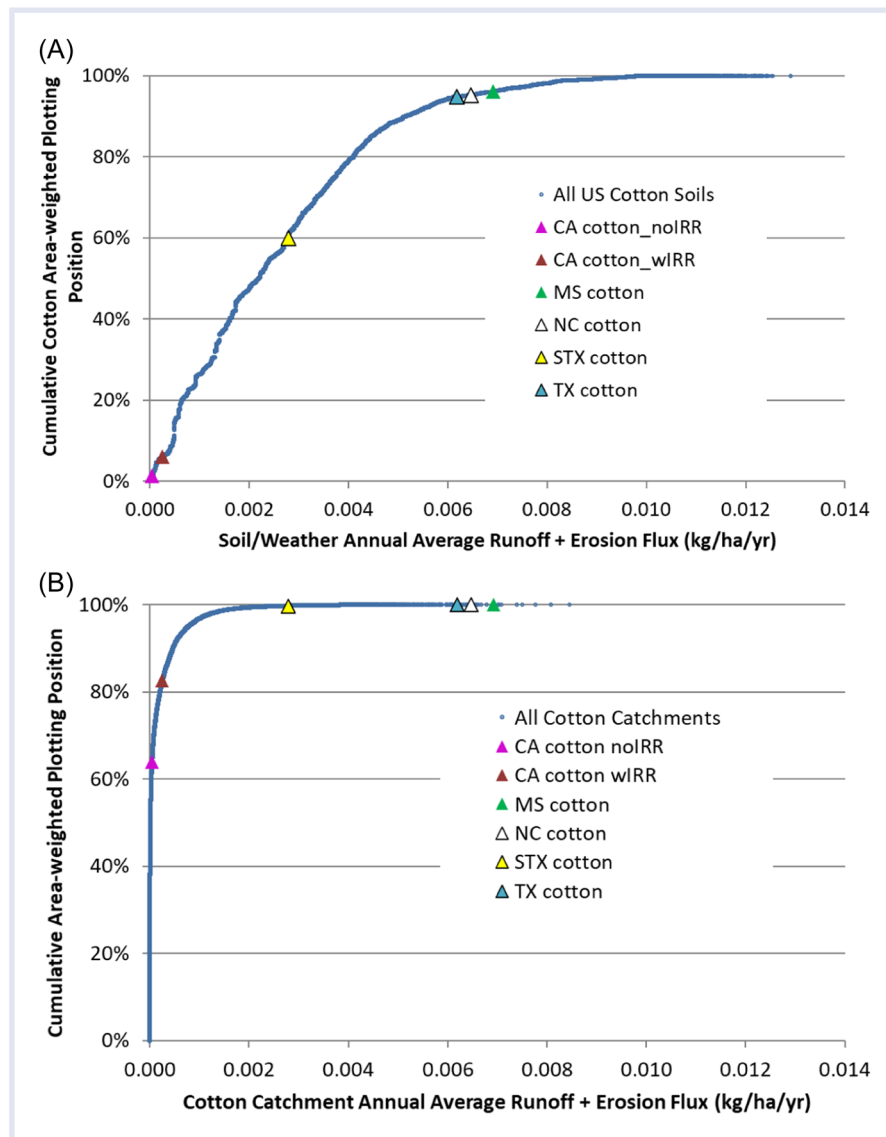


FIGURE 4 Hypothrin Sum_{RE} annual average total mass flux (kg/ha/year) from USEPA standard cotton scenario (colored shapes) plotted on the distribution of (A) soil/weather Sum_{RE} flux (blue) indicating the cumulative soil and weather area coincident with cotton exceeds a specific average annual total Sum_{RE} mass flux and (B) NHD+ catchment-level Sum_{RE} mass flux (blue) indicating the cumulative total catchment area containing some portion of cotton exceeds a specific average annual total Sum_{RE} mass flux. NHD+, National Hydrography Dataset Plus; noIRR, no irrigation; Sum_{RE} , pesticide runoff + erosion; wIRR, with irrigation

and completely treated with a pyrethroid. Figure 4B displays the plotting position of each catchment based on the cumulative percent of total national/regional catchment area containing the Col (y-axis) with the corresponding hypothrin average annual total Sum_{RE} mass flux per unit area (ha) of the catchment (x-axis) for cotton. Figure S3 shows the graphs for each of the nine Cols evaluated (addressing 36 USEPA standard crop scenarios). Using cotton as an example for interpretation, Table 5 and Figure 4B indicate that, when the average year total Sum_{RE} mass flux predicted using the standard USEPA MS cotton scenario is superimposed on the full distribution for the 138 707 catchments, the standard scenario is more extreme than 99.99% of the total catchment area containing at least some cotton in the USA. In fact, only eight of the 138 707 catchments cropping cotton in the USA in 2012 can be expected to experience an

average annual total Sum_{RE} mass flux as or more severe than that scenario in an average year. Similarly, Table 5 shows that the severity of the NC and TX standard cotton scenarios are extreme; also falling at the 99.99th percentile of the national distribution with only 14 and 21 of 138 707 catchments growing any cotton in 2012 expected to experience pyrethroid Sum_{RE} mass flux equal to or greater than this, respectively. However, on a catchment scale, the USEPA CA cotton and CA corn standard scenarios fall below the 90th percentile when ranked with all the catchments containing the Col in the US. The overall range for all the regulatory scenarios (i.e., a 100% cropped single-soil catchment) evaluated relative to their catchment scale distributions was 64–100% for the long-term annual average total Sum_{RE} mass fluxes per ha per year. There are three scenarios that have zero catchments more severe than the

TABLE 6 USEPA standard scenarios soil loss

Scenario	Soil loss, tons/ac		Scenario	Soil loss, tons/ac		Scenario	Soil loss, tons/ac	
	30-year Avg.	Max. year		30-year Avg.	Max. year		30-year Avg.	Max. year
CA alfalfa	0.08	0.19	TX-south cotton	2.75	7.02	MS corn	52.7	155.9
IL alfalfa	0.42	1.42	TX cotton	12.2	53.4	NC corn E	6.50	10.9
MN alfalfa	0.002	0.01	GA pecans	3.98	11.5	NC corn W	1.87	5.02
NC alfalfa	0.05	0.14	MS soybean	6.94	19.5	ND corn	0.41	1.13
PA alfalfa	0.30	1.60	ND wheat	0.71	3.46	NE corn	2.71	5.78
TX alfalfa	0.01	0.03	CA corn	1.92	6.13	OH corn	10.1	37.3
CA almond	0.12	0.57	IA corn	12.6	34.4	PA corn	5.27	31.9
FL citrus	1.69	3.11	IL corn	11.0	23.9	TX-south corn	2.16	5.56
CA cotton	0.13	0.69	IN corn	1.02	3.22	TX corn	18.7	59.7
MS cotton	33.0	93.8	KS corn	1.91	4.60	FL sweet corn	1.58	2.85
NC cotton	30.0	54.2	MN corn	1.09	4.66	OR sweet corn	9.17	14.0

Note: Scenarios considered unsustainable (30-year average or maximum year soil loss above 5 tons/ac) are shown in bold.

USEPA standard scenario (IL alfalfa, PA alfalfa, and GA pecan) and 25 scenarios are greater than the 99th percentile. Only five of the 36 USEPA scenarios evaluated fall below the 90th percentile of catchment scale Sum_{RE} vulnerability, indicating that the great majority of the standard scenarios are significantly more vulnerable than the intended assumption that scenarios would approximate the 90th percentile of the real-world Sum_{RE} vulnerability distribution when using real-world soil and weather and crop co-occurrences at the catchment scale.

SOURCES OF UNCERTAINTY

The present study used publicly available data to develop a modeling framework to assess the mass flux of a generic pyrethroid from Sum_{RE} after treating nine Col across all soil and weather co-occurrences with the Col both nationally and when aggregated on a catchment scale across the USA. Just as the USEPA conservative standard scenario (10-ha field 100% cropped and 100% treated with a pesticide) is based on a series of simplifying assumptions, modeling the average annual total Sum_{RE} mass flux generated nationally or regionally on a catchment scale has certain inherent assumptions and uncertainties. This section describes a few such sources of potential uncertainty in our estimates; Table S1 provides a more comprehensive analysis.

As described in detail above, a key assumption in this study is the relevance of the spatial scale of the NHD+ catchments to farm-scale operations when considering the delivery of runoff and erosion to USA flowing waters. The authors believe that the spatial scale of NHD+ catchments is highly relevant for evaluating the landscapes that deliver runoff and erosion. Critically, the comparison of catchment sizes to farm sizes indicates the NHD+ catchments cover a similar range of areas, which makes them relevant to farm-

scale management of the land; the median catchment size (160 ha) is equivalent to the 2019 USA average farm size (180 ha) (USDA, 2020). However, catchment sizes vary considerably based on topography and will be more or less representative of a single or small set of farms accordingly. In addition, several other potential sources of uncertainty can serve to either increase or decrease our estimates of Sum_{RE} mass flux.

Firstly, there are already many well-documented sources of uncertainty associated with the multiple assumptions (e.g., storm characteristics, planting and harvest dates, and curve number) embodied in the USEPA PRZM scenario definitions. For example, SAMSON weather precipitation data were assigned to all model runs across catchments. In reality, rainstorm intensity may vary at an even more local scale and vary across the cropped fields during a given day. Similarly, the maximum number of permitted applications of a pesticide is only infrequently used to counter extreme pest pressures since these rarely occur. Additional assumptions inherent in regulatory Sum_{RE} modeling are listed in Table S1.

An additional source of uncertainty is that the modeling assumed that all Sum_{RE} pyrethroid residues would potentially be available to be transported to a stream and leave a catchment. In reality, transport of eroded soil and associated pyrethroid residues typically depends on the proximity of a field (in this case a soil component) to the stream, with deposition en route greatly depending on slope and channeling. It is generally accepted that sediment delivery at the catchment scale is considerably lower than for small plot studies (Almendinger et al., 2014). In that sense, the present study estimates of average total transport to the stream are most likely overestimates.

The present study used an extremely hydrophobic compound, and thus, results are driven primarily by

erosion processes and results could be significantly different for a more soluble chemical, which would have a lower tendency to sorb to soil and be transported via erosion. Soil erosion is a site-specific phenomenon dependent on very localized conditions with respect to rainfall intensity, soil erosivity, slope, slope length, soil cover, and conservation practice. Therefore, it is not practical to consider the PRZM simulations reported here as precise predictors of erosion. Rather, these simulations are comparative, providing a useful standardized method for a national ranking suitable for identifying areas of higher and lower potential crop-specific vulnerability. As previously discussed, the simulated eroded sediment may result in an HEL condition but growers with fields considered to have highly erodible soils generally will install management practices (e.g., reduced or no tillage, contouring, etc.) to reduce soil erosion.

There is also spatial and temporal uncertainty of crop–soil relationships and catchment cropping density. While CDL change annually, and therefore the soil and crop associations may vary, the extremely large population size of cropped catchments and five years of soil/crop combinations provides sufficient soil/weather/crop combinations to be representative of any single year.

DISCUSSION

This study has created a novel dataset by using a runoff + erosion modeling approach to estimate the potential for off-target transport of a highly hydrophobic molecule from every co-occurrence of nine Col across a f-year span with particular soil and slope combinations identified in the SSURGO databases. Each co-occurrence was modeled using daily data from the most appropriate weather station with typically 30 complete years of daily measurements. This enormous new dataset has then been used to provide context to better understand the output from the USA standard pesticide aquatic exposure assessment procedure, which uses a small number of crop-specific scenarios for 30-year daily modeling. These standard scenarios were designed, often many years ago, with the intention that they should represent the 90th percentile of crop-specific vulnerability.

In the first comparison, the runoff + erosion flux modeled with the standard scenarios for nine Col was compared with the national distribution of Sum_{RE} flux for all co-occurrence of the Col and soils (on an area-weighted basis). The results showed that several of the important standard scenarios generate output higher (in some scenarios much higher) than the expected 90th percentiles while in other instances the standard scenarios were not severe enough.

More importantly, a second analysis aggregated the Sum_{RE} flux data at the NHD+ catchment scale since these are the best representation of the farm-scale areas, which actually deliver runoff and erosion to the USA stream network. The extent of soil and weather co-occurrences with a Col in each catchment as a fraction of the total delivery area becomes a significant factor in this second analysis.

Comparing these results with standard scenario output shows that, in most cases, the standard scenarios are exceptionally over predictive when compared with the actual range of Sum_{RE} flux likely to occur from real-world delivery areas.

While it is important to consider the sources of potential uncertainty listed above when examining this approach, there are several reasons why these results are realistic. Firstly, many of the sources of uncertainty (Table S1) are equally applicable to output from both the modeling in this paper and also the standard scenario modeling such that any associated uncertainty applies equally to both approaches. Secondly, the potential uncertainty associated with catchment scale might be concerning if a few individual catchments were being considered; however, the range of catchment numbers across all the Col (~7500–~750 000) suggests that many individual uncertainties will have been normalized across the data distributions. Finally, reports have indicated that regulatory predictions of runoff and erosion are overestimates, which supports these overall findings (e.g., USEPA, 2020b, 2021).

It is also worth mentioning that, while this hypothetical modeling output is directly applicable to sediment transport and other highly hydrophobic pesticides, the general observation of overestimation of runoff and erosion will likely also apply to regulatory aquatic exposure modeling for hydrophilic pesticides.

CONCLUSIONS

Pesticide registrations rely on prospective exposure estimations from models to make important decisions regarding whether a potential product is approved for safe use. Over the past few decades, USEPA has developed a set of standard crop scenarios for use in the pesticide registration process to predict waterbody annual maximum concentrations that are assumed not to be exceeded more than one year in 10 at every Col location in terms of Sum_{RE} pesticide transport vulnerability (USEPA, 2004). However, the present analysis using a hypothetical pyrethroid shows that, compared to the distribution of catchment-scale crop-specific Sum_{RE} mass flux at either national or regional spatial extents, the majority of the USEPA crop scenarios that were simulated (comparable to a 100% cropped single-soil catchment) were more severe than 90% of the total national or regional catchment area that has been cropped at least in part to the Col (31 scenarios out of 36). Twenty-five of those standard scenarios were more severe than the 99th percentile of the total national or regional catchment area.

The USEPA recently acknowledged the overconservative nature of its scenarios and stated that the majority of its standard crop scenarios were more vulnerable than the intended 90th percentile (USEPA, 2020b) and have started to make revisions. This means that the current regulatory process, including the past 20+ years when these scenarios have been used, is more protective than the desired protection goals when these (and possibly other) standard scenarios are used since they imply that the potential for

aquatic exposure is higher than is likely for the 90th percentile goal. This does not mean that the exposure estimates from the USEPA standard scenario results are wrong; it just indicates that they are less likely to occur than the intended 90th percentile goal.

While being overly protective ensures risk-averse outcomes, there are associated implications. For example, one consequence might be that over predicted pesticide transport in a particular scenario could mean that the Col may not be included as a registered crop use on a pesticide label. One possible effect of this is that growers might be restricted in the variety of tools available to produce safer and less expensive food using fewer cropped acres, ultimately resulting in less impact on the environment.

To understand why the overprediction of Sum_{RE} flux in USEPA's standard scenarios is not simply a sensible way of introducing conservatism into the regulatory process, it is important to consider the intent of parameterizing the standard scenarios (i.e., soils prone to runoff and erosion; HSG C and D) as well as the many conservative factors already built into the simulation framework. The framework-related assumptions (23 of which are documented in Table S1) include using protective estimates of pesticide dissipation, the use of the maximum application rate, application numbers, and intervals, assuming 100% cropping intensity, 100% of Sum_{RE} mass drains to a waterbody, lack of parameterization of best management practices, and so forth. These factors, as parameterized in the standard regulatory modeling approaches, all tend to lead to the simulation of higher exposures than expected in the real world and are acknowledged to be generally protective. However, until now, the Sum_{RE} flux potential of the standard scenarios based on soil and weather factors was understood to reflect the regulatorily defined severity for a given crop/region (i.e., 90th percentile). The findings in this paper indicate that this assumption was invalid in many scenarios, and thus Sum_{RE} flux is overestimated beyond the acknowledged levels of precaution to an unexpected and unintended extent (especially for hydrophobic active ingredients). This overestimation is on top of the nonsoil/weather-related assumptions already used in the estimation of environmental concentrations (i.e., Table S1). Consequently, USEPA risk managers should factor this information into their evaluation of potential risks under FIFRA and should also consider modifying the current standard scenarios.

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DATA AVAILABILITY STATEMENT

Data and associated calculation tools for this manuscript are available as Supporting information or from Ms. Amy Ritter (rittera@waterborne-env.com).

SUPPORTING INFORMATION

The Supporting Information file consists of additional and supporting data, tables, and figures.

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