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Methodology for evaluating pesticides for surface water protection: Spatial modeling for aquatic exposure assessment

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1 Introduction

The Surface Water Protection Program (SWPP) of the California Department of Pesticide Regulation (CDPR) is developing a more consistent and transparent method for pesticide fate and transport in surface water. The methodology was first developed for evaluating registration packages and implemented in the Pesticide Registration Evaluation Model (PREM) (Luo and Deng, 2012a, 2012b; Luo, 2014, 2017a). Later, the modeling capabilities of PREM were extended for post-use risk assessment of pesticides in agricultural and urban settings in California (Budd and Luo, 2016; Luo, 2017b, 2017d; Xie *et al.*, 2018). In summary, two modeling approaches are incorporated in the current version of PREM:

1) "Registration evaluation". With this model application, PREM makes registration recommendations for pesticide products based on the chemical properties (environmental fate data and aquatic toxicology data), product label information, and predefined modeling scenarios. Documents for registration evaluation are posted on CDPR's webpage for Surface Water Models (cdpr.ca.gov/docs/emon/surfwtr/sw_models.htm).
2) "Exposure assessment". This approach is applied to pesticides already registered and used in California. It examines risks to aquatic organisms from reported pesticide uses and evaluates the effectiveness of mitigation practices proposed after registration. Case studies for exposure assessments are documented in analysis memos and peer-reviewed papers (Budd and Luo, 2016; Budd *et al.*, 2017; Luo, 2017b, 2017c, 2017d; Xie *et al.*, 2018; Luo, 2019, 2020).

Currently, both approaches are based on *unit* simulations, where pesticide applications are modeled in one template (a field of 10 ha). The only difference is how they represent pesticide applications in terms of rate, frequency, timing, and extent. Registration evaluation follows the proposed product label (e.g., the maximum application rate and the maximum number of applications) and makes the most conservative assumptions on pesticide applications, while exposure assessment considers additional data for pesticide uses reported or observed in California. For example, the frequency and time frame of agricultural uses of bifenthrin were summarized from Pesticide Use Report (PUR) data (CDPR, 2019) and incorporated into the baseline simulations by PREM to replicate the current exposure levels observed in monitoring data (Luo, 2017d). For urban uses, survey results for the treatment extent and frequency (Winchell and Cyr, 2013) were used in the exposure assessments for fipronil (Budd and Luo, 2016; Budd *et al.*, 2017) and bifenthrin (Luo, 2017b, 2017c). Essentially, both approaches simulate the worst-case conditions of pesticide uses in California, either registered with the product labels or reported in actual applications. Therefore, the primary limitation of the current PREM-based exposure assessment is that the unit modeling is not able to capture the spatial variabilities of pesticide uses and environmental conditions.

In this study, a new modeling approach called "spatial modeling of PREM" is proposed in order to generate more realistic, yet protective, predictions for exposure assessment. The new approach is based on *spatial* modeling with reported pesticide uses and associated field conditions. This approach enhances the modeling capability of PREM for exposure assessment of agricultural pesticide uses with a more detailed spatial perspective. The spatial modeling approach is developed to automatically prepare spatially distributed input data, manage individual PREM runs, and post-process modeling results. Compared to the unit simulations, the spatial modeling of PREM considers the spatial variability of field size, pesticide application data, dilution from untreated fields, and environmental and landscape conditions (crop, soil, and weather). Two spatial scales are involved: simulations for individual fields with reported pesticide uses, and spatial aggregation at section level (1×1 mi^2). Each field is modeled for the estimated environmental concentrations (EECs) in a hypothetical receiving water body. The size of the water body is proportional to that of the field with a ratio of 1 ha (water) to 10 ha (field), which is derived from the United States Environmental Protection Agency) (USEPA) standard pond scenario. For all fields in a section, the model-predicted EECs are summarized as the average weighted by the corresponding field sizes, which are reported as the representative EECs for exposure assessment in each section. In this study, the predicted representative EECs are compared with monitoring data for model validation.

2 Review of relevant studies

Table 1 summarizes representative modeling approaches for pesticide exposure assessment. All demonstrated models are based on the Pesticide Root-Zone Model developed by the USEPA (2022a) as the simulation engine for landscape processes. Pesticide transport processes in a receiving water body are simulated via various modeling approaches, e.g., VVWM (Variable Volume Water Model), EXAMS (Exposure Analysis Modeling System), AGRO-2014, or SWAT (Soil Water Assessment Tool).

Both PREM and PWC (Pesticide in Water Calculator) conduct screening-level evaluation, and they have no major differences for agricultural uses of pesticides in California. As deterministic models, PREM and PWC only report one single value of an estimated environmental concentration (EEC) for each set of output variables (e.g., the aqueous EEC in the water column of a certain period of moving average).

Probabilistic modeling for pesticide exposure assessment is usually developed with stochastic simulations of multiple screening-level model runs, similar to sensitivity analysis. First, the spatial variabilities on weather data, application dates, soil properties, and percent treated area (PTA) are summarized as probabilistic distribution functions. For example, a uniform distribution can be defined by the observed minimum and maximum values or from an empirical distribution derived from observed percentiles. A large number of input datasets are then generated from the identified probability distributions. Finally, the model runs over all individual datasets and reports results as a distribution of EECs. While screening-level models answer the question "whether or not the pesticide applications could potentially cause adverse effects to surface water", probabilistic models further estimate the probabilities of the effects at various levels and statistically (not spatially) identify the ranges of input parameters associated with higher risks. Note that probabilistic modeling is still a scenario-based approach. Input datasets are statistically sampled from probability functions, not necessarily geo-referenced to acute field conditions.

Table 1. Existing and proposed modeling approaches for pesticide exposure assessment [1]

Approach	**Screening-level**	**Probabilistic**	**Spatial with label rates**	**Spatial with PUR data**	**Spatial with PUR data**
Examples [2]	PWC, PREM	Probabilistic exposure assessment	SAM v1.0a	CoPST	This study
Type of modeling	Unit	Unit	Spatial	Spatial	Spatial
Modeling unit	Template field	Template field	10×10 m	HRU	Field
Spatial resolution	NA	NA	NHD catchment	Section (1×1 mi^2)	Section
Environment (weather, soil, PTA)	Crop modeling scenarios (USEPA, 2022b)	Probability distribution	Site-specific data	Site-specific data	Site-specific data
Pesticide applications	From labels	From labels [3]	From labels [3]	PUR	PUR
Receiving waterbody	USEPA pond [4]	USEPA pond [4]	Flowing water [5]	NA	USEPA pond with surface area varying with drainage area [6]

Notes:

[1] Abbreviations: HRU = hydrological response unit, usually as unique combinations of soil and land use at a given spatial resolution; PTA = percent treated area; NHD = National Hydrography Dataset; PUR = Pesticide Use Reporting database in California.

[2] References for the example models: PWC = Pesticide in Water Calculator (USEPA, 2022a), probabilistic exposure assessment (Whitfield-Aslund *et al.*, 2017), SAM = Spatial Aquatic Model (USEPA, 2015), CoPST = Co-occurrence Pesticide Species Tool (Hoogeweg *et al.*, 2011)

[3] Local weather data and crop operation calendars were considered to determine the time windows for pesticide applications.

[4] The USEPA pond has a surface area of 1 ha and depth of 2 m.

[5] SAM version 1.0 alpha only reports aqueous concentrations of pesticide in water column.
[6] This study models a hypothetical receiving water body with a surface area determined from the drainage area with a ratio of 10 ha field to 1 ha pond, and other properties taken from the USEPA pond scenario.

Spatial modeling for pesticide exposure assessment is based on site-specific field conditions. SAM (Spatial Aquatic Model) is a spatially continuous model developed by USEPA, with 10×10-m grid cells for landscape simulation. The publicly available version of SAM (alpha 1.0) was only developed for Ohio River Basin with atrazine as a test agent. Model simulations are driven by spatially distributed data of land use, soil, and weather prepared for each cell. Modeling results are further aggregated at the spatial resolution of the National Hydrography Dataset (NHD) catchment for estimating EECs. Unlike the probabilistic modeling approach, each input dataset in spatial modeling is specific to a spatial unit (e.g., a field or grid cell). So, the model outputs reflect the spatial variability of predicted pesticide exposure over the simulation domain.

With pesticide use data available from the PUR database, more efforts for spatially continuous modeling are observed in California. One of the first studies was to predict the distribution of diazinon concentrations in the Sacramento River Basin's main drainage canal (Snyder and Williams, 2004). Similar approaches were used to model organophosphate and pyrethroid pesticides in the Central Valley (Dasgupta *et al.*, 2008; Luo *et al.*, 2008; Luo and Zhang, 2009c, 2009a, 2009b, 2010, 2011). In the development of CoPST (Co-occurrence Pesticide Species Tool), this modeling approach was extended to the risk assessment of 40 pesticides in California's Central Valley and Bay-Delta area (Hoogeweg *et al.*, 2011). All spatial modeling studies with PUR data were developed with a resolution of *section* (about 1×1 mi area) in the Public Land Survey System (PLSS), consistent with that of the PUR. Each section may include multiple properties and commodities and thus requires multiple model runs.

3 Model development

3.1 Modeling overview

This study proposes incorporating a spatial modeling approach into the PREM framework. Offsite movement of pesticides is simulated for each treated field in a section. Compared to other spatial modeling of pesticides, the proposed approach is designed to provide EECs more consistent with the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) Tier 2 modeling framework for ecological risk assessment. Specifically, reported pesticide use data for a field in a certain year are repeatedly modeled for 30 years under the historical meteorological conditions observed in a nearby National Climatic Data Center weather station by National Centers for Environmental Information (NCEI, formerly the National Climatic Data Center). Similar to the previous PREM results for registration evaluation, the new approach reports one set of EEC results for each field and each year of PUR data. In addition, the new approach manages multiple model runs over fields and years of PUR data to represent spatial variability and temporal trends of aquatic ecosystem exposure to pesticides. In summary, the proposed modeling approach is implemented by spatially distributed modeling of PREM with site-specific data of landscape properties and reported pesticide uses.

Spatial modeling of PREM is developed with two components (Figure 1):

1) S*ite-specific simulations* by extending the existing modeling capabilities in the PREM framework. “Site” here refers to a field with reported pesticide uses and follows the terminology in the PUR. Each site is modeled with a hypothetical receiving water body. Based on the pesticide use data, crop modeling scenarios, and environmental characteristics, EECs in the water column and benthic region of the water body are predicted for each site.
2) A new component for *spatial aggregation* of the results from individual PREM runs. The EECs predicted at individual sites within a section are summarized as field-size weighted averages. Untreated fields or areas in the section are set with zero EECs and also considered in spatial aggregation. Finally, the model reports average EECs for each of the sections in the simulation domain.

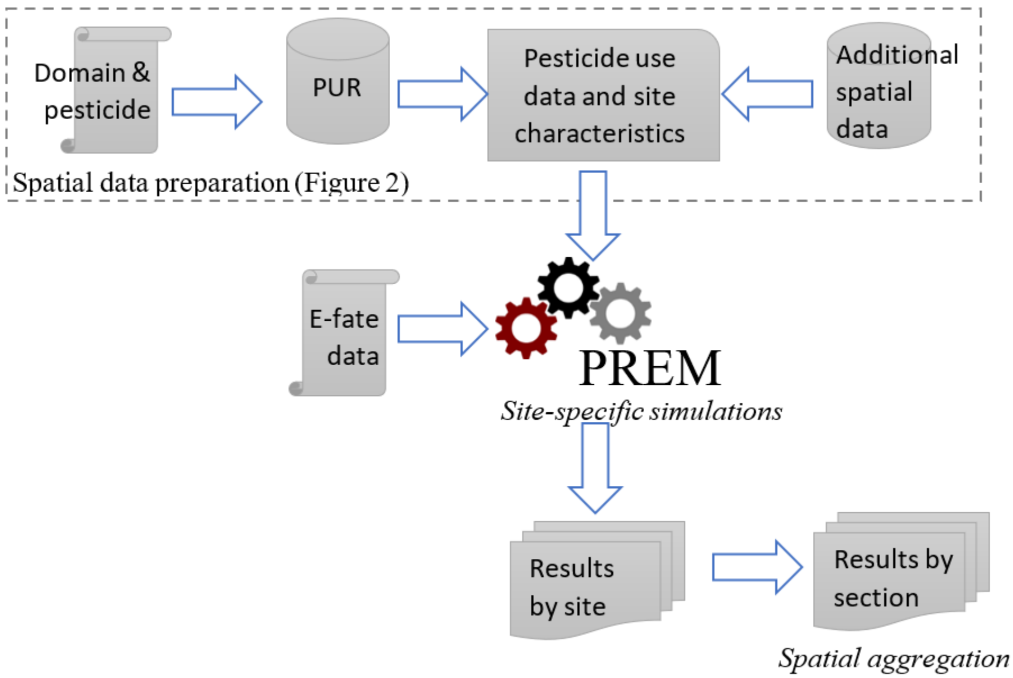


Figure 1. Spatial modeling approach for PREM

3.2 Site characterization

Unlike the screening-level modes for a template field, site-specific simulations are conducted for each site over the entire modeling area. “Site” here is defined in each section by two variables of the PUR: site location ID (SITE_LOC_ID) and site code (SITE_CODE). The site location ID spatially locates the field within a section, while the site code specifies the land use type of the field. The site location ID indicates a particular location (field) where an application occurs. No consistent format exists for SITE_LOC_ID. It is assigned as unique characters (by year and by section) at the discretion of County Agricultural Commissioners (CACs) and growers. Site code, also known as commodity code, indicates the target site to which a pesticide product is applied. SITE_CODE is from a list established by the USEPA and modified by CDPR. For example, lettuce (head) is assigned the site code of 13045. Table 2 shows an example of pesticide use records in the PUR indexed by the two variables. More details on the PUR data query and pre-processing for spatial modeling of PREM are provided in the next section.

Table 2. Example of SITE_CODE and SITE_LOC_ID in the PUR, showing records for agricultural uses of imidacloprid in the section M12S03E17 during 2016

SECTION	SITE_LOC_ID	SITE_CODE	Acre treated	Pound applied	Application date
M12S03E17	710001	13045	13	0.61	4/28/2016
M12S03E17	710001	13031	12.5	0.58	4/28/2016
M12S03E17	710002	13031	11.5	0.53	4/28/2016
M12S03E17	710001	13045	13	0.61	5/10/2016
M12S03E17	710001	13024	12.5	0.61	7/11/2016
M12S03E17	710001	13024	12.5	0.61	7/11/2016
M12S03E17	710002	13024	11.5	0.52	7/12/2016

Site-specific simulations are conducted for each unique combination of section, SITE_CODE, and SITE_LOC_ID (the first three columns in Table 2) retrieved for the pesticide of interest over the modeling domain. Taking the data in Table 2 as an example, five "sites" for modeling are identified for the section M12S03E17 in 2016: spinach (SITE_CODE=13024) in the field with SITE_LOC_ID=710001, spinach in 710002, lettuce (leaf) (SITE_CODE=13031) in 710001, lettuce (leaf) in 710002, and lettuce (head) (SITE_CODE=13045) in 710001.

Spatial data are prepared for each identified site. Spatial data here refer to modeling input data for pesticide use and environmental conditions. Other input data such as physicochemical properties and reaction half-lives will follow the same guideline for PREM (Luo, 2017a; Luo *et al.*, 2019).

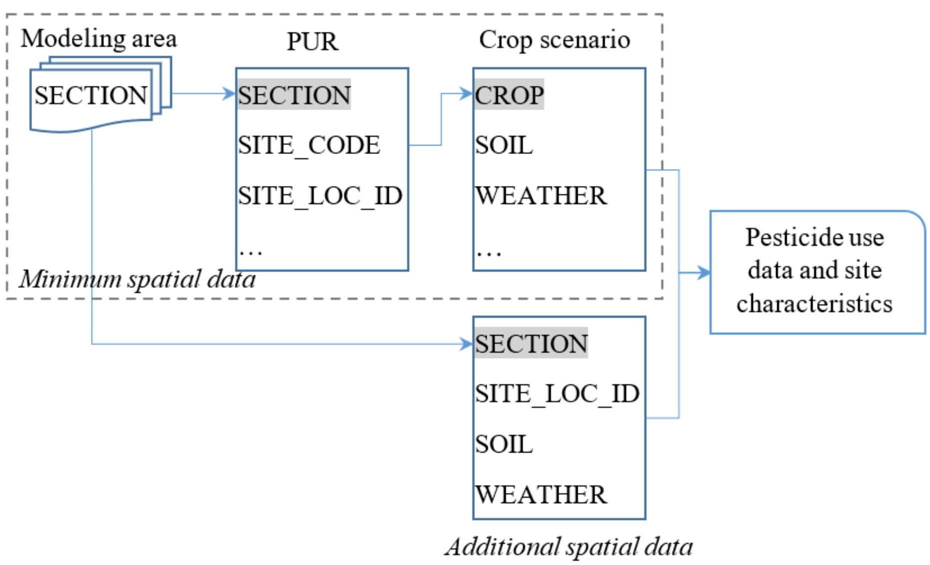


Figure 2. Preparation of pesticide use data and site characteristics

A modeling area is geographically defined by sections (Figure 2). The approach is similar to that in the Surface Water Monitoring Prioritization (SWMP) model, which is also based on PUR data at the section level for agricultural uses (Luo *et al.*, 2013; Luo and Deng, 2015). For each section in the area, pesticide use records are retrieved from the PUR during the modeling period. In addition to the PUR variables demonstrated in Table 2, the general description of spray method, AER_GND_IND, is also used to separate ground (AER_GND_IND =“G”) and aerial (“A”) applications. However, the PUR does not specify different ground application methods, such as air blast, ground boom, and soil incorporation. Pesticide label review may be needed to determine the spray method for a reported ground application.

In addition to pesticide use data, the PUR also provides information for site characterization. A SITE_CODE could be linked with a crop scenario for pesticide runoff modeling (USEPA, 2022a), which summarize representative data for the crop and associated environmental conditions (soil, weather, and other hydrometeorological parameters) in a state or region. Crop scenarios are widely used in pesticide modeling; the screening-level models directly use the predefined parameters in the scenarios, while other models alter the parameter values by considering their probability or spatial distributions (Table 1).

In the spatial modeling of PREM, the input parameters for crop management and landscape descriptions are first initiated from the crop scenarios. A scenario is usually named after a representative crop, but actually developed for a group of crops (i.e., multiple SITE_CODEs). In the ecological risk assessment (ERA) for imidacloprid (USEPA, 2016a), for example, the “onion” scenario (“CAonion_WirrigSTD”) was used for both onion and leek, and all crops in the group of leafy greens are simulated with the “lettuce” scenario (“CAlettuceSTD”). This development incorporates all 29 crop scenarios for California, including the 16 scenarios which have been utilized in PREM for registration evaluation (Luo, 2017a). To link the two data sources of PUR and crop scenarios, a lookup table is developed to assign SITE_CODEs to each scenario (Figure 2). The lookup table is built based on the modeling settings in the previous ERAs on various pesticides by USEPA and other organizations. The 2017 assessment on malathion (Clemow *et al.*, 2017) provides a comprehensive summary of the use of the crop scenarios in California.

Soil data in the crop scenarios are derived from the representative cropping areas for the corresponding crop in California. This data can be improved by extracting soil properties at the exact location of a section (or a field, if field boundaries are available) from a soil database such as SSURGO (Soil Survey Geographic Database). Pre-processing of SSURGO data for hydrological and pesticide modeling has been documented previously (Luo *et al.*, 2012).

Integrated in the crop scenarios are meteorological data from 237 weather stations in the Solar and Meteorological Surface Observation Network (SAMSON) throughout the United States from 1961 to 1990 (USEPA, 2006). The data have been recently extended to 2014 using National Oceanic and Atmospheric Administration (NOAA) products (Fry *et al.*, 2016). Other weather data, such as California Irrigation Management Information System (CIMIS), can be optionally used in the spatial modeling of PREM to override the built-in data from SAMSON or NOAA. To be consistent with the previous model settings for registration evaluation and exposure assessment, a minimum period of 30 years is required for weather data.

3.3 Hypothetical receiving water body for each site

To be consistent with the FIFRA modeling framework for ecological risk assessment, each site is modeled with a hypothetical receiving water body. The surface area of the water body is determined from the field size with a fixed ratio of 10 (field):1 (water). Note that the total field size, including both treated and untreated portions, is used in the characterization of its receiving water body. Pesticide application is assumed to be evenly distributed over the field, and the effective application rate (mass applied normalized by total field size) reflects the PTA for exposure assessment.

The value of 10:1 used in this study is derived from the modeling scenario of the USEPA standard farm pond, which assumes a 10-ha field draining to a 1-ha pond. This scenario has been widely accepted for pesticide risk assessment and incorporated into PREM for registration evaluation. Previous studies suggest that the field:water ratio derived from the pond scenario is appropriate for regulatory exposure assessment for agricultural (Xie *et al.*, 2018) and urban (Luo, 2014) settings in California.

Except for the surface area, other input parameters for the hypothetical water body are taken from the pond scenario (Table 3). For each identified site, the spatial modeling of PREM predicts the 1-in-10-year EECs of a pesticide in the water column and benthic region of the hypothetical water body, referred to as site-specific EECs, which will be further aggregated at the section level (more details in the next section). The same statistics have been used by the USEPA and CDPR for pesticide registration evaluation and post-use exposure assessment. EECs can be calculated at user-specified time periods for averaging, such as daily average for acute exposure and 21-d moving average for chronic exposure. In the case study of this report (Section 4), both daily and 21-d EECs are reported; daily EECs are presented as the primary outputs for illustration and model validation.

In addition, site-specific simulations also report pesticide loadings from the treated field. The loadings include the contributions by water runoff, soil erosion, and spray drift. Each of these loadings is calculated as the cumulative amount normalized by the total mass applied, called the load as percent of use (LAPU). For example, LAPU(runoff)=1% indicates that the predicted pesticide loading in dissolved form from the treated field is 1% of total mass applied to the corresponding area and period of modeling. The total LAPU is the sum of three components: runoff, erosion, and drift.

Table 3. Input parameter values for the hypothetical receiving water body in the spatial modeling of PREM

Parameter	Value
Surface area (m^2)	[Field area]/10
Water column depth (m)	2
Benthic depth (m)	0.05
Water column suspended solids (SS, mg/L)	30
Water column fraction of organic carbon (foc, -)	0.04
Water column dissolved organic carbon (DOC, mg/L)	5
Water column biomass (mg/L)	0.4
Benthic porosity (-)	0.5
Benthic bulk density (g/cm^3)	1.35
Benthic foc (-)	0.04
Benthic DOC (mg/L)	5
Benthic biomass (g/m^2)	0.006

Note: the surface area varies with the field size; other parameters are set at the default values in the USEPA standard pond scenario (Young, 2019).

3.4 Spatial aggregation of site-specific EECs

The simulation design for the spatial modeling of PREM is similar to that previously used for a complex landscape where model simulations are managed for multiple modeling units and the results from individual units are aggregated at a given spatial resolution. For example, two urban "surfaces" are used in USEPA's nationwide suburban scenario (USEPA, 2012, 2013) and surface-specific model outputs are aggregated in a predefined 10-ha urban watershed. Similarly, four surfaces are incorporated in PREM for urban pesticide evaluations in California (Luo, 2014). Modeling "site" in the spatial modeling of PREM is conceptually equivalent to the modeling "surface" used in urban evaluations, while a section represents the resolution for spatial aggregation.

Although the field sizes and surface area of the hypothetical water body vary from site to site, they have the same drainage area normalized to capacity (DANC) (USEPA, 2017). That means the predicted EECs for each site are independent of the field size (and thus the water body area), but only related to application data and crop modeling scenario. Note that PREM simulations are based on pesticide application rate (kg/ha, calculated as [mass applied]/[acre treated] and converted for unit) rather than mass applied (kg). For a given application rate (or multiple applications characterized by individual rates) and modeling scenario, for example, a modeling unit of "20-ha field, 2-ha water" and another unit of "40-ha field, 4-ha water" would be predicted with the same values of EECs.

This property greatly simplifies site-specific simulations: all sites can be modeled with the same field size (thus the same surface area of water body) with their application rates normalized by a predefined spatial resolution. This study considers a spatial resolution of section; therefore, the normalized application rate is calculated as the ratio between mass applied retrieved from the PUR for each application and the size of a section (usually about 1 mi^2 or 259 ha):

[Normalized rate] = [reported rate]/[size of a section]

Compared to the actual application rate reported in the PUR, the normalized rate reflects the fraction of the treated field size over the entire section, or the PTA. In spatial modeling, the PTA represents the dilution effects on EECs from the untreated area in the domain, including the untreated portions of a site and untreated areas in a section.

Note that there is no hypothetical water body modeled for a section. All model simulations for EECs are conducted at field scale with a hypothetical water body modeled at each site, and their results are aggregated at the section level for exposure assessment. In spatial aggregation, sites are grouped by section. The average value, weighted by modeled field sizes, of EECs or LAPUs predicted for sites within a section is reported as the representative EEC or LAPU at the section level. Finally, there are two EEC values (EEC in the water column and EEC in the benthic region) and a total LAPU value reported for each section. The representative EECs at the section level processed from the spatial aggregation are considered the primary outputs from the spatial modeling of PREM.

In addition to the section level, spatial aggregation can be conducted at other spatial resolutions. One example is the aggregation by crop groups, as demonstrated in the case study (Section 4) of this report: EECs and LAPUs are summarized for all sites in the simulation domain with crops in the same group.

4 Case study: agricultural uses of imidacloprid

4.1 Problem statement

Imidacloprid is a neonicotinoid insecticide used on a wide variety of agricultural crops in California. Imidacloprid has been monitored by CDPR's SWPP since 2010 (Starner and Goh, 2012); its monitoring has been extended to three regions: Salinas, Santa Maria, and Imperial. The overall detection frequency was 58%, and all of the detected concentrations exceeded the lowest chronic USEPA benchmark (10 ng/L) (Deng *et al.*, 2019).

Nationwide ERAs for imidacloprid have been conducted by the USEPA (2016b) and Intrinsik Environmental Sciences (Whitfield-Aslund *et al.*, 2017). Their modeling approaches (Table 1) are based on screening-level and probabilistic simulations, respectively. Some of the relevant modeling parameters and options from the two ERAs are used in this study.

The modeling area is defined by four counties (Imperial, Monterey, San Luis Obispo, and Santa Barbara) covering all CDPR agricultural monitoring sites (active and historical) for imidacloprid. Following the settings in the Surface Water Prioritization Model (Luo and Deng, 2015), this study uses the most recent three-year PUR data (2014-2016). There are about 1,240 sections per year (varies slightly by year) with reported uses of imidacloprid in the modeling area. No temporal trend is detected for the modeling area as a whole: the annual average application intensities are 29.2, 29.4, and 28.5 kg/section/year, for 2014, 2015, and 2016, respectively. Over the three years, imidacloprid was mainly used on lettuce (head and leaf, 28% of total use), wine grapes (22%), and broccoli (17%).

4.2 Modeling inputs

Application methods for agricultural uses of imidacloprid include applications to soil and the canopy, and seed treatments. Seed treatment is not reported in the PUR. In addition, imidacloprid-treated seeds are not commonly used in the study areas, so it is not considered in the case study. Three types of application methods are modeled: soil, foliar (including ground boom and airblast), and aerial applications.

As mentioned before, the PUR only separates ground vs. aerial applications. Soil and foliar methods are all reported as ground applications. They are further identified based on the product label review from the previous ERAs (USEPA, 2016a; Whitfield-Aslund *et al.*, 2017). Foliar applications are generally associated with lower application rates than soil incorporations. The maximum label rates for foliar applications are generally lower than 0.2 lb/ac (actually, most of them are ≤0.1 lb/ac), while ≥0.2 lb/ac rates are frequently observed for soil applications. Therefore, 0.2 lb/ac is used as the critical value to separate PUR-reported imidacloprid uses by soil or foliar applications (Table 4). Ground boom and airblast still cannot be differentiated using data from the PUR. With a higher drift fraction, the method of ground boom is selected to model all foliar applications.

Table 4. Application methods for imidacloprid and associated modeling parameters

Method	**AER_GND_IND**	**Application rate (lb/ac)**	**Required buffer (ft)**	**CAM**	**Application efficiency**	**Drift fraction**
Soil	G	≥ 0.2	-	1	100%	0
Foliar/boom	G	< 0.2	25	2	99%	0.0267
Foliar/airblast	G	< 0.2	25	2	99%	0.0150
Aerial	A	Any	150	2	95%	0.0385

Note: CAM = Chemical Application Method: CAM=1 (under-canopy application, linearly decreasing incorporation between soil depth 0-4cm), or CAM=2 (above-canopy applications with linear interception, linear decreasing incorporation between soil depth 0-4cm).

For soil applications, its drift fraction is assumed to be zero. For other methods, USEPA (2016a) estimated the drift fractions according to the label-required buffers, and the results are used in this study (Table 4). Application efficiency is set at 100% for soil applications, 99% for ground-boom and airblast, and 95% for aerial applications. The settings are consistent with the modeling guidance (USEPA, 2009) and the USEPA ERA for imidacloprid.

Field boundaries are not used in this case study. Environmental descriptions are based on the minimum input data sets, such as the built-in soil properties in crop scenarios and weather data from a nearby SAMSON station. Chemical properties and reaction half-lives of imidacloprid (Table 5) are taken from the USEPA ERA (USEPA, 2016a). Other environmental fate data are set at the default values following the USEPA guidance.

Table 5. Physicochemical properties of imidacloprid

PREM input variables	**Value**
Water solubility (mg/*l*)	610
KOC (*l*/kg[OC])	266
Hydrolysis half-life (HL, d)	Stable
Aerobic soil metabolism HL (d)	254
Aerobic aquatic metabolism HL (d)	236
Anaerobic aquatic metabolism HL (d)	81
Molecular weight (g/mol)	255.7
Vapor pressure (torr)	1.5E-9
Aqueous photolysis HL (d)	0.2

4.3 Result interpretation

The spatial modeling of PREM is applied to agricultural uses of imidacloprid in the modeling domain (four counties and three PUR years). Using year 2016 as an example, there are 29,768 agricultural application records of imidacloprid over the modeling area, reported in 15,292 sites (i.e., unique combinations of section, SITE_CODE, and SITE_LOC_ID). Site-specific simulations are conducted for each site. Results are first aggregated by sections and presented for the spatial distribution of predicted concentrations over the modeling area. In addition, modeling results are grouped by monitoring region for model validation and by crop group for management implications.

Spatial distribution

Modeling results are reported as 1-in-10-year daily aqueous EECs in water column (EECs or predictions, thereafter) for each section with agricultural uses of imidacloprid in the modeling domain. Predictions are plotted for the entire modeling area (Figure 3) and for each of the monitoring regions (Figure 4). The general spatial pattern of the EECs is consistent with the areas monitored by CDPR and the impaired water bodies in the 2018 303(d) list for pesticides from agricultural sources by California State Water Resources Control Board (SWRCB, 2020). Note that all Imperial Valley drains are listed as impaired streams by pesticides, but their sources are not explicitly identified (labelled as “unknown” in the list).

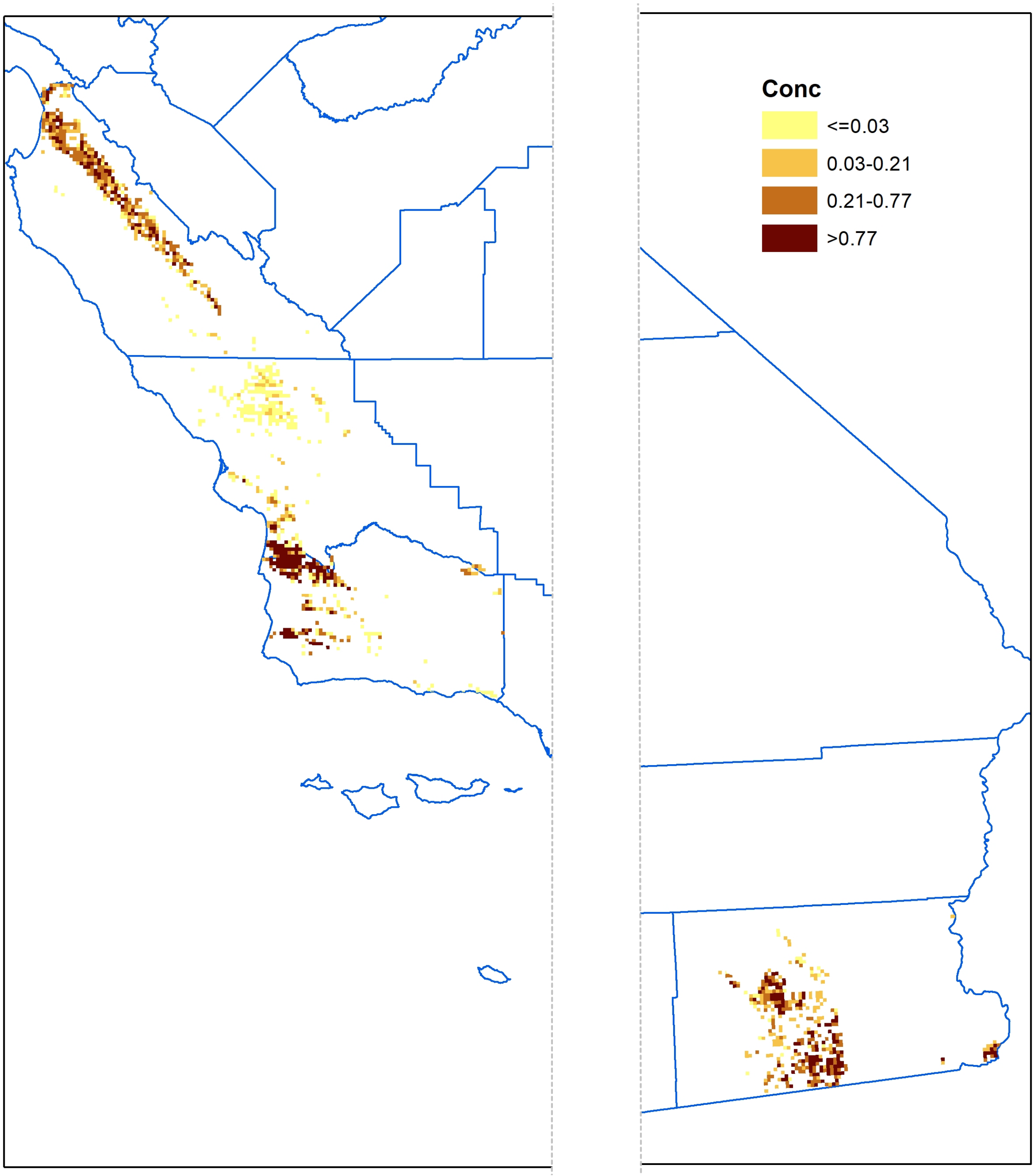
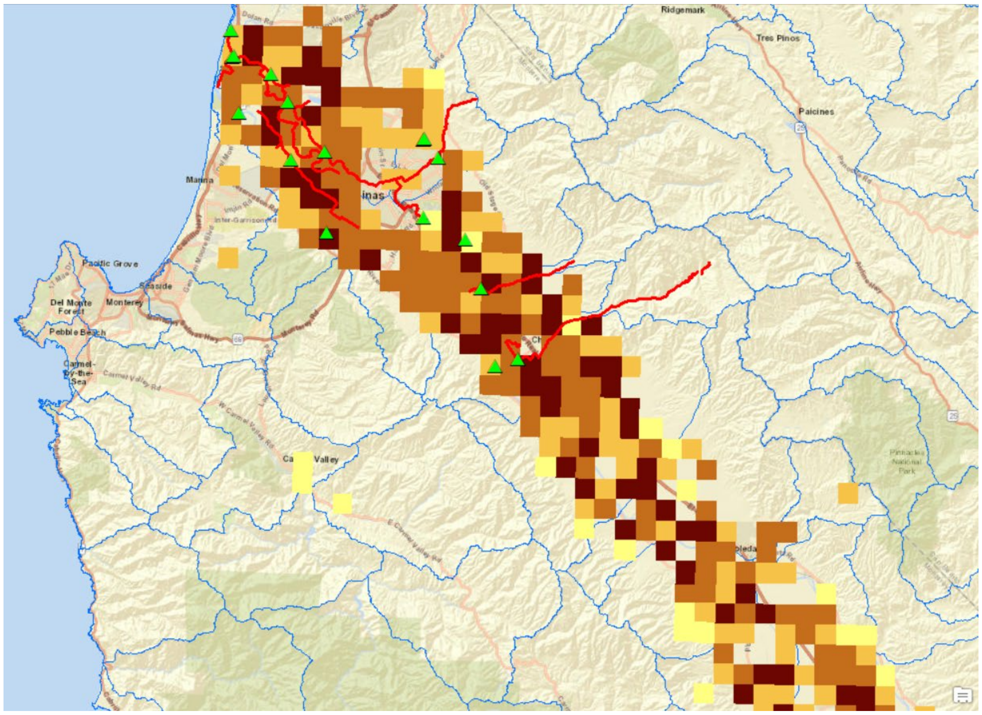


Figure 3. Model-predicted EECs of imidacloprid (ppb) from agricultural uses in the PUR years 2014-2016. Range classification of the EEC values is based on the “Quantile” option in ArcGIS

(a)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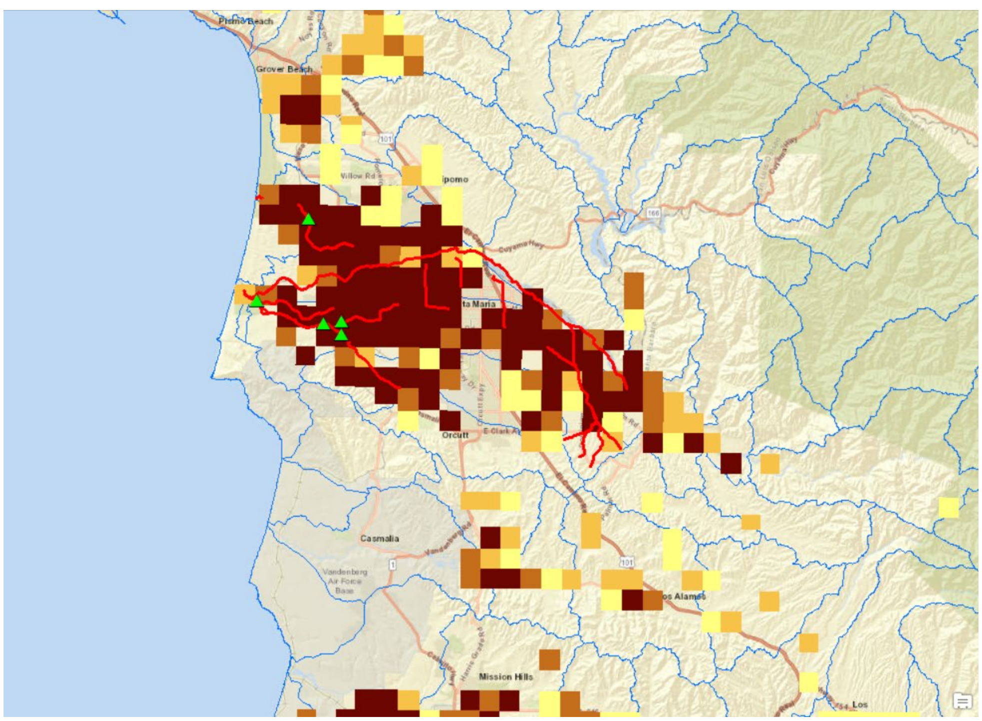
Marina
Pacific Grove
Seaside
Del Monte Forest
Monterey
Pebble Beach
Carmel-by-the-Sea
Pinnacles National Park

(b)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Grover Beach
Orcutt
Casmalia
Vandenberg Air Force Base
Mission Hills

(c)

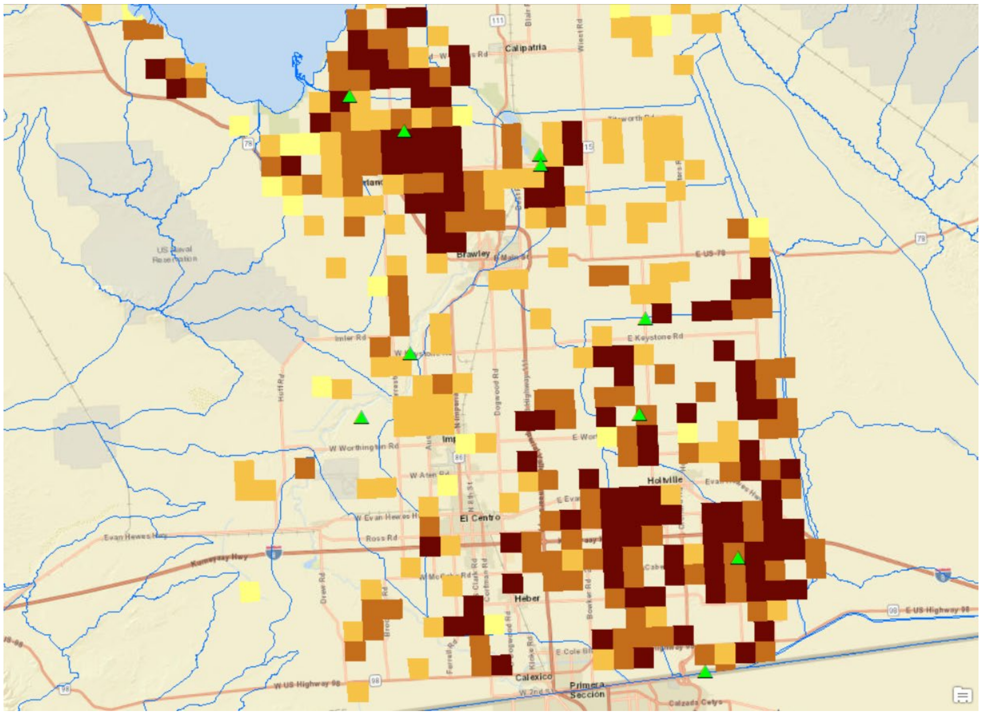

Figure 4. Model-predicted EECs of imidacloprid (ppb) over the monitoring regions of (a) Salinas, (b) Santa Maria, and (c) Imperial. All maps are drawn to the same scale of 1:300,000. EECs are displayed with the same value classification as in Figure 3. The maps also show CDPR monitoring sites (green triangles) (CDPR, 2022), 12-digit hydrologic unit code (HUC12, blue polygons) and river segments in the 303(d) list impaired by pesticides from agricultural sources (red lines).

Model Validation

Modeling results are evaluated using monitoring data. A monitoring dataset for imidacloprid has been compiled from Surface Water Database (SURF) (CDPR, 2022), including 421 grab samples collected by SWPP from 33 sites in three monitoring regions of Imperial, Salinas and Santa Maria valleys. For consistent comparison, the monitoring regions are delineated by HUC12s (watersheds with 12-digit Hydrologic Unit Code) which enclose the corresponding monitoring sites (Figure 4). For example, the five monitoring sites in the region of Santa Maria are located in two HUC12s ("180600060704 Oso Flaco Creek" and "180600080503 Corralitos Canyon"), so their monitoring data are compared to the model predictions for all sections in the two HUC12s.

Measured concentrations of imidacloprid are associated with various drainage areas, but higher concentrations are more likely observed near to the source before dilution in the stream network. This assumption is used in previous ERAs where model predictions are expected to capture the observed high concentrations. The same approach is implemented in the case study. For each region, the upper percentiles (90^{th} and 95^{th}) and maximum values of the monitoring data are compared to the same statistical summaries of EECs (Table 6). Results of the comparison indicate that the spatial modeling of PREM conservatively and reasonably predicts the observed concentrations of imidacloprid in the monitoring regions. The statistical summaries of predictions and observations (Figure 5) are significantly correlated (r=0.98 and p<0.001). The P/O ratio (prediction to observation, as statistical summaries) range from 0.9 to 2.6 with a median of 1.3, indicating that the model generally overestimates the monitoring data within a factor of 1-2.

Table 6. Predicted EECs compared to monitoring data, summarized as the maximum, 90th percentile (90%ile), and 95th percentile (95%ile). All values are in ppb

Monitoring region	**Observed 90%ile**	**Predicted 90%ile**	**Observed 95%ile**	**Predicted 95%ile**	**Observed Max**	**Predicted Max**
All (33 sites, 16 HUC12s)	1.80	2.39	2.58	3.42	9.86	13.2
Imperial (11 sites, 7 HUC12s)	0.60	1.59	0.85	2.08	3.48	4.28
Salinas (17 sites, 7 HUC12s)	1.58	1.45	2.16	1.92	9.86	13.2
Santa Maria (5 sites, 2 HUC12s)	2.75	4.95	5.05	6.18	9.14	9.57

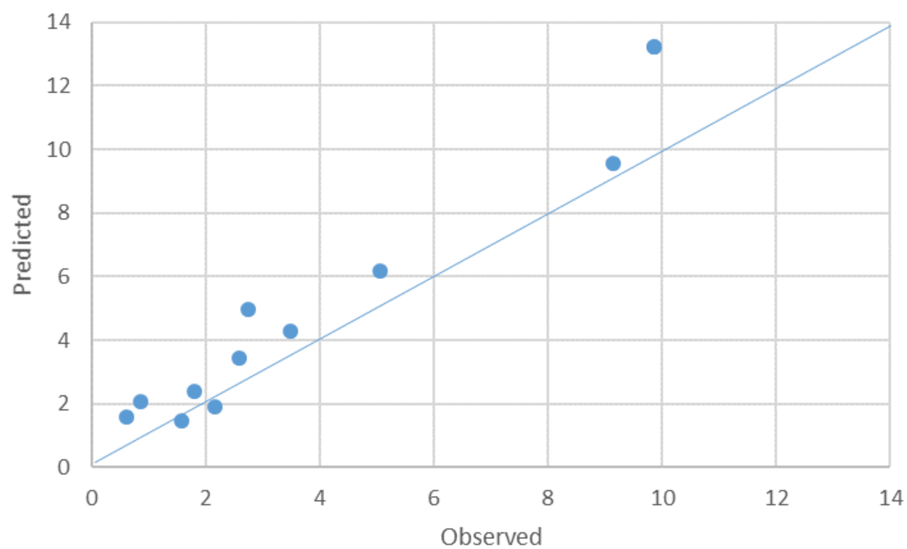

Figure 5. Comparison of the statistical summaries of the predicted and observed concentrations (ppb, Table 6)

In addition to the comparison of the maxima and upper percentiles, the probability distributions on all observed and predicted concentrations in the monitoring regions are compared (Figure 6). The underlying distributions for the two data sets are not statistically identical, but similar based on the Kolmogorov-Smirnov 2-sample test (test statistic = 0.109, and the critical value = 0.081 under significance level of 0.05). For all probabilities, predictions are within a factor of 2 of the corresponding observations. The model successfully captures the maximum concentrations in monitoring data (Table 6); however, it underestimates the observed probability of peak concentrations (>1.2 ppb, Figure 6). This is related to the different periods used in modeling and monitoring: the model continuously simulates for days and months in a year, while sampling events were prioritized for months with high-use and high-concentration of imidacloprid.

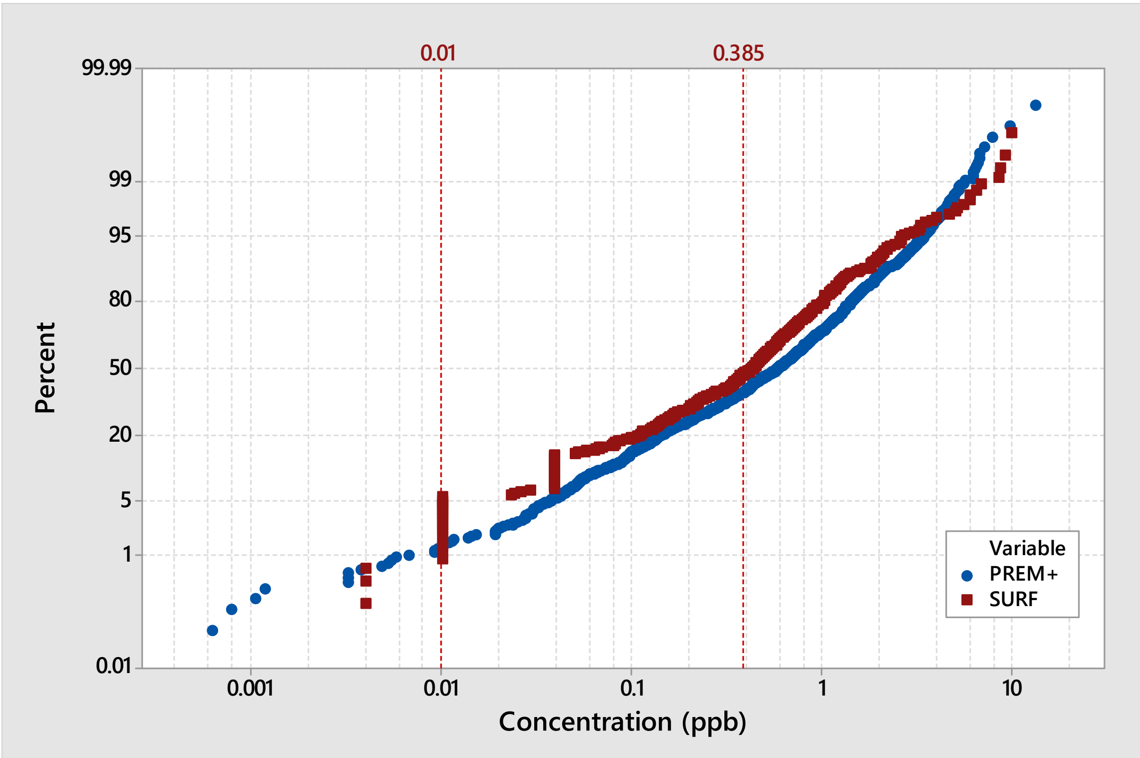

Figure 6. Probability plots of observed (SURF) and predicted (PREM+) concentrations for the monitoring regions over the four counties. Non-detects are replaced with the corresponding method detection limit for display purpose. The reference lines at x=0.01 and 0.385 ppb indicate the lowest chronic and acute benchmarks, respectively. Note that the displayed variables are based on different statistics: observations as instantaneous grab samples, prediction as 1-in-10-year daily EEC, and benchmarks with various toxicity test durations.

Management implications

Compared to screening-level models, results from spatial modeling better represent the current condition of pesticide residues and their distribution. In addition to the EEC grouping by region (Table 6), summaries by crop provide useful information for developing management and mitigation practices. Table 7 shows the average EEC and total LAPU for each crop group. Over all crops in the simulation domain, the total LAPU is mainly (96%) contributed by water runoff, thus indicating the high runoff potential of imidacloprid.

Table 7. Modeling results for selected crops

Crop group	Representative crops in the modeling area	Use	Average EEC (ppb)	Total LAPU
4 (leafy vegetables)	Lettuce, spinach	32%	1.07	2.2%
5 (brassica leafy vegetables)	Broccoli, cauliflower	27%	1.23	2.1%
13-07F (grape)	Wine grape	22%	0.04	0.1%
13-07G (strawberry)	Strawberry	4.1%	1.39	1.5%

Notes: Crop groups follow the Code of Federal Regulations, section 180.41. LAPU = loading as percent of use. [Use]×[Total LAPU]=[Total loadings] by definition.

According to the use amounts and predicted LAPUs, leafy vegetables and brassica leaf vegetables (the crop groups #4 and 5) are identified as the major contributors to the detection of imidacloprid in surface water over the modeling domain. The two groups together explain 59% of reported uses of imidacloprid and more than 80% of predicted total loadings. They are associated with the highest runoff potentials (LAPU=2.2% and 2.1%) over all crops. To further investigate the effects of application method on runoff potential, screening-level model (original PREM) is conducted with label rates. Taking lettuce as an example, two application sequences are modeled: [1] one soil application on February 9, 2022, at 0.30 kg/ha, and [2] five foliage applications started on February 16, 2022, at 0.05 kg/ha with a 5-d interval. Results suggest significantly higher EEC and LAPU with soil application compared to foliage applications. In the modeling area, about 75% imidacloprid for leafy vegetables and brassica leaf vegetables is used as soil application. Based on modeling results, mitigation practices to reduce imidacloprid runoff from soil application are recommended for the two crop groups.

Table 8. Screening-level modeling with hypothetical application methods for the "lettuce" scenario.

Run ID	Application method	EEC	Total LAPU
1	Soil application (2/9, 0.296 kg/ha ×1)	9.57	2.5%
2	Foliar application (2/16, 0.053 kg/ha ×5 @ 5-d interval)	3.09	1.3%
3	Both soil and foliar applications	9.61	2.0%

Notes: EEC is reported as the 1-in-10-year daily concentration; Application methods are retrieved from previous label reviews for imidacloprid (USEPA, 2016a; Whitfield-Aslund *et al.*, 2017) where the run #3 (combined method) was used.

The contribution from strawberry production is predicted with the highest average EEC but its total use of imidacloprid is relatively small (Table 7). The high concentrations predicted for strawberry are related to the application timing: about 80% of imidacloprid uses on strawberry were applied during the winter rain season of California (November to February). Grape production is associated with the lowest average EEC and LAPU. In the crop scenario for "grape", the low runoff curve number limits both overland flow generation and soil erosion from treated fields (Luo, 2017d).

4.4 Demonstration and discussion of modeling capability

The spatial modeling of PREM can test various scenarios, assumptions, and parameterizations for mathematical representation of pesticide applications. It also generates EECs in various forms according to modeling objectives. Below are some examples based on the case study:

1) **Cutoff value for application rates.** Both soil incorporation and foliar application are reported as ground applications in the PUR. In the case study, a critical value of 0.2 lb/ac is used to separate the two methods: all PUR-reported ground applications with <0.2 lb/ac are modeled as foliar application, all others as soil incorporation. A higher cutoff value of 0.3 lb/ac is also tested. This new value allocates more use amounts (about 4% of total uses of imidacloprid in the modeling area) to foliar methods, especially for leafy vegetables and brassica leaf vegetables (the crop groups #4 and 5). Since the predicted EECs are mainly contributed by soil applications (Table 8), the use of 0.2 lb/ac represents a conservative estimation of EECs. In addition, by using 0.2 or 0.3 lb/ac as the cutoff value no significant changes occur in the modeling results (in terms of average EECs) for the two crop groups or for all crops.
2) **Ground boom vs. airblast.** Although foliar applications are identified with a cutoff rate, there is no sufficient information to further separate the two associated methods of ground boom and airblast. From a modeling viewpoint, the two methods are only differentiated by drift fraction (Table 4). AgDRIFT modeling results showed that drift fractions for airblast and boom applications are similar at most distances (Whitfield-Aslund *et al.*, 2017). In the case study, all foliar applications are modeled as boom due to its higher drift fraction (Table 4). Simulations with airblast are also tested, resulting in a decrease of 0.15% to the average EEC compared to model results from ground boom application.
3) **Averaging periods for EEC reporting.** In addition to the daily averages presented previously, 21-d moving averages of aqueous EECs of imidacloprid in the water column are also predicted. In the USEPA ERA, the 21-d averages were used for characterizing chronic risks (USEPA, 2016a). The 1-in-10-year 21-d EECs show a modest decline from the daily values. The 90th percentile of 21-d EECs over all monitoring regions is 1.78 ppb, or a 26% drop compared to that for daily EECs (2.39 ppb, Table 6).
4) **EECs in the benthic zone.** The spatial modeling of PREM predicts EECs in both the water column and benthic zone. For example, the 90th percentile of the 1-in-10-year aqueous daily EECs of imidacloprid in the benthic zone is predicted as 0.71 ppb over all monitoring regions. This is much lower than that in water column (2.39 ppb, Table 6), but exceeds the lowest acute benchmark (0.385 ppb).

5 Conclusion

A spatial modeling approach is developed to extend PREM capability for pesticide exposure assessment. This new approach, “spatial modeling of PREM”, utilizes reported pesticide uses and associated environmental descriptions for more realistic modeling of pesticide fate and transport in surface water. In the case study, the new modeling approach is tested with agricultural uses of imidacloprid in California’s Central Coast and Imperial Valley. The model reasonably replicates monitoring data with a factor of 2. This suggests a refined exposure assessment compared to the factor of 10 (i.e., one order of magnitude) or more commonly observed in the evaluation of screening-level modeling approaches (Giddings *et al.*, 2016; USEPA, 2016b; Luo, 2017d). Furthermore, the model predicts the distribution and variability of pesticide exposures to aquatic system, either by a spatial resolution (sections or regions) or by site characteristics (crop groups). In summary, the spatial modeling of PREM provides a new understanding of continuous pesticide loadings from treated areas and EECs in receiving water bodies. This allows assessment of aquatic impacts with much greater certainty, which facilitates further evaluation and implementation of mitigation strategies.

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