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Chapter 22

Development of a Spatial-Temporal Co-occurrence Index To Evaluate Relative Pesticide Risks to Threatened and Endangered Species

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A decline in pelagic species has been observed in the San Francisco Bay-Delta, triggering questions as to whether contaminants are contributing to the decline. An index method was developed to evaluate the spatial and temporal co-occurrence of pesticides and threatened and endangered species for this large ecosystem. The co-occurrence index combines monthly species abundance with statistical distributions of pesticide indicator days for 40 widely used pesticides. The frequency of co-occurrence was determined for 12 aquatic and semi-aquatic threatened or endangered species to help guide future research and monitoring priorities, and the placement of best management practices in the study area.

Introduction

A decline in pelagic species in the San Francisco Bay-Delta region has been reported (*1*), causing speculation as to whether contaminants may be playing a role in organism decline. The objective of this study was to evaluate the potential co-occurrence of pesticides with several threatened and endangered species (TES) in the Sacramento River, San Joaquin River, Bay-Delta estuary, and their

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tributaries to help guide research and monitoring priorities, and the placement of best management practices (BMPs) in the study area.

Forty pesticides (Table I) were considered in this project. The list is slightly modified from a list published by the Central Valley Regional Water Quality Control Board (*2*) of pesticides that pose the highest overall risk to aquatic life in surface water in the Central Valley based on usage in the region, aquatic life toxicity, and chemical properties.

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Table I. Pesticides Evaluated

Chemical Name	*Chemical Name*	*Chemical Name*
(S)-Metolachlor	Deltamethrin	Oxyfluorfen
Abamectin	Diazinon	Paraquat Dichloride
Bifenthrin	Dimethoate	Pendimethalin
Bromacil	Diuron	Permethrin
Captan	Esfenvalerate	Propanil
Carbaryl	Hexazinone	Propargite
Chlorothalonil	Imidacloprid	Pyraclostrobin
Chlorpyrifos	Indoxacarb	Simazine
Cyhalofop-butyl	Lambda-cyhalothrin	Thiobencarb
Clomazone	Malathion	Tralomethrin
Copper Hydroxide	Mancozeb	Trifluralin
Copper Sulfate	Maneb	Ziram
Cyfluthrin	Methomyl	
Cypermethrin	Naled	

The twelve species addressed in the study include: four runs of Chinook salmon (*Oncorhynchus tshawytscha*), Central Valley steelhead (*Oncorhynchus mykiss*), Southern North American Green Sturgeon (*Acipenser medirostris*), Delta Smelt (*Hypomesus transpacificus*), Striped Bass (*Morone saxatilis*), San Francisco Longfin Smelt (*Spirinchus thaleichthys*), Threadfin Shad (*Dorosoma petenense*). California Red-legged Frog (*Rana draytonii*), and California Freshwater Shrimp (*Syncaris pacifica*). The runs of Chinook are Sacramento River winter-run, Central Valley spring-run, Central Valley fall run, and Central Valley late fall run.

Co-occurrence Method Development

Existing Co-occurrence Methodologies

Co-occurrence studies have been used to evaluate a wide variety of topics, including predator-prey relationships (*3*, *4*), invasive species (*5*, *6*), or competing species (*7–9*). Researchers have relied on a number of different methods to determine co-occurrence such as basic geographic information system (GIS) analysis (*9*, *10*), statistical approaches (*11*, *12*) or co-occurrence networks (*13*), and C-scores (*14–17*). The most common GIS assessments use standard overlay, predictive surfaces (*10*), and cluster analysis (*9*) to determine if two species co-occur. Statistical approaches to determine co-occurrence range from basic joint probability assessment (*18–20*), to more complex approaches such as multivariate logistic regression (*11*) or probabilities of occurrence based on multiple presence/absence surveys (*12*). The C-score or checker box approach, which produces a presence/absence matrix, has been demonstrated to work well for two species and for multiple paired species over a period of time (*21*).

The methods listed above function well when only a few entities are compared, but they cannot accommodate multiple species and multiple pesticides on a landscape level with a temporal component whilst ranking co-occurrence areas of concern. Therefore, a new approach was developed.

Co-occurrence Matrix

For this study, co-occurrence was determined by partitioning the landscape into discreet segments based on the likelihood that at least one pesticide is above a set benchmark and that one or more species are present at that location during the same period. The segments enabled us to account for local spatiotemporal patterns. The model assumes that species richness is sufficient to rank and determine co-occurrence for any time period. To account for temporal variability, a monthly time step was applied to the chemical occurrence and species richness. Rather than calculating a joint probability (*18–20*), the co-occurrence is expressed in a 2-dimensional unitless number in a matrix. Each part of the number expresses the contribution of the two entities considered. Higher numbers indicate greater co-occurrence and lower numbers indicate lesser co-occurrence.

The public land survey system (PLSS) section was used as the spatial computational element because historical pesticide use in California is reported at this level (*22*). For each landscape segment the potential ecological risk was calculated using the concept of a risk quotient (RQ). The RQ is calculated as the estimated exposure concentration (EEC) divided by the toxicity (*23*).

Generally in risk assessment, RQ $\geq$ 1 indicates pesticide exposure may adversely impact species. To avoid confusion over RQ, which implies adverse effects, the term "indicator event" is used. An indicator event is one in which toxicity has the potential to occur if the species is present.

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One dilemma faced in the development of the co-occurrence matrix was whether to conduct the analysis based on the number of chemicals causing indicator events in a landscape segment on the same day or if any chemical produced an indicator event on that day. Because the effects of multiple pesticides (i.e., mixtures) not all interactions are understood (*24*), co-occurrence was evaluated using indicator days. An indicator day is a day in which at least one indicator event occurs. The rate of indicator days (I_n) was calculated for each landscape segment for each for the set time period:

$$I_n = \frac{I}{(N_y \times N_d)}$$

Where

I_n = rate of indicator days for the analysis period

I = number of indicator days per time period (month)

N_y= number of years considered

N_d = number of days in the time period

For long time periods, I_n has the potential of becoming large and meaningless. However, I_n can be expressed by percentile level. In this study 10 percentile classes were used (e.g., 10th, 20th, 90th and 100th percentiles) in order to normalize results and accommodate a range of conditions, such as a different numbers of pesticides, analysis time steps (e.g., seasons instead of months), or analysis periods (number of years).

In order to determine if the species under question were present, distribution maps were assembled that associate the aquatic TES with landscape segments. Once the maps were in place, a species richness assessment was performed to determine the fraction of species estimated to be present relative to the number under consideration in this study. That fraction is called the species richness fraction, S_n, and is calculated as:

$$S_n = \frac{M}{N}$$

Where

M is number of species present in the time period considered

N is the number of species considered in the study

Like I_n, percentile fractions (the 10th, 20th, ..., 90th and 100th) were determined for each landscape segment and time period in order to normalize results when considering a different number of species.

Both pesticide concentrations and species are dynamic in space and time. The landscape segment anchors the spatial aspect and does not influence the temporal aspect. The environmental fate models used for the analysis, which are discussed

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later in this document, operate on a daily time step (*25*, *26*). However, since species distribution was available on a monthly basis, the ecological risk temporal windows were up scaled from day to month. As such the co-occurrence model embeds a monthly temporal window. A monthly time step was deemed to provide sufficient temporal resolution to detect any potential trends over the course of a year.

Because I_n and S_n are expressed as percentiles at a monthly time step, a single score or joint probability would obscure some of the information. To circumvent this, a 2-dimensional co-occurrence matrix was created. The matrix is an 11 x 11 grid (Figure 1) with indictor day percentiles along the abscissa and species richness percentiles along the ordinate. The grid axes are divided into bins representing percentile intervals -- that is, the 1st to 10th percentile is bin 1, 11th to 20th percentile is bin 2, and so on. The bins are numbered 0 to 10 from left to right and from top to bottom. The matrix values are simply a two-digit juxtaposition of the bin numbers and range from 0000 to 1010, i.e., 0000 indicates that neither species nor indicators days are present and 1010 indicates that all species and indicator days are very likely to co-occur. Because the bins are scaled to the population, the maximum fractions (and thus 100th percentiles) are not necessarily 1.0, but could be smaller. This approach enables the user to determine for the considered populations areas where, relatively speaking, more frequent co-occurrences of pesticides and species are located in the landscape.

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Co-occurrence Model Input Development

Modeling Estimated Environmental Concentrations

Daily pesticide loads to aquatic systems in the study area were estimated for historical applications of 40 pesticides to agricultural fields, rice paddies, and urban areas. Modeling for a ten-year period (2000 - 2009) necessitated the development of a framework to account for the dynamic aspects such as variable weather, changing application locations, and temporal changes in agricultural landscapes. The framework for this study was the PLSS section. Using a GIS, each PLSS section was further divided into hydrologic response units (HRU; (*27*)). Each HRU is uniform in land cover (e.g., agriculture, urban), soils (USDA Soil Survey Geographic Database (SSURGO); (*28*)), climate (California Irrigation Management Information System (CMIS); (*29*)), and agricultural management practices (irrigation from the California Department of Water Resources 2001 county survey; (*30*)). To account for a changing landscape, the land cover layer was updated every two years based on data from the California Farm Mapping and Monitoring Program (*31*).

Pesticide mass loadings for runoff and erosion were calculated using model simulations for each HRU. The total mass loading at the PLSS section level was calculated by aggregating the mass loadings. The sub-aggregated mass loadings were then used as input for the receiving water model, which in turn estimated environmental concentrations (EECs). Using data from California's Pesticide Use

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Reporting (PUR) database (*22*), historical applications were linked to use sites (28 different crop categories and urban) for each PLSS sections for a 9-year period (2000–2008).

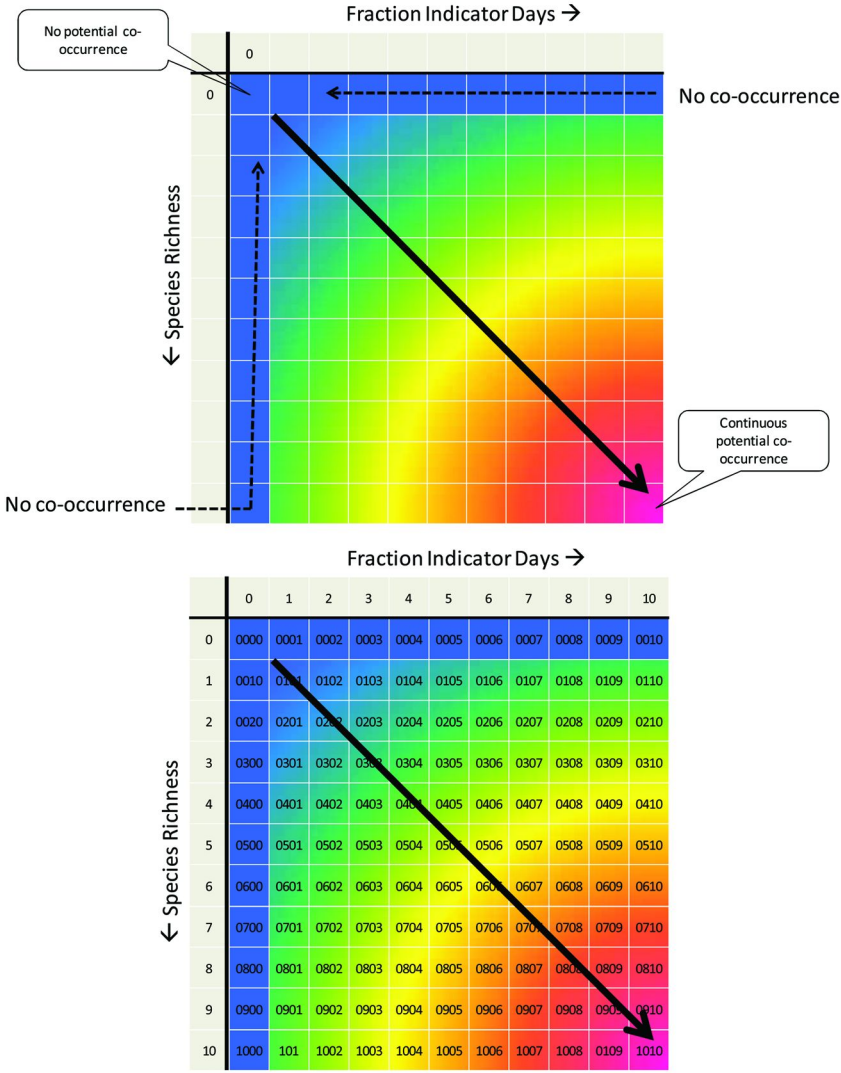

Figure 1. Co-occurrence matrix basic design (top), filled in (bottom). (see color insert)

Daily pesticide mass loadings resulting from agriculture and urban applications were simulated using the Pesticide Root Zone Model (PRZM). PRZM is a dynamic, compartmental model developed by the U.S. Environmental Protection Agency (USEPA) for use in simulating water and chemical movement

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in unsaturated soil systems within and below the plant root zone (*25*). PRZM is the standard model used for ecological and drinking water risk assessments for pesticides by the USEPA's Office of Pesticide Programs (USEPA OPP; (*32*)). The model has undergone an extensive validation effort against numerous field-scale runoff and leaching studies conducted for pesticides in the United States (*25*, *33*) and the model has been integrated into several watershed assessments in the U.S., including the Sacramento River watershed, which resides in the study area (*34*).

Pesticide mass loadings from wet seed application rice agriculture were simulated using the rice water quality model, RICEWQ 1.7.3 (*26*). RICEWQ has the ability to simulate the unique water management practices associated with rice production and because of the relative ease in using the model for bulk scenario processing. The model has been validated against field and watershed applications to flooded rice paddies in Australia, Italy, Greece, Japan, and the U.S. (*35–50*).

A further issue that can impact the aquatic environment, and needs to be considered, is spray drift. Spray drift is the offsite movement of pesticide during application. The drift can end up in a water body depending on a number of factors, including application rate, method of application, pesticide formulation, wind speed, wind direction, humidity, barometric pressure, height and velocity of the application apparatus, proximity of the water body to the treated field, and presence and effectiveness of interception barriers. Unfortunately, the PUR gives only the application rate and a general description of the application method. Therefore, drift load (M_{drift}) for an application was estimated with a simple linear equation:

$$M_{\text{drift}} = \text{Rate} \times D_{\text{FRACT}} \times \sum_{i=1}^{n} (L_i \times W_i) \times \frac{\text{PUR}_{\text{area}}}{\text{Ag}_{\text{area}}}$$

Where

M_{drift} = Mass loading (kg) resulting from drift for a single pesticide.

Rate = pesticide application rate (kg /ha^{-1}) for the pesticide.

D_{FRACT} = Drift fraction (unitless), based on values used by the USEPA for pesticide risk assessment (*51*). For aerial applications a drift of 5% of the application rate is assumed. For ground applications, a drift of 1% of the application rate is assumed.

L_i = Stream length (m) associated with the treated field.

W_i = Width of the stream (m).

$\text{PUR}_{\text{area}}/\text{Ag}_{\text{area}}$ = Area-weighted correction (unitless) for the treated area, PUR area (ha), and the PLSS land area (ha).

This equation applies only to a single event, but the daily concentration is what is of interest. So, to calculate that for a generic pesticide mass loading (M_i), a receiving water body was defined from the total stream length within each PLSS section. The volume (V) of this water body is calculated based on the linear length of each stream order in the PLSS according to the following equation:

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$$V = \sum_{i=1}^{n} (L_i \times W_i \times D_i),$$

Where
L_i = length,
W_i= width,
D_i = depth,
i = one of n channel segments.

As data for a more complex stream definition was not readily available for all streams in the study area, the stream geometry was fixed by stream order, with lengths derived from the National Hydrography Dataset (NHD+; (*52*)). For a natural stream, the depth and width were obtained from USEPA Reach File 1 (RF1; (*53*)). A linear regression equation was developed based on the RF1 from streams in the study area to estimate the depth of a stream given the width. The resulting relationship was used to compute the depth of each stream order based on assumed standard width. For man-made agricultural ditches, the dimensions were obtained from expert opinion (Wrysinski, J. Yolo County Resource Conservation District, Woodland, CA. Personal Communication, 2010).

The final calculation for estimating environmental concentrations is:

$$[C_i] = \frac{M_i}{V_i},$$

where
M_i = total daily mass (kg) for a chemical i in a PLSS section,
V_i = volume of water (m3) in the PLSS section,

M_i represents the total daily off-target mass for each of the 40 pesticides determined by summing the modeled mass agricultural loadings from runoff (dissolved and adsorbed to eroded soil), releases from rice paddies, drift from spray, and runoff from urban areas, and then mixing the total off-target mass in a volume of water. The computed concentration was then compared against a reference benchmark to determine if the computed concentration is above a benchmark.

Aquatic Life Benchmarks

Benchmark values were derived for each pesticide. The primary data source was the lowest acute fish or invertebrate benchmark value from the OPP Aquatic Life Benchmarks database (*54*). The benchmarks, which contain a safety factor of 2, were divided by an additional safety factor of 10 to account for TES. The toxicity of copper is influenced by a number of physicochemical characteristics (in particular water hardness), which, influences speciation and bioavailability of copper. A representative hardness and a hardness equation acute criterion maximum concentration equation (*55*) were calculated for both

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copper-based pesticides. The OPP database did not contain benchmarks for abamectin, indoxacarb, cyhalofop-butyl, or pyraclostrobin; the benchmarks for these pesticides were from other sources (*56*).

Species Distribution

The next piece needed for the co-occurrence analysis is a sense of what species are at risk and where they are located. The U.S. Fish and Wildlife Service (USFWS) critical habitat data (*57*) provides some of this information. However, the USFWS only gives federally listed species; no convenient dataset existed for state listed species (e.g., the California freshwater shrimp). In addition, the critical habitat data lack a clear temporal aspect. Given these limitations, a dataset for each species was required, specifically, one which showed, for each water segment, monthly species presence or absence.

Developing these species-specific datasets required life-cycle and presence information from a variety of sources. The primary references used were from Moyle (*58*, *59*). The resultant fish species range maps are considered high water year ranges; some of the stream reaches included are ephemeral and would not contain adults or juveniles during low water years. The California Red-legged frog was a special case. The distribution and abundance representations relied only on the USFWS critical habitat data (*57*), which is likely to under represent the actual species distribution.

Co-occurrence Assessment

The first step in the co-occurrence assessment was the development of the two required input datasets: the frequency distribution of the sum of indicator days and the frequency distribution of the species richness. Results concerning the off-target mass loadings and predicted concentrations are not included in this chapter, but are included in separate report by Hoogeweg and coworkers (*60*).

Indicator Days

Indicator days provide insight into the potential of an estimated pesticide concentration exceeding the benchmark for one or more pesticides. The maximum number of indicator events in a PLSS section was 2,876 in this study. Computed indicator days for several randomly selected PLSS sections (Figure 2) demonstrate that the number of indicator days is highly variable by location and by month due to factors such as application timing relative to rainfall and irrigation practices. The modeled decrease in the number of indicator days in the months of August through October for the PLSS section shown in Figure 2 might be due harvest of the crops in that time period.

The frequency distribution for indicator days by month for the period 2000–2009 is shown in Figure 3. Overall, the distribution appears to follow a log-normal curve, but with additional peaks at roughly the 0.15 and 0.50 bins. The tri-modal pattern is caused by differences between the application schemas

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of pesticide use in the urban environment, on rice paddies, and on other crops. The drivers of this are differences in application timing, for example urban applications are comparatively higher in the winter and early spring. Without urban applications the graph followed a log-normal pattern. The highest and most frequent indicator days were predicted to be in the San Joaquin River watershed in June through August. In these months, a majority of the agricultural areas fall in the upper percentile range (90th–100th percentile).

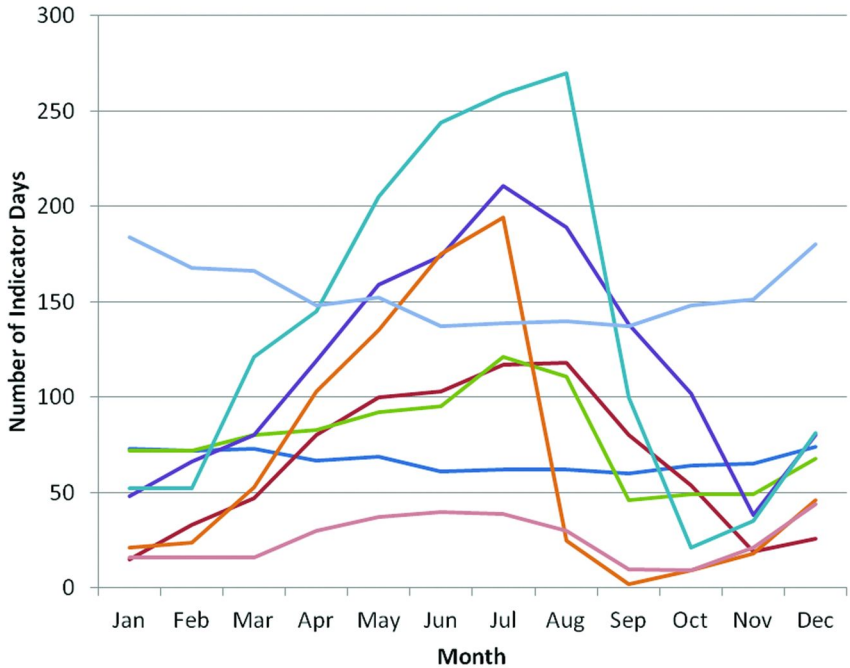

Figure 2. Temporal trend of the number of indicator days for selected Public Land Survey System sections by month for random locations in the study area. (see color insert)

In order to characterize the statistical distribution of indicator days, the frequency distribution was organized into percentile fractions (Table II). As shown in the table, the 80th percentile represents those months (and sections) where half of the time an indicator event took place. The 90th percentile is slightly higher at 0.589. The maximum value of 0.994 is noteworthy, since it indicates that there are a few instances (sections and months) in which the pesticide concentrations have the potential to be above a benchmark nearly every day of a year and month.

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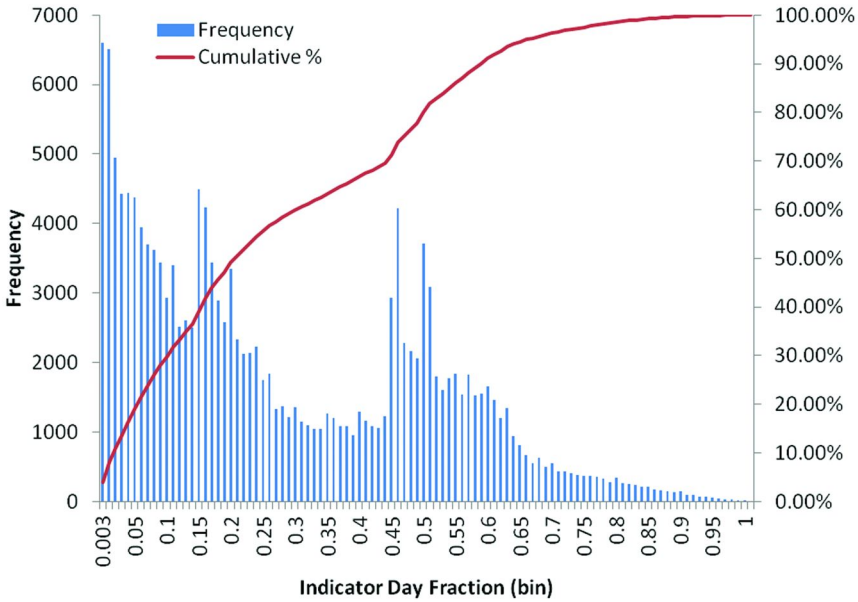

Figure 3. Frequency and cumulative distribution of all indicator days. (see color insert)

Table II. Statistics for the Indicator Day Distribution

Percentile	*Fraction*	*Bin*	*Bin Range*
10	0.017	1	0–0.017
20	0.055	2	0.018–0.055
30	0.100	3	0.056–0.100
40	0.153	4	0.101–0.153
50	0.206	5	0.154–0.206
60	0.303	6	0.207–0.303
70	0.447	7	0.304–0.447
80	0.500	8	0.448–0.500
90	0.589	9	0.501–0.589
100	0.994	10	0.590–0.994

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Species Richness

The physical distribution of the species under consideration was limited by the presence of partial and full barriers (e.g., dams) that prohibit upstream or downstream movement of the species. As such, many species are not present in the streams at higher elevation and were limited to aquatic habitats within the traditional agricultural areas in the Central Valley and to lower elevations in the mountains.

Although the distribution maps indicate where the species is present, they do not show when the species is present. This is significant, since while the results show that species richness changed little throughout the year, temporal changes are present in the system (Figure 4). Salmon migrations, for example, influence the species richness at certain times of year. Irrespective of the time period considered, the highest species richness was located in the Delta and along the Sacramento River.

The frequency distribution of the species richness data (Figure 5) depicts a strong bias at the 30th and 50th percentiles. This means that up to six of the species are present in most streams throughout the year.

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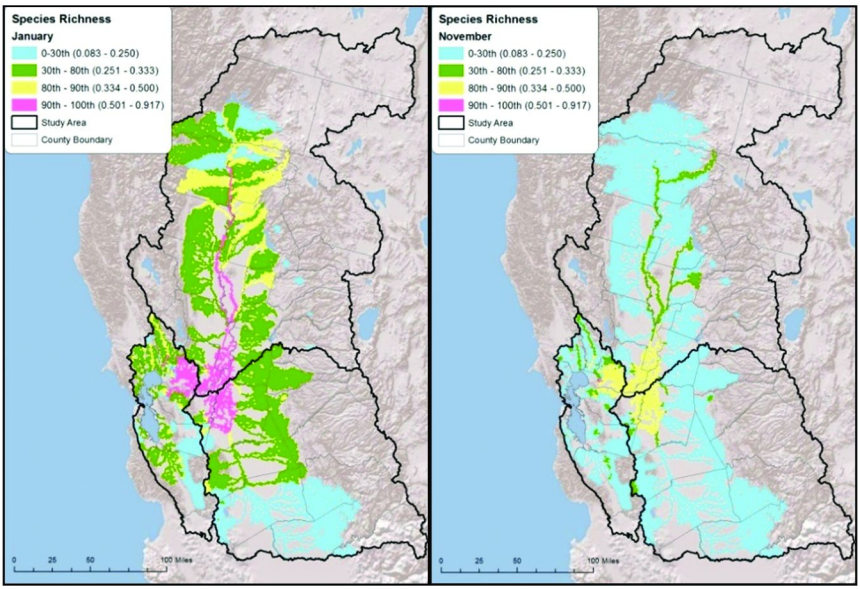

Figure 4. Species richness distribution for January (left) and November (right). (see color insert)

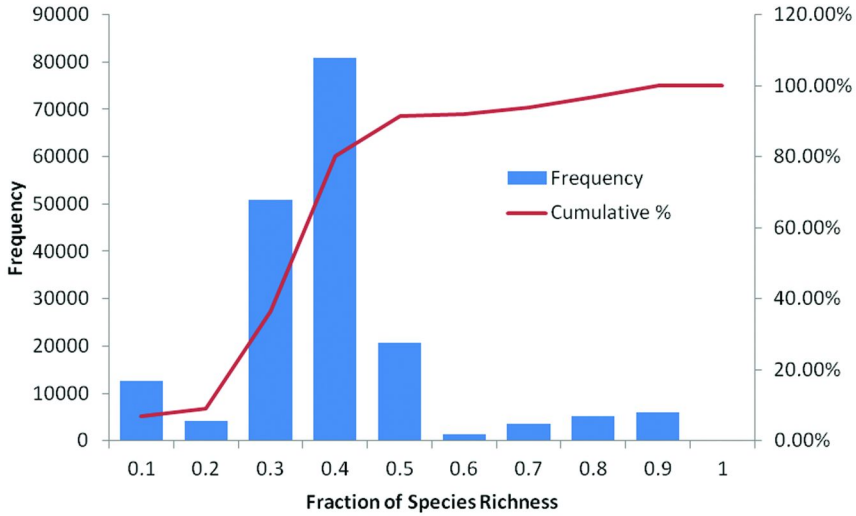

Figure 5. Frequency and cumulative distribution of the species richness. (see color insert)

Table III. Statistics for Species Richness Distribution

Percentile	*Fraction*	*Bin*	*Bin Range*
10	0.250	1	0.001–0.250
20	0.250	2	0.001–0.250
30	0.250	3	0.001–0.250
40	0.333	4	0.251–0.333
50	0.333	5	0.251–0.333
60	0.333	6	0.251–0.333
70	0.333	7	0.251–0.333
80	0.333	8	0.251–0.333
90	0.500	9	0.334–0.500
100	0.917	10	0.501–0.917

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Because the frequency distribution of the species richness is dominated by the 0.3 to 0.5 range, the calculated percentiles of species richness (Table III) show little variation. For example, the 10th to 30th percentile are 0.250 and the 40th to 80th percentiles are 0.333. The maximum (100th percentile) species richness value is 0.917. This indicates that no area has all 12 species present. This is due to the fact the California Red-legged frog is not found in the Delta, and California freshwater shrimp have a very limited distribution.

Colusa Basin Drain Case Study

To demonstrate the utility of the co-occurrence matrix for assessing co-occurrence of pesticides and TES, case studies were conducted to determine where potential areas of concern. The Colusa Basin Drain (primarily agricultural) is presented in this paper as an example. As was described in the previous sections, the co-occurrence matrix uses a relative ranking based on percentile distributions. The higher the individual percentile level, the higher the likelihood of co-occurrence. However, for co-occurrence to transpire, both the species and the indicator day must coincide in same temporal window and location.

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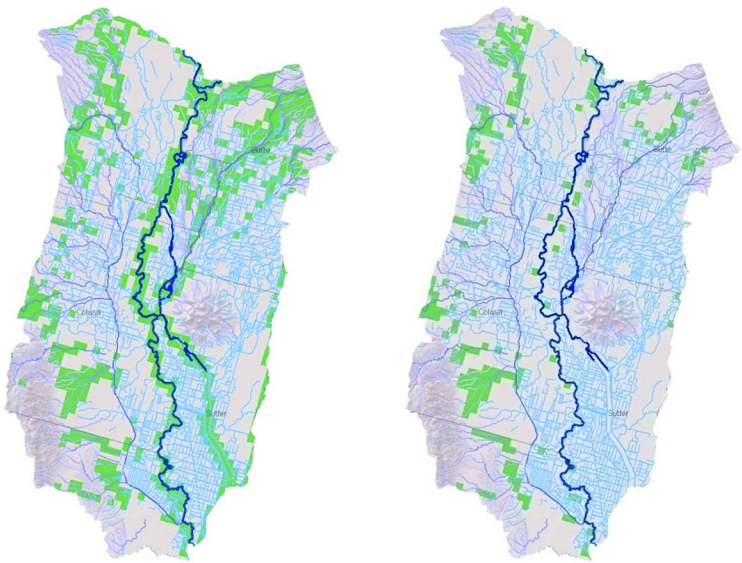

Figure 6. Percentile areas (shown in green), 50th (left) and 80th (right), for co-occurrence of pesticides and threatened and endangered species in the Colusa Basin Drain. The blue lines represent natural streams and agricultural ditches. (see color insert)

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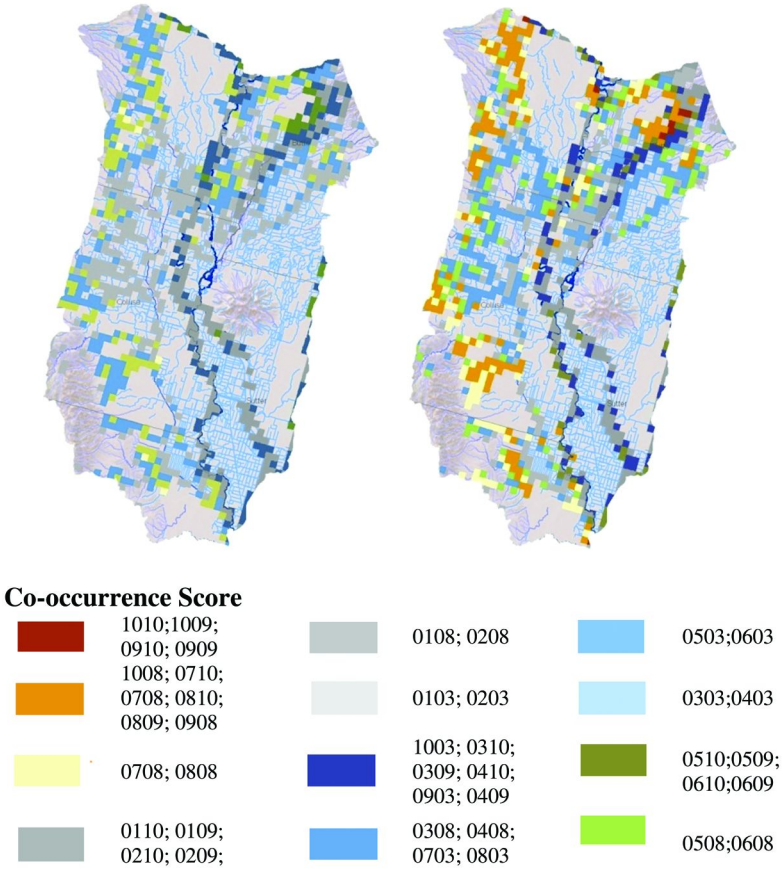

Figure 7. Co-occurrence for January (left) and May (right) of pesticides and threatened and endangered species in the Colusa Basin Drain (see color insert)

Varying Percentile Levels

To demonstrate the utility and versatility of the developed co-occurrence approach, regions were determined that adhere to predefined percentile levels using a 12-month time window. Next, the 50th, 80th, and 90th percentile levels were calculated for the Colusa Basin Drain. The 50th percentile represents the median case and had values of 0.206 for indicator days and 0.333 for species richness. However, 0.333 represents the 40th to 80th percentile range for the species richness. Therefore, the 80th percentiles for both indicator days and species richness were considered as well. The 90th percentile was used as the worst case, following the normal procedure in risk assessments (*61*). Using the

co-occurrence matrix approach, the 90th percentile values are 0.5 for species richness and 0.589 for indicator days. As the percentile level increases, fewer sections adhere to the predefined 50th and 80th percentile levels (Figure 6). At the 90th percentile level (not shown) two PLSS sections were found in the Colusa Basin Drain that met this scenario.

Temporal Assessments

The final component to consider is the temporal assessment. Both pesticide use and species richness vary over time; therefore co-occurrence should be time dependent as well. Figure 7 illustrates the co-occurrence for two example months (January and May) for the Colusa Basin Drain. In January the overall co-occurrence is lower than in May. This is due to increases in both pesticide use and species richness in the month of May. Co-occurrence ranged from 0103 to 0710 in January and 0103 to 1010 in May. Areas with no co-occurrence (i.e., either no indicator days or no species present during the time period) are not shown on the maps.

The lowest co-occurrence value in both January and May was 0103, which represents the 10th percentile level for indicator days and the 30th percentile level for species richness. At the upper range, January had a co-occurrence of 0710 and May of 1010. The percentile levels for the indicator days ranges from bin 7 (60th–70th percentile level) to bin 10 (90th–100th percentile range). For both months, the species richness was in the 10th bin, which represents the 90th–100th percentile range, or near maximum likelihood that all species were present.

Because this assessment shows the intersection in time and space of aquatic species and pesticide use, there are many different potential applications for the co-occurrence matrix. Resources agencies tasked with protecting aquatic species will now be able to better predict optimal times and places to monitor within watersheds, and thus will be able to make optimal use of BMPs to mitigate pesticide loadings. The information could also be parsed out for risk managers attempting to understand the specific locations of higher co-occurrence of a particular species and a particular pesticide or the joint co-occurrence of multiple pesticides in the same class (i.e., pyrethroids).

Conclusions

The growing need to determine if pesticides may be coming into contact with threatened and endangered species prompted the creation of a new approach that juxtaposes modeled pesticide concentrations in surface water and species richness data to determine where co-occurrence is most probable. Comparing these two sets was done with a monthly timescale, as that best represented both species richness and the distribution of pesticide exposure events (indicator days).

The results of this analysis are both positive and negative. Given sufficient data, a co-occurrence assessment is certainly possible and the information it yields can be valuable on a variety of levels. In addition to that, the majority of information needed to conduct the study was publicly available or could be

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processed from public sources. However, there are limitations and assumptions that lead to uncertainty in predictions of co-occurrence. Degradation products, chronic toxicity, and indirect effects were not addressed. There are gaps in the data, particularly in the estimation of water volumes and channel routing that compromise the ability to estimate exposure concentrations. Therefore, predictions of co-occurrence do not mean that adverse effects will occur. As a result, they should only be used to provide a relative ranking of potential areas of risk to the threatened and endangered species in the study area and the general time of year when these risks would be most likely to occur.

Yet, the co-occurrence matrix is flexible and scalable and can be adapted to answer a variety of potential questions depending on the needs of the risk assessor. The method could easily be expanded upon to give it greater complexity and utility by incorporating more detailed information about the hydrodynamics and the temporal distribution of species abundance and presence in the watershed, and could include additional species, pesticides, endpoints, and/or other water quality constituents. While this work done was specific to California's Central River Valley, the same method could be applied to other species, geographical areas, time windows, or pesticide classes. Large watersheds are difficult to manage, requiring very large sets of both modeling and monitoring data, and the co-occurrence method can give resource managers a way to focus and refine their impact evaluations. By applying these tools, resource managers can identify higher risk areas, giving them a better idea of when and where they may occur during a year. It also gives managers a way to test solutions, such as alternative pesticide use and optimized location of BMPs. Others may find this model useful in predicting effects of changing pesticide use instructions on labels (e.g., different application rates, targeted vs. broadcast applications, use of buffer zones).

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