Environmental Release Tool
Pesticide Mitigation Prioritization Model
User Guide v1.0

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September 2022
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Preface

Throughout the United States, a high degree of pesticide toxicity is introduced into the environment and has been observed to have severe effects on pollinators and aquatic taxa.[1–7] In California, 13% of river and stream reaches assessed for non-point sources by California Environmental Protection Agency under section 303(d) of the Clean Water Act are impaired by pesticides[8]. Other mitigation tools are available to derive toxicity reduction strategies which include fate models[9,10], toxicity/risk maps[11,12], risk indices[13–15], and summaries of pesticide use[16,17]. However, the individual tools are limited by their ability to evaluate large extents, toxicity sources, cumulative toxicity, and ability to consider the economic benefits of application sites. To improve the information available for pesticide mitigation via integrating features that address these limitations, we have developed the Environmental Release Tool (ERT) for experts, stakeholders, and the public. The tool is the first stage of development for the Pesticide Mitigation Prioritization Model (the second stage is a companion fate model) and quantifies the spatiotemporal distribution of applied toxicity, defined here as the mass of pesticide released into the environment, weighted by toxicity to user-defined priority species.

The ERT accommodates analyses anywhere users can provide pesticide use data but is particularly useful in California. The California Department of Pesticide Regulation (CDPR) hosts the world’s most comprehensive pesticide use data[18]. Their Pesticide Use Reports (PUR) database[19] comprises agricultural pesticide applications recorded at the daily time step and 1 square mile (2.6 km²) area by application site. We have leveraged the database directly into the ERT to quantify the applied toxicity by active ingredient, source, and watershed across California in seconds to minutes. While many regions have minimal pesticide use data relative to California, new resources are being developed to provide use estimates for common crops and
pesticides such as PEST-CHEMGRIDS[17]. These datasets, or future pesticide use collection efforts, can be leveraged with tools such as the ERT to explore mitigation opportunities for reducing environmental toxicity. For study areas where data is unavailable, users may consider employing pesticide use rates for crops observed in California due to pesticide use being recorded for over 400 unique agricultural application sites over more than 400,000 km², the mass of pesticides applied is ~20% of that used in the US.[20,21]

1.0 Environmental Release Tool Methods

The ERT quantifies toxicity reduction targets by chemical, application site, and watershed for the study area of interest. Reduction targets are quantified by the applied toxicity, defined herein as the mass of pesticide released into the environment as weighted by toxicity to species targeted by tool users. Each pesticide may have very different applied toxicity relative to applied mass, with some being hundreds to thousands of times more toxic for the same amount applied. It is suitable for designing toxicity reduction strategies and planning monitoring campaigns by identifying areas where higher toxicity is released in the environment, which could introduce health hazards to aquatic taxa, terrestrial taxa, or humans. The tool ranks application sites and watersheds by their applied toxicity.

This tool does not quantify fate or exposure but rather illustrates the location and amount of applied toxicity[22] for designing toxicity reduction strategies and planning monitoring campaigns by identifying areas where higher toxicity is released in the environment, and its sources. Although the ERT is a spatial tool designed for large extents, the tool works best to understand sources of pesticide exposures for species with a small habitat range. For organisms whose activities are more widespread, such as feeding behaviors, and who have less direct
contact with environmental compartments where pesticides are most likely to persist, the location of applied toxicity may be less useful for understanding sources of potential exposure. For aquatic organisms, though the transport of pesticides to surface water bodies is sensitive to their physicochemical properties[23], physicochemical property correlation to surface water detection frequencies has been demonstrated to be weaker than for pesticide sales data. Halbach et al. (2021) performed a 2-year monitoring campaign of over 100 streams. They investigated the explanatory power of pesticide frequency of detection with pesticide sales data, the half-life of pesticides in water and soil, and solubility for 76 active ingredients. The most robust relationship was for pesticide sales, and significance for the other factors was only observed for the half-life in water.[24] Though simulating and monitoring the fate of pesticides and organism exposure is imperative to risk assessment, given data paucity for many pesticides and environments for model parameterization and calibration[25], we determined an applied toxicity tool to be important to informing mitigation efforts.

The ERT has two platforms: a web application for California and a desktop version for all study areas in the United States, which offer different advantages. The web-based tool is accessible on any internet-accessible device, summarizes applied toxicity in seconds, and provides a more straightforward user interface. The offline tool offers a high degree of customization, more detailed information, and custom simulations. To assist experts and non-experts, the ERT web tool and desktop version were built in RStudio[26] version 1.4. The development environment accommodates full customization of model code for experts and the ability to run unique simulations for non-experts via editing spreadsheet files in Google Sheets and clicking a start button.
The user interface of the ERT provides a heatmap of applied toxicity. Within the map, users can zoom in, pan to find a watershed of interest, and click to see applied toxicity summaries by source and chemical for the watershed (Fig 1). In addition to graphical summaries, tabular outputs are provided with summaries of applied toxicity for the analysis period and the daily time step. Currently, the online tool only accommodates analyses of applied toxicity to aquatic organisms (fish, aquatic invertebrates, and nonvascular and vascular plants) within California for the most recent 5-year pesticide use data and is not customizable. There is also a couple of years lag in pesticide use data availability, and at the time of this guide’s publication (2022), the most recent 5-year period of available data is 2014-2018. The chief advantage of the online platform is that it is accessible from any device and provides applied toxicity summaries for watersheds across California in seconds. The offline tool is advantageous because it works for any species, state, or analysis period and offers a high degree of customization. The online application is available at this web address [https://nicol-parker.shinyapps.io/Environmental-Release-Tool/], and the desktop tool is downloadable from the scientific digital repository Dryad. The tool can be located via this link [https://datadryad.org/stash/share/7a-F-jEXmLvWi3-xeRx_X4osZqXrr8Nh97tmx2bBOSk] or searched for as ‘Pesticide Mitigation Prioritization Model (PMPM) - Environmental Release Tool and Results’.
**Fig A. User interface.** The clickable and graphical user interface of the Environmental Release Tool. Note that other graphical summaries are not shown in this image, which summarizes crop values, applied toxicity by chemical, and illustrates economic and health indices. Base map imagery is a product of OpenStreetMap [https://www.openstreetmap.org/copyright](https://www.openstreetmap.org/copyright).
1.1 Pesticide Sources

To evaluate targets for pesticide toxicity reduction, the Environmental Release Tool requires manually inputting pesticide use data, or for California, the tool can autoload pesticide use report data from statewide agricultural applicators[18]. The Environmental Release Tool internally hosts the pesticide use data. Using an autoload script, the tool aggregates data for the area of interest to the user, which watersheds or counties may define. The data retrieved by the autoload feature is discussed in the remainder of this section.

Pesticide use data are retrieved by active ingredient (AI) and for the 432 site types from CDPR Pesticide Use Reports[18] that are agricultural. Agricultural applications are estimated to account for ~90% of the applied pesticide mass in the United States[21]. In Pesticide Use Reports, applications are recorded at the daily time step and by site type at the County Meridian Township Range Section (referred to as Section) spatial scale (2.6 km$^2$). Urban applications are not included within the CDPR pesticide use database records for household applications, and most professional urban applications are recorded at the county level as well as monthly time-step, which cannot be allocated to a specific watershed or date.

To enable evaluations of the variability of toxicity reduction opportunities over large extents, the tool summarizes pesticide applications and toxicity by watershed. The data is summarized by watershed and applications sites as well as pesticides since pesticide losses via runoff and eroded sediments share a common outlet. Summarizing applied toxicity by watersheds is important to conceptualize areas that share common hydrologic routes for pesticide transport. Though the Environmental Release Tool does not simulate loss processes, it is the first stage of development of the Pesticide Mitigation Prioritization Model. The product of the second
stage of development is a companion, mechanistic fate and transport tool where loss processes are simulated.

To derive watershed-specific applied toxicity, pesticide use data, which is recorded by Section, is assigned to watersheds via geospatial intersection analyses. Section geospatial data is provided by the California Pesticide Information Portal[18], while watershed geospatial data for the United States is available in the Watershed Boundary Dataset[27]. The Watershed Boundary Dataset delineates watersheds as hydrologic unit codes (HUCs) by hydrologic connectivity and at multiple scales. Watersheds with shorter HUCs, such as HUC 2-digit codes, are large watersheds that encompass hundreds of thousands of square kilometers, while longer HUCs, such as HUC 8-digit codes (HUC8) represent subwatersheds of the shorter digit codes (e.g., HUC2) that are tens to hundreds of square kilometers. The assignment of pesticide use data to watersheds can be conducted at three watershed spatial scales in the Environmental Release Tool to enable users to adjust the resolution of analysis, which are HUC8, HUC10, and HUC12, whose watershed mean square areas are ~3,600, ~440, and ~100 km² respectively. For Sections where pesticide use data is reported that overlaps multiple watersheds, the area fraction of overlap is used to weight the mass of AI applied.

In addition to assigning pesticide use data to a specific watershed, a key feature of the Environmental Release Tool is the ability to preserve information relating to the applied toxicity of application site types. However, too many application sites make the interpretation of results difficult. The tool thus enables users to group similar AIs and application sites (e.g., alfalfa and alfalfa-grass mixture) by assigning the same ID to multiple site types. By default, 432 agricultural application site types from Pesticide Use Reports are simplified to 116 based on the
similarity of the crops. Groupings can be viewed and modified in the tool input file for application sites.

1.2 Affected Compartment

Areas impacted by pesticide applications for terrestrial and aquatic investigations can be estimated with agricultural land use datasets such as the National Land Cover Dataset[28] or the Cropland Data Layer[29]. In California, the impacted area can be retrieved from Pesticide Use Reports, which provide the application and planted area of crops[19]. However, there are known inaccuracies. The planted area is often recorded for all the grower’s land; although reported for a specific crop, fields are subject to multiple crop rotations within a year, and multiple applications are typical for a crop which renders the net-application area unknown. Due to these concerns, alternative land use datasets were evaluated for use[28–30].

The most accurate, high-resolution dataset reviewed was the California Department of Water Resources land use surveys (https://data.cnra.ca.gov/dataset/statewide-crop-mapping) with a median accuracy of 97.5% and positional quality of 8m. However, a limitation of the dataset, as well as the others, is that it provides fewer site types (43) compared to Pesticide Use Reports (432). Using this dataset to determine the affected area of specific application site types would require highly reducing the resolution of pesticide source data. Attempts to recategorize crops to fit available land use data did not obtain reliable results. As a result, we chose to consider the affected area to be all agricultural land in the California Department of Water Resources dataset. The representation of the affected compartment to all agricultural land was deemed appropriate because only 5% of agricultural fields in California employ organic cultivation practices[31] and use non-synthetic pesticides recorded in use reports.
1.3 Applied toxicity

Applied toxicity refers to the mass of pesticide applied to an area with the potential to do harm[22]. The applied toxicity for the $i^{th}$ pesticide in the $j^{th}$ watershed is calculable from applications to the of the $k^{th}$ site type and toxic endpoint of the $m^{th}$ taxon of interest as:

$$TI_{j,i} = \sum \frac{M_{i,j,k,m}}{r_{i,j,k,m}} \quad Equation \ (1)$$

Where $TI$ is the Toxicity Index (kg-m$^3$/kg), $M$ (kg) is the mass of applied AI, and $T$ (kg/m$^3$) is the adverse health-effect concentration of concern (e.g., the lethal concentration of fifty percent of the test organism population) for the species or taxonomic groups of interest. Within a simulation, the tool is suitable for quantifying the applied toxicity to taxa within the same compartment, not across environmental compartments, because variation in the transport of pesticides based on physicochemical properties is not simulated. The tool illustrates applied toxicity within the soil compartment or available for transport to the compartment of interest. While the transport of pesticides from the application site is sensitive to their physicochemical properties[23], property correlation to surface water detection frequencies has been demonstrated to the more robust for pesticide sales data than physicochemical properties in a monitoring campaign of 72 pesticides of diverse properties in over 100 streams[24]. Though this approach is not suitable for risk assessments, it facilitates an understanding of where mitigation opportunities exist[57] without data requirements and uncertainty of fate and transport models over large extents[26,27,58].

For pesticides, the tool facilitates the summarization of similar AIs. This feature is useful because many AIs have a similar chemical make-up (e.g., isomers or are produced in several forms, including acids, salts, amines, and esters) but have no or limited toxicity data for the
various AI forms. Provided that AI forms can have very different affect concentrations, where possible, the user should provide AI form-specific toxicity. To accommodate AI form-specific endpoints where available but to simplify tool outputs, unique toxicity endpoints are accepted and calculated for pesticides within a user-defined pesticide group, and the group’s total applied toxicity is reported by the group ID in tool output. In this investigation, we considered AIs detected (2014-2018) within California’s surface waters with available toxicity data (n = 151). From the CDPR’s Pesticide Use Reports, 290 forms of the AIs were observed (e.g., 12 unique esters and 15 salts of 2,4-D).

Our investigation considers the applied toxicity of pesticides for fish, as well as aquatic invertebrates, nonvascular plants, and vascular plants. Toxicity endpoints employed were acute values from the United States Environmental Protection Agency (USEPA) Aquatic Life Benchmarks Database. The USEPA derives Benchmarks from the concentration at which fifty percent of a species sample in single-dose laboratory investigations experience severe effects, derived from mortality endpoints, or for plants, significant changes in growth/biomass (LC50 or EC50). A genera endpoint is then calculated based upon a 0.05 cumulative probability of toxicity for represented species, which typically reflects the most sensitive species within the taxonomic group. For fish and invertebrates, the USEPA calculates the final acute value as the product of the taxonomic group endpoint multiplied by a safety factor of 0.5 and does not adjust plants. Where no toxicity endpoints were reported for the pesticide in the Aquatic Life Benchmark database (n = 10), the Pesticide Properties DataBase acute toxicity endpoints were employed, and unverified data were excluded.
The first applied toxicity index reported by ERT for pesticides, sites, and watersheds is the Relative Toxicity Index (RTI). The index weights the toxicity of the $i^{th}$ applied pesticide by the size of the application area within the $j^{th}$ watershed as:

$$RTI_{j,i} = \frac{TI_{i,j}}{A_j} \quad Equation \ (2)$$

where $A$ (m$^2$) is the area of the affected compartment.

As the quantification of the affected compartment area is frequently limited, and the fraction of a watershed subject to pesticide application is highly variable, we provide a second applied toxicity index independent of area, the Net Toxicity Index (NTI). The NTI is a relative rank toxicity index to determine if the applied toxicity is greater than what is typical for the $i^{th}$ pesticide in the $j^{th}$ watershed. As our reference of what is typical, we calculate for the study area the 50th percentile ($perc_{50}$) of the applied toxicity for any applied pesticide ($pst$) in watershed ($w$). The NTI is calculable from the TI of the $i^{th}$ pesticide in the $j^{th}$ watershed as:

$$NTI_{i,j} = \frac{TI_{i,j}}{perc_{50} (TI_{pst_1,w_1},TI_{pst_1,w_1},TI_{pst_1,w_2},TI_{pst_2,w_2},...,TI_{pst_n,w_n})} \quad Equation \ (3)$$

The NTI approach can quickly identify applied toxicity above typical levels in the study extent. For example, if the 50th percentile of the applied toxicity of pesticides to a watershed in the study area is applications of imidacloprid in the San Joaquin Watershed, 1000 TI, to calculate the NTI, the TI of the pesticide and watershed of interest is divided by 1000 TI. Using this approach, pesticide applications within a watershed over the simulation period with an NTI greater than unity have applied toxicity above typical levels. This normalization provides a unitless applied toxicity index that does not affect the relative rank of the applied toxicity for pesticides, sites, or watersheds and can identify effective toxicity reduction targets specific to the study area.
For single taxonomic group investigations with the ERT (e.g., only fish), the cumulative applied toxicity, the potential of all pesticides released to the environment and under investigation to do harm to the taxon, is calculable via an adaption of the concentration addition method[60,61]. We calculate the cumulative toxicity indices of pesticides for each index for $n$ pesticides for a watershed (here $w_1$) as:

$$RTI_j = \sum RTI_{pст_1,w_1} + RTI_{pст_2,w_1} + RTI_{pст_3,j,w_1} ... RTI_{pст_n,j,w_1} \quad \text{Equation (4)}$$

$$NTI_j = \sum NTI_{pст_1,w_1,k} + NTI_{pст_2,w_1,k} + NTI_{pст_3,w_1,k} ... NTI_{pст_n,w_1,k} \quad \text{Equation (5)}$$

The method used in this study relies on the assumption of additive toxicity and non-interacting chemical species. While this assumption is theoretically unsound for chemicals of diverse modes of action, and this limitation is not addressed by the ERT, pesticides rarely express synergism at environmentally relevant concentrations, and cumulative addition has been empirically demonstrated to be a reliable method for quantifying pesticide mixture toxicity[62]. For example, in studies with hundreds of pesticide mixtures, the method has predicted mortality within a factor of 2 for 90% of samples[63–65]. Additionally, the method is robust to independent modes of action[64]. However, the approach is not suited to simultaneously understand the effects of pesticide mixtures on diverse taxa due to the presence of unique organism receptors and responses[66]. Where multiple organisms are included for analysis, the net applied toxicity is interpretable as where toxicity reduction opportunities are greatest for all taxa considered.

1.4 Health and Economic Indices

Health and Economic Scores

The health and economic impacts of application sites are quantified over the study extent with a Health Score (ha/NTI), an Economic Score (USD/ha), as well as an Economic and Health
Score (USD/NTI per ha). These indices are calculated over the study extent (California) rather than in specific watersheds due to the low resolution of reliable land use data (see Section 2.2 Affected Compartment). For health and economic scores, higher values represent more favorable outcomes. Health and economic scores are calculated for the application site areas of the study extent as:

\[
Economic\ Score = \frac{\text{Gross Value (USD)}}{\text{Harvested Hectares}} \quad \text{Equation (6)}
\]

\[
Health\ Score = \frac{\text{Harvested Hectares}}{\text{Toxicity Index (NTI or RTI)}} \quad \text{Equation (7)}
\]

The Economic and Health Score penalizes crops with high applied toxicity and is calculated as:

\[
Economic\ and\ Health\ Score = \frac{\text{Gross Value (USD per Harvested Hectare)}}{\text{Toxicity Index (NTI or RTI per Harvested Hectare)}} \quad \text{Equation (8)}
\]

For health and economic scores, the harvested hectares and gross value of application site types were compiled from the United States Department of Agriculture National Agricultural Statistics Service (https://www.nass.usda.gov/). We considered the median economic value and harvested hectares for a crop in California from 2014-2018 to minimize single-year anomalies.

In addition to numeric scores, users are also provided with categorical scores based upon percentiles for the study area to facilitate interpretation. Scores are divided into 20th percentiles and range from ‘Very Low’ (0-20th percentile) to ‘Very High’ (80-100th percentile).

**Table A. Application site summary.** Environmental Release Tool outputs for pesticide application sites which introduce 90% of the applied toxicity in California to fish, invertebrates, nonvascular aquatic plants, and vascular aquatic plants from 2014-2018, where: AI (kg) represents the mass of active ingredients applied; NTI the Net Toxicity Index; NTI (%) the percent of the total NTI of the application site type; Economic, Economic Health, and Health Scores the numeric score of sites; and the Economic, Economic Health, and Health Values the quantiles of scores where 0-20th quantile is ‘Very Low’ and 80-100th ‘Very High’.
<table>
<thead>
<tr>
<th>Site Type</th>
<th>Applied Mass (kg)</th>
<th>NTI (%) Total</th>
<th>Economic Score (USD/ha)</th>
<th>Economic Health Score (USD/NTI)</th>
<th>Health Score (NTI/ha)</th>
<th>Relative Economic Score</th>
<th>Relative Economic Health Score</th>
<th>Relative Health Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>Almond</td>
<td>1.49E+07</td>
<td>1.41E+08</td>
<td>1.32E+04</td>
<td>2.78E+02</td>
<td>2.11E-02</td>
<td>3-Medium</td>
<td>2-Low</td>
<td>2-Low</td>
</tr>
<tr>
<td>Pistachio</td>
<td>3.27E+06</td>
<td>1.07E+08</td>
<td>1.32E+04</td>
<td>1.86E+02</td>
<td>1.42E-02</td>
<td>3-Medium</td>
<td>2-Low</td>
<td>1-Very Low</td>
</tr>
<tr>
<td>Alfalfa</td>
<td>4.37E+06</td>
<td>6.08E+07</td>
<td>1.58E+03</td>
<td>1.64E+02</td>
<td>1.04E-01</td>
<td>1-Very Low</td>
<td>1-Very Low</td>
<td>4-High</td>
</tr>
<tr>
<td>Lettuce</td>
<td>1.48E+06</td>
<td>4.59E+07</td>
<td>1.75E+03</td>
<td>2.67E+02</td>
<td>1.53E-01</td>
<td>2-Low</td>
<td>2-Low</td>
<td>4-High</td>
</tr>
<tr>
<td>Walnut</td>
<td>2.96E+06</td>
<td>2.96E+07</td>
<td>9.95E+03</td>
<td>2.54E+02</td>
<td>2.55E-02</td>
<td>3-Medium</td>
<td>2-Low</td>
<td>2-Low</td>
</tr>
<tr>
<td>Rice</td>
<td>5.87E+06</td>
<td>2.84E+07</td>
<td>1.21E+03</td>
<td>1.91E+03</td>
<td>1.58E+00</td>
<td>1-Very Low</td>
<td>1-Very Low</td>
<td>3-Very High</td>
</tr>
<tr>
<td>Cotton</td>
<td>2.73E+06</td>
<td>2.09E+07</td>
<td>1.24E+02</td>
<td>6.74E+00</td>
<td>5.45E-02</td>
<td>1-Very Low</td>
<td>1-Very Low</td>
<td>3-Medium</td>
</tr>
<tr>
<td>Tomato</td>
<td>2.43E+06</td>
<td>2.03E+07</td>
<td>8.57E+03</td>
<td>4.00E+02</td>
<td>4.67E-02</td>
<td>2-Low</td>
<td>2-Low</td>
<td>3-Medium</td>
</tr>
<tr>
<td>Corn</td>
<td>2.47E+05</td>
<td>1.53E+07</td>
<td>5.74E+03</td>
<td>5.27E+01</td>
<td>9.17E-03</td>
<td>2-Low</td>
<td>1-Very Low</td>
<td>1-Very Low</td>
</tr>
<tr>
<td>Broccoli</td>
<td>4.56E+05</td>
<td>8.71E+06</td>
<td>8.98E+03</td>
<td>2.70E+02</td>
<td>3.01E-02</td>
<td>3-Medium</td>
<td>2-Low</td>
<td>2-Low</td>
</tr>
<tr>
<td>Cherry</td>
<td>3.94E+05</td>
<td>7.66E+06</td>
<td>5.84E+03</td>
<td>8.68E+02</td>
<td>1.48E-01</td>
<td>2-Low</td>
<td>4-High</td>
<td>4-High</td>
</tr>
<tr>
<td>Peach</td>
<td>5.50E+05</td>
<td>6.36E+06</td>
<td>8.61E+03</td>
<td>3.25E+02</td>
<td>3.77E-02</td>
<td>2-Low</td>
<td>2-Low</td>
<td>3-Medium</td>
</tr>
<tr>
<td>Strawberry</td>
<td>6.44E+05</td>
<td>5.93E+06</td>
<td>1.02E+05</td>
<td>8.57E+02</td>
<td>6.88E-03</td>
<td>3-Very High</td>
<td>4-High</td>
<td>1-Very Low</td>
</tr>
<tr>
<td>Orange</td>
<td>1.50E+06</td>
<td>5.67E+06</td>
<td>4.51E+02</td>
<td>1.29E+01</td>
<td>2.86E-02</td>
<td>1-Very Low</td>
<td>1-Very Low</td>
<td>2-Low</td>
</tr>
<tr>
<td>Onion Misc.</td>
<td>6.17E+05</td>
<td>4.09E+06</td>
<td>1.83E+04</td>
<td>3.05E+02</td>
<td>1.67E-02</td>
<td>3-Medium</td>
<td>2-Low</td>
<td>2-Low</td>
</tr>
<tr>
<td>Bean (Dry)</td>
<td>1.87E+05</td>
<td>3.75E+06</td>
<td>1.42E+03</td>
<td>1.77E+02</td>
<td>1.25E-01</td>
<td>1-Very Low</td>
<td>1-Very Low</td>
<td>4-High</td>
</tr>
</tbody>
</table>
2.0 Environmental Release Tool Installation and Operation

To prepare to use the web-based platform, users can navigate to the tool via this link: https://nicol-parker.shinyapps.io/Environmental-Release-Tool/ and skip to Section 4.0 of this guide. Desktop users will need to follow the stepwise instructions provided for tool installation and use in this section and read Section 3.0, model parameterization.

The desktop ERT is run through the RStudio user interface. All model parameterization is done using spreadsheets which can be modified in google sheets or Microsoft Excel. When executing tool simulations in RStudio, a pop-up window with a clickable user interface (see Fig 1) is produced with graphical summaries of the data and tabular exports (in spreadsheet format).

2.1 Installing RStudio

I. Establish an internet connection with your device.

II. Download R version 4.1, the software environment of RStudio. The software is freely available for Mac, Windows, and Linux users here https://cran.rstudio.com/.

III. Download RStudio version 1.4; the software is freely available for Mac, Windows, and Linux users here: https://www.rstudio.com/products/rstudio/download/#download.

IV. Follow the RStudio download and install instructions.

V. Open RStudio; for new users, some quick tutorials may be helpful to familiarize yourself with the software, but they are unnecessary. The first time you open the software, you’ll need to install packages which will take just a few minutes. Packages are functions employed by the ERT and are installed within the RStudio user interface. The packages which need to be installed include ProjectTemplate, data.table, dplyr, stringr, lubridate, zoo, rgdal, shiny, leaflet, and plotly. To install packages, follow these steps for instructions (see Fig 2 to view the RStudio interface):

1) Within the RStudio Window, navigate to the ‘Packages’ tab in the lower right window.

2) Click the ‘Install’ button.

3) In the pop-up window, data field ‘Install From’, set the option to ‘Repository (CRAN)

4) Type the list of packages separated by a comma above or copy this list of packages and paste into the ‘Packages’ field:

data.table, tidyverse, stringr, lubridate, zoo, leaflet, plotly, shiny, rgdal
5) Ensure ‘Install dependencies’ is checked.

6) Select the ‘Install’ button at the bottom of the pop-up window.

7) Packages should install without error; if errors are encountered, they will be displayed in the Console as ‘Error:’ followed by an issue-specific note. If issues are discovered, try installing packages one at a time. To troubleshoot the package-specific problems, typically, another package must be installed for which the name is displayed in the RStudio console. If difficulties persist, RStudio is a widely used platform for which internet searches for error codes will provide troubleshooting assistance for your operating system (macOS, Windows, or Linux).
Fig B. RStudio package installation. RStudio interface with required user steps/features for package installation.

2.2 Installing the Environmental Release Tool

1) Navigate to the ERT model download via this link  
[https://datadryad.org/stash/share/BJwLp5INjd3ybsATDQ2fJLvRdH3uDobvBMnFVEmC7M, the temporary link for reviewers and publishers, needs to be updated for the public]
2) Download the tool zip file and save it to your computer.
3) Unzip the ERT download. The ERT model requires a small fraction of the downloaded file memory, 0.6 GB. Still, the entire download package requires 6 GB of memory due to the millions of pesticide use data points for the most recent 10-year period of data availability for California (as of this guide’s publication 2009-2018). To substantially reduce the space the ERT requires on your personal computer; you may delete all pesticide use data not of interest to your analyses (see the sub-directory ‘EnvironmentalReleaseTool/data/inputs_simulation/cdpr_pur’ to delete from years not of interest to your analyses. For users seeking to conduct analyses beyond this period for
California, the required files can be downloaded in minutes, see Section 3.4 for download instructions.

2.3 Running a Simulation Environmental Release Tool

1) **Open RStudio.**

2) Prior to running the ERT in RStudio, the user needs to provide the path to where they have saved the ‘EnvironmentalReleaseTool’ directory (folder) on their computer. Setting the path tells RStudio and the ERT where to retrieve and save model files. To set the path:
   a. Navigate to the top of the RStudio window to the tab ‘Session’, click once, and hover over ‘Set Working Directory’ (do not click yet).
   b. Scroll down on the sub-menu that pops up and click once on ‘Choose Directory’.
   c. Browse to where the ‘EnvironmentalReleaseTool’ directory is saved and click once; then, at the bottom of the pop-up window, select open. The path has now been set.

3) To open the clickable user interface, a user must open the ‘PMPM_EnvironmentalRelease.R’ file in the ERT directory (where you saved the downloaded model). To open the file, in the RStudio window, navigate to the ‘File’ tab at the top left. In the drop-down menu, select ‘Open File’. Navigate to the ‘EnvironmentalReleaseTool’ directory and open the ‘PMPM_EnvironmentalRelease.R’ file.

4) The model can now be run with default inputs. Select the ‘Run App’ button in the RStudio window (Fig 3). By default, the model will display ERT outputs for pesticide-applied toxicity at the HUC8 watershed scale (mean watershed size ~3,600 square kilometers) for 2014-2018 in California. For new simulations with the ERT, refer to ‘Section 3.0 Parameterization’ of the user guide for instructions to customize the simulation.

5) The clickable user interface will now display (Fig 1). Click around to view graphical summaries of data. To view tabular data, open the ‘output’ sub-directory. See Section 5. Outputs for more information on available outputs. Note that model values are displayed in scientific notation for graphical summaries because they are often large values that are otherwise messy to display and difficult to read. Scientific notation expresses the number
of zeros that follow or precede a number. 1,000,000 is written in scientific notation as \(1 \times 10^6\), 0.1 is written as \(1 \times 10^{-1}\). A quick web search of ‘scientific notation’ will provide useful details on the number format, which is common scientific practice.

6) New simulations will require a few minutes to an hour to summarize results and display them in the clickable user interface (Fig 1), depending on your operating system and the number of watersheds and pesticides analyzed. Once a simulation has been run, a user can display an existing simulation result in the user interface in less than a minute. To do so, see Section 3.1 instructions.

**Fig C. RStudio interface.** RStudio interface with key user features for the Environmental Release Tool. 1) Top of the window where tabs for navigating RStudio menus are located. 2) The name of the tool execution file (‘PMPM_EnvironmentalRelease.R’). 3) The button the user clicks to run the script; alternatively, the user can highlight all text in the file and press enter. 4) The code in the ‘PMPM_EnvironmentalRelease.R’ file initiates the module's running and opening of the user interface. 5) The RStudio console window updates the user on what the model is processing. It displays errors if the model does not run correctly. 6) Window within which directories on your computer can be navigated (similar to File Explorer in Windows or Finder in Mac).

### 3.0 Parameterization

This section describes each input file for the ERT, the parameters (input file fields), and provides specific notes on formatting. For inputs, formatting must match the input files; see the
Template’ input folder with input files and formatting required in the ERT (located in the ‘EnvironmentalReleaseTool/data/inputs_simulation/simulations’ directory). To modify module inputs discussed below, navigate to the input file of interest, open, edit, and save the files which are editable in Google Sheets, Microsoft Excel, or text editors (format comma-separated files).

The ERT summarizes pesticide applied toxicity by watershed. Watersheds are delineated using the United States Geological Survey Watershed Boundary Dataset[27]. Watersheds in this dataset are delineated as hydrologic unit codes (HUCs), with longer-digit watersheds of higher resolution. Users can choose between three default watershed resolutions to use for the ERT; from lowest to highest resolution, they are eight-digit HUCs digits (HUC8), ten-digit HUCs (HUC10), and twelve-digit HUCs (HUC12). The mean area of the watersheds varies by state, and in California are ~3,600 square kilometers for HUC8 watersheds, ~440 square kilometers for HUC10 watersheds, and ~100 square kilometers for HUC12 watersheds. Other watershed delineation options are available, which the user may choose from, but require manual parameterization of the input files for watersheds and application site types, as well as for the user to download the spatial dataset for the resolution of interest (see Section 3.3).

Within the ERT, all default parameters (including pesticide use data) are available at each of the three watershed resolutions in California (see Section 1.1). Users seeking to analyze pesticides in areas outside of California will need to modify most input files. By default, the inputs for pesticide use and toxicity consider pesticides detected in statewide surface monitoring campaigns in California that are recorded in the CDPR Surface Water Monitoring Database[18] for 2014-2018 (n=151). Pesticide use data is derived from the CDPR PUR database[19] (see Section 1.1). Toxicological data was derived from the United States Environmental Protection Agency Aquatic Life Benchmarks Database[33] (see Section 1.3).

3.1 Default Simulations

Default simulations are available at three spatial scales for aquatic species in California’s watersheds for 2014-2018 (defaults will be updated when pesticide use reports for later years are publicly available). Two types of simulations can be conducted with toxicity endpoints. One considers the most sensitive taxonomic group per pesticide. For the toxicity endpoints used, the Aquatic Life Benchmarks[33], 18% of the most sensitive endpoints for investigated pesticides
were from fish, 38% for aquatic invertebrates, 27% for nonvascular aquatic plants, and 17% for vascular aquatic plants. The second approach employed toxicity endpoints for the individual taxonomic groups. By default, the active pesticide ingredients analyzed are those detected (2014-2018) within California’s surface waters (n = 151). From the CDPR’s Pesticide Use Reports, 308 forms of the 151 AIs were observed (e.g., 30 unique salts and esters of 2,4-D). If multiple toxicological endpoints exist for the active ingredient, the more sensitive endpoint was employed as a conservative toxicity estimate; pesticides were evaluated, and default groupings can be viewed in the default module input file for pesticides. The custom simulations are under the ‘EnvironmentalReleaseTool/data/inputs_simulations/simulations’ directory. See the next section to customize input parameters to evaluate other species (terrestrial or aquatic), pesticides, and study areas.

3.2 Custom Simulations

Within the ‘EnvironmentalReleaseTool/data/inputs_simulation’ directory, there exists a file, the ‘Simulation_Information.csv’. This input file informs the tool which simulation file to run, the analysis period, and how output data will be summarized.

- ‘Simulation_Information.csv’ fields:
  - simulation_name: Name of the simulation input file to run. The simulation input file contains information on the pesticides, application sites, and watersheds to be analyzed (see Section 3.2). This field's format can employ characters, underscores, and periods (.). The name used in this field must match exactly match (capitalization sensitive) the name of the simulation file (see Section 3.2) BUT not include the file extension (.csv). This name also creates a directory for the simulation to store model outputs.
  - watershed_resolution: Input what resolution to analyze pesticides at for watersheds. Users can choose between three default watershed resolutions to use for the ERT; from lowest to highest resolution, they are eight-digit HUCs digits.
(HUC8), ten-digit HUCs (HUC10), and twelve-digit HUCs (HUC12). To analyze at the HUC8 scale, enter ‘huc8’ in the field for a HUC10 analysis ‘huc10’, and a HUC12 analysis ‘huc12’. The mean area of the watersheds varies by state, and in California are ~3,600 square kilometers for HUC8 watersheds, ~440 square kilometers for HUC10 watersheds, and ~100 square kilometers for HUC12 watersheds.

- tox_summary: For the graphical summaries provided by the module, this field indicates whether to display the NTI or RTI in the heat map summary of pesticide applied toxicity; see Equations (2) and (3) in Section 1.0.
- new_simulation: Enter ‘yes’ to run a new simulation or ‘no’ for the ERT to display existing data. The simulation must have data in the ‘output’ and ‘cache’ sub-directories under the simulation name (automatically generated when a simulation is run) to display graphical summaries for existing simulations.
- print_daily_summary: Provides the option to print daily output of pesticide toxicity by watershed, site, and chemical. To provide daily output, insert 'yes'; to increase the model speed and reduce the memory consumed by ERT outputs, choose not to print daily summary data by entering a 'no'. Tabular summaries will always be provided for the analysis period, and graphical summaries by month and year.
- manual_pest_application: Indicates whether to use manually input pesticide use data or the auto-load pesticide use feature (available only for California, see details in Section 3.4). To employ manual data, enter ‘yes’; to use CDPR data, enter ‘no’.
- filter_by_county: This parameter is only used by the module for evaluations in California, where the autoload feature is used for pesticide use data. The field indicates whether the model filters the study area by counties specified by the user or watersheds. If data are filtered by counties, this information will be employed to select watersheds within counties specified by the user in the simulation input file (see Section 3.2), and all model outputs will still be summarized by watershed. To function, the user must ensure all watersheds in California are present in the simulation input file ‘Watersheds.csv’ input file (see Section 3.2.2)
for the desired scale of analysis (e.g., HUC8). Watershed data is available for HUC8, HUC10, and HUC12 watersheds in California in the default simulation files provided in the ‘EnvironmentalReleaseTool/data/input_simulations/simulations’ directory. To filter by county, insert 'yes', and to filter by watershed, 'no'.

- start_day: First day of simulation with format 'dd'.
- start_month: First month of simulation with format 'mm'.
- start_year: First year of simulation with format 'yyyy'.
- end_day: Last day of simulation with format 'dd'.
- end_month: Last month of simulation with format 'mm'.
- end_year: Last year of simulation with format 'yyyy'.
- affected_depth: This value represents the depth of soil impacted by pesticide application and is with the affected area per watershed provided in the simulation input file (see Section 3.2) to calculate the NTI (Equation (3)). The default value is 0.01m.
- percentile_NTI: Percentile of the applied toxicity of pesticides in watersheds used to calculate the NTI, see Equation (3). The default is the 50th percentile.
- econ_val: For study areas with uncertain harvested hectares or gross value for pesticide application site types, the user can select to use a gross economic value for the study area provided by default in the ‘ApplicationSite.csv’ input file. To use the economic value for the entire study area to calculate the economic score, insert ‘yes’. To use user-defined harvested hectares and gross crop value to calculate the economic score for the study region, insert ‘no’.
- health_val: For study areas with uncertain harvested hectares for pesticide application site types within the study region, the user can select to use the health score calculated from the application site area across the study area provided by default in the ‘ApplicationSite.csv’ input file. To use the health score for the entire study area, insert ‘yes’. To use user-defined harvested hectares to calculate the economic score for the study region, insert ‘no’.
3.2 Simulations

The simulation files describe the pesticides to be evaluated, toxic endpoints to employ, the extent of analysis, and the output summarization method. Each simulation will have a folder with the simulation name and all input files. The user customizes the folder name to represent their unique scenario. Section 3.2.1 lists the steps to prepare the ERT to run a new simulation. Section 3.2.2 discusses simulation parameters and data resources.

3.2.1 Simulation Overview

1) To run a new simulation, a user can employ one of the simulations provided in the ‘EnvironmentalReleaseTool/data/inputs_simulation/simulations’ or customize a simulation using input files in the ‘Template’ folder.
   a. By default, the ERT is parameterized to analyze pesticide-applied toxicity in California for 2014-2018 at the HUC8 watershed resolution (~3,600 km², 140 watersheds). Default simulation files are also available for users seeking to summarize applied toxicity in California at the resolution of HUC10 watersheds (~440 km², 1,038 watersheds) or HUC12 (~100 km², 4,463 watersheds) for 2014-2018. These simulation inputs are in the directory ‘EnvironmentalReleaseTool/data/inputs_simulation/simulations’.
   b. Custom simulations must follow the field names and formats of the files in the ‘EnvironmentalReleaseTool/data/inputs_simulation/simulations/Template’ folder. For custom scenarios, save a copy of the ‘Template’ input folder and rename it to reflect the new simulation (e.g., ‘SacramentoWatershed_2021’).

2) To employ the correct simulation files in an ERT model run, the user must enter the unique simulation file name into the ‘Simulation Information.csv’ input file (located in the ‘EnvironmentalReleaseTool/data/inputs_simulation’ directory) field ‘simulation_name’. The simulation name must NOT include the input file extension (*.csv) and is capitalization sensitive. The simulation name must also match the folder containing all simulation input files in the ‘EnvironmentalReleaseTool/data/inputs_simulation/simulations/’ directory (e.g., folder name ‘SacramentoWatershed_2021’).

3) For simulations in California, no further parameterization is necessary. For simulations outside of California, watershed spatial data acquisition is required. This effort requires
only a few minutes; see Section 3.3. The simulation file specifies the number of
watersheds and chemicals to analyze. Typically, the ERT can handle simulations at the
state level. However, analyses over five years for more than 200 chemicals and 5,000
watersheds may cause the ERT to run out of RAM and for the model not to run. If an
error is encountered for large simulation spaces, reduce the number of watersheds,
chemicals, or years considered.

3.2.2 Simulation Parameters

The simulation input files required are in the
‘EnvironmentalReleaseTool/data/inputs_simulation/simulations/Template’ directory. The
simulation run is based on the simulation name provided in the ‘Simulation_Information.csv’
input file (see Section 3.1). Default simulation files are available, or users can create a custom
scenario with the template files. A simulation employs six input files: ‘Pesticides.csv’,
‘Pesticide_Application.csv’.

• ‘Pesticides.csv’ fields:
  o pesticide_id: Unique identifier which will be used to summarize highly similar
    pesticides. This may be unique from the ‘pesticide’ field to merge similar applied
    chemicals such as isomers. IMPORTANT NOTE, for pesticide use reports in the
    CDPR PUR database, many active ingredients with slight variation in form (e.g.,
    2,4-D and 2,4-D LITHIUM SALT) exist. If using the autoload feature or
database, a user will want to ensure they explore all chemical names similar to
    their active ingredient of interest, or the applied toxicity may be underestimated.
    To ensure all pesticide loads associated with an active ingredient are included, list
    all relevant CDPR PUR chemical names in the ‘pesticide’ field. For each
    chemical for which the same toxicity value will be used, provide the same
    ‘pesticide_id’ field value; see Table 2.
  o pesticide: Name of the active ingredient of the pesticides under investigation. If
    the user seeks to use the autoload feature for pesticide use data, the module
    requires this field to match pesticide names within the CDPR PUR[19] database
    (including capitalization). The chemical name formatting can be found in the ERT
directory under ‘EnvironmentalReleaseTool/docs/ChemicalFormatting.csv’.
o tox_1: Toxicity endpoint (kg/m³) used to calculate applied toxicity. Numeric formatting with no commas must be employed (e.g., no thousands placeholder nor comma used as the decimal); to represent decimals, employ a period (.) For sediment or soil toxicity endpoints, typically (mg/kg), convert to (kg/m³) using a typical value for the compartment density (e.g., 1,400 kg/m³). For example, if the soil toxicity endpoint is 0.001 mg/kg, then:

\[
0.001 \frac{mg \ pst}{kg \ soil} = 1000 \frac{kg \ pst}{kg \ sol} \\
\]

\[
tox_1 = 1000 \frac{kg \ pst}{kg \ soil} \times 1,400 \frac{kg \ soil}{m^3 \ soil} = 1,400,000 \frac{kg \ pst}{m^3 \ soil}
\]

o tox_2 to tox_10: The user has the option to add toxicity endpoints for a total of 10 species; however, species evaluated in the same simulation must all have toxicity endpoints in the same environmental compartment (see Section 1.3).

The Environmental Release Tool is a relative ranking tool that quantifies the net applied toxicity to species, showing where the relative applied toxicity is highest. When multiple species are considered, in tool outputs, the net applied toxicity to all species of interest (sum of all applied toxicity to individual species). Note that to evaluate the cumulative applied toxicity of pesticides to a specific species, a user must run individual simulations (provide only a value for tox_1). By default, tox_1 to tox_4 are provided and are the toxicity endpoints, obtained from the USEPA Aquatic Life Benchmarks[33] (or Pesticide Properties DataBase[32] where USEPA benchmarks were unavailable) for fish, invertebrates, nonvascular aquatic plants, and vascular aquatic plants respectively.

<table>
<thead>
<tr>
<th>pesticide_id</th>
<th>pesticide</th>
<th>tox_1</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,4-d ester</td>
<td>2,4-D, BUTOXYETHANOL ESTER</td>
<td>152</td>
</tr>
<tr>
<td>2,4-d ester</td>
<td>2,4-D, ISOOCTYL ESTER</td>
<td>152</td>
</tr>
<tr>
<td>2,4-d salt</td>
<td>2,4-D, DIMETHYLAMINE SALT</td>
<td>299</td>
</tr>
<tr>
<td>2,4-d ester</td>
<td>2,4-D, BUTYL ESTER</td>
<td>152</td>
</tr>
<tr>
<td>2,4-d salt</td>
<td>2,4-D, TRIISOPROPanOLAMINE SALT</td>
<td>299</td>
</tr>
</tbody>
</table>

Table B. Pesticide groups. Example inputs that group chemical names in the pesticide use data to chemical names used in model outputs.
• ‘Watersheds.csv’ fields:
  o huc: Unique hydrologic unit code watershed identifier. Formatting is character, with the string ‘HUC’ followed by the digits of the HUC watersheds of interest (e.g., HUC18070301 for HUC8 or HUC1807030111 for HUC10).
  o huc_name: Name of hydrologic unit code watershed. Users can use WBD default names or create custom names that employ characters, numbers, or underscores (no special characters).
  o affected_area_ha: Area (ha) of the watershed impacted by pesticide application in hectares (whole watershed area may be used if the affected area is unknown). The tool converts the value from ha to m² internally for toxicity index calculations. Numeric formatting with no commas must be employed (e.g., no thousands placeholder nor comma used as the decimal); to represent decimals, employ a period (.)

• ‘Counties.csv’ fields only need to be populated if the user opts for the autoload feature for pesticide use data (available only for California study areas) and to filter pesticide use data by county (see Section 3.1).
  o county_cd: County code employed by the CDPR. Formatting must match codes in the ‘county_cd.txt’ file in the ERT directory under the ‘data/model_configuration/cdpr_pur’ sub-directory.
  o county_name: Name of the county. Formatting is up to the user.

• ‘ApplicationSites.csv’ fields provide information about which application sites to consider in watersheds (e.g., agricultural sites). The input file also enables users to group similar site types considered into one toxicity index (e.g., table grapes and wine grapes to a toxicity index for ‘GRAPES’). The fields also describe the value of the application sites per hectare. For crop values, default data was aggregated from the United States Department of Agriculture National Agricultural Statistics Service (USDA NASS)[34] for California for the most recent 5-year pesticide application data (2014-2018). For users seeking to customize crop values, the same database provides crop values at the state and county levels for the United States.
‘app_site_id’: Unique pesticide application site identifier. For users employing the CDPR PUR database, the ‘app_site_id’ must match the ‘site_code’ field identifier in the CDPR PUR database (see ‘EnvironmentalReleaseTool/docs/ApplicationSiteForamtting.csv’). If the user manually inputs pesticide use data (via the ‘Pesticide_Applications.csv’ input file), the ‘app_site_id’ used here must match the pesticide use data.

‘pmpm_id’: Unique application site identifier in outputs of the Environmental Release Tool (ERT) of the Pesticide Mitigation Prioritization Model (PMPM). This field can summarize outputs from unique application sites in pesticide use data into application site type groups, see Table 3.

Table C. Application site groups. Example Environmental Release Tool inputs that group application site names (app_site_id) into a ‘pmpm_id’ to enable summarization of applied toxicity across similar sites.

<table>
<thead>
<tr>
<th>app_site_id</th>
<th>pmpm_id</th>
<th>harvested_ha</th>
<th>gross_usd</th>
</tr>
</thead>
<tbody>
<tr>
<td>AIRPORT</td>
<td>Urban</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>ALFALFA</td>
<td>Alfalfa</td>
<td>308,864</td>
<td>1,027,626,000</td>
</tr>
<tr>
<td>ALFALFA-GRASS MIXTURE</td>
<td>Alfalfa</td>
<td>308,864</td>
<td>1,027,626,000</td>
</tr>
</tbody>
</table>

‘harvested_ha’: The statewide harvested hectares for each crop type. Numeric formatting with no commas must be employed (e.g., no thousands placeholder nor comma used as the decimal); to represent decimals, employ a period (.). This data is available in the USDA NASS[34] database.

‘gross_usd’: Gross value of crop per year. Numeric formatting with no commas must be employed (e.g., no thousands placeholder nor comma used as the decimal); to represent decimals, employ a period (.). This data is available in the USDA NASS[34] database.

‘health_val’: Health score calculated for the entire study area for application site types.

‘econ_val’: Economic score calculated for the entire study area for application site types.
‘PesticideApplications.csv’ fields to input pesticide use data; populating this file is ONLY required for users manually inputting pesticide use data (not employing the ERT autoload feature). We recommend that users who evaluate California agricultural study sites employ the module's automatic pesticide use population feature; see Section 3.4 for more information about the autoload feature. Users with analyses external to California may benefit from exploring the pesticide use databases provided by the United States Geological Survey[35,36] or PEST-CHEMGRIDS[17].

- date: Date of pesticide application, format dd/mm/yy.
- huc: Unique hydrologic unit code watershed identifier. Formatting is the number of digits of the HUC with no characters (e.g., eight, ten, or twelve) and must match values in the ‘huc’ field of the ‘Watersheds.csv’ input file.
- huc_name: Name of hydrologic unit code watershed. Formatting is up to the user. Users can use WBD default names or create custom names that employ characters, numbers, or underscores (no special characters).
- app_site_id: The name of the application site should match the name of the source data frame, but this is not a requirement. This field must match the ‘app_site_id’ present in the ‘Application_Sites.csv’ input file.
- pesticide: Name of pesticide applied; the field must match the names employed in the ‘pesticide’ field in the ‘Pesticides.csv’ input file (can be unique from the ‘pesticide_id’ field).
- pesticide_kg: Mass of active ingredient applied. Formatting is numeric with no commas (employ ‘.’ to indicate decimal places).

3.3 Watershed Spatial Data

The watershed spatial data is employed to visualize the distribution of pesticide applied toxicity across watersheds in the graphical user interface. The watershed spatial data file formats are shapefiles (*.shp) stored in the directory ‘EnvironmentalReleaseTool/data/inputs_watershed.spatial_data’. Users conducting simulations in California are provided with watershed spatial data files by default in the ERT; for other states/counties in the United States, the files can be downloaded from the Natural Resources Conservation Service Geospatial Gateway in a few minutes[37]. The watershed file for the area of interest (e.g., the entire state) will likely be large (>5 MB). For the ERT to run efficiently, the
polygons should be simplified if the user has the technical expertise. An efficient method for simplifying the polygons is to employ the ‘ms_simplify’ function in the ‘rmapshaper’ package for RStudio (other software users may be more familiar with can be used to simplify polygons such as QGIS). Polygons should be simplified to less than 2 MB; the smaller the file, the more efficiently the tool will run. Simplifying polygons does NOT affect the analysis resolution, only the graphical summary heatmap in the user interface.

Follow these steps to download the watershed shapefile:

1) Navigate to the Geospatial Data Gateway via this link: https://datagateway.nrcs.usda.gov/
2) In the lower right-hand corner, select the link to ‘Order by County or Counties’ or ‘Order by State’.
3) Choose the study area of interest (State or Counties) from the drop-down list.
4) Scroll down to the heading ‘Hydrologic Units’ (headings are in alphabetical order).
5) Select the resolution to download by 8 Digit Watershed Boundary Dataset (HUC8), 10 Digit Watershed Boundary Dataset (HUC10), 12 Digit Watershed Boundary Dataset (HUC12), or other.
6) Select the ‘Continue’ button at the bottom of the page.
7) Under the ‘Format’ heading, select the ‘ESRI Shape’ files from the list. Do not select ‘Separate ESRI Shapefiles’.
8) Under the ‘Projection’ heading, select ‘Geographic NAD83’.
9) Press ‘Continue’ at the bottom of the page.
10) Enter your email address to receive a link to the requested data, and press ‘Continue’ at the bottom of the page.
11) Review your order and click ‘Place Order’ on the window's lower left.
12) Open the data download link on your device. Save the downloaded data files (shapefiles have multiple files associated with them to display spatial data) into the ‘inputs_watershed_spatial_data’ directory under the sub-directory of the watershed delineation downloaded. For example, save HUC8 watershed data under the ‘EnvironmentalReleaseTool/data/inputs_watershed_spatial_data/huc8’ directory and HUC10 watershed data under the ‘EnvironmentalReleaseTool/data/inputs_watershed_spatial_data/huc10’ directory. If saved under the incorrect directory (e.g., HUC10 data under ‘huc8’), the module will not
run. Also, ensure the file extensions *.shp, *.prj, *.dbf, and *.shx are present. Other files will be present from the data download, which can be copied into the folder but are unnecessary for the ERT.

3.3 Pesticide Autoload Feature

Pesticide use for agricultural applications can be autoloaded in the ERT for California study areas if opted for by the user (see Section 3.1). The data employed are derived from the CDPR pesticide use reports[19] and are stored in the ‘EnvironmentalReleaseTool/data/cdpr_pur’ directory. The pesticide use is reported at the daily time step by application site type at a resolution of 2.6 km$^2$ (1 mi$^2$), the county/range/township/section (COMTRS). This data is assigned to a given watershed in the ERT via geospatial intersect analyses. For pesticide use reporting units (COMTRS) overlapping multiple watersheds, the fraction of the total area of the pesticide reporting unit within a given watershed is used to weigh the amount of pesticide applied.

By default, pesticide use reports are available for the most recent 10-year period for available pesticide use data (2008-2018 at the time of this guide’s publication). They are not to be modified by the user without the potential for model disruption. For users seeking to conduct analyses before this period, follow these instructions to download data for additional years (1990 onward). This is a quick process that will take a few minutes. This data is not included by default because they are large files that require a lot of memory on your device (~60 MB per year of data).

1) Visit the California Pesticide Information Portal website operated by the CDPR and navigate to the ‘Data Archives’. At the time of this guide’s publication, the link to the homepage with the ‘Data Archives’ link is [https://calpip.cdpr.ca.gov/main.cfm](https://calpip.cdpr.ca.gov/main.cfm). Windows users may need to use Firefox or Internet Explorer as their web browser to avoid known issues with Chrome.

2) Download data for years of interest to your analyses.

3) Drag or copy data from all years of interest to the ERT sub-directory ‘EnvironmentalReleaseTool/data/cdpr_pur’. Unzip each file in this location (may be done by opening the zip file for many users or using a secondary software on your device for exporting zip files).

4) The ERT can now use data for additional years.
4.0 Outputs

The ERT offers users graphical and tabular summaries to prioritize toxicity reduction strategies detailed in this section.

4.1 Graphical Outputs

When the ERT is opened in the web application, the user can summarize applied toxicity by HUC8 watersheds (~3,600 km²) or HUC10 watersheds (~440 km²); for more information on the watershed delineations, see the Watershed Boundary Dataset.[27] They can then choose to summarize data by month or year. Default data summarizations are by HUC8 watershed, time-step year, with the first year 2014 and last 2018 (Fig 1). In the desktop application, the watershed resolution displayed will depend on the watershed identifier employed in the simulation inputs file (‘Simulation_Information.csv’). If an 8-digit value is entered in the ‘Watersheds’ sheet of the input file in the ‘huc’ field, the tool will automatically display HUC8 watersheds; if a 10-digit value is entered, HUC10 watersheds, etc. To change the watershed scale at which applied toxicity is summarized graphically, a user can display simulations that have been run previously (see Section 3.1) or run a new simulation for watersheds at a different spatial resolution. The desktop tool can summarize applied toxicity by at any scale of interest to the user (Fig 1). The HUC12 is not offered in the web tool due to the high memory storage required for the high-resolution data.

To view watershed-specific data, click the watershed of interest on the map; see Fig 4. The watersheds are partially transparent, so users can see the names of cities and water bodies on the map to help orientate their search. When hovering over the map, the following information is provided: the name and number of the HUC, the date by which the data is currently summarized, the applied toxicity during the time step, and the applied toxicity relative to other watersheds. The applied toxicity relative ranking of low to very high is determined via the percentiles of watersheds analyzed; very low represents watersheds in the lower 20th percentile of toxicity, low 20-40th percentile, medium 40-60th percentile, high 60-80th percentile, and very high 80-100th percentile. Watersheds with no pesticides applied are not considered in the percentile analysis and are depicted as having no pesticides applied.

Relative toxicity index in the heat map and other graphical summaries are displayed in the side panel. The toxicity index presented on the map in the graphs are in scientific notation, a
standard format for writing large or small numbers in science. The format indicates where the
decimal place is relative to the reported digits. For instance:

<table>
<thead>
<tr>
<th>Scientific Notation</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.00E+06</td>
<td>1000000</td>
</tr>
<tr>
<td>1.00E+05</td>
<td>100000</td>
</tr>
<tr>
<td>1.00E+04</td>
<td>10000</td>
</tr>
<tr>
<td>1.00E+03</td>
<td>1000</td>
</tr>
<tr>
<td>1.00E+02</td>
<td>100</td>
</tr>
<tr>
<td>1.00E+01</td>
<td>10</td>
</tr>
<tr>
<td>1.00E+00</td>
<td>1</td>
</tr>
<tr>
<td>1.00E-01</td>
<td>0.1</td>
</tr>
<tr>
<td>1.00E-02</td>
<td>0</td>
</tr>
</tbody>
</table>
**Fig D. Clickable heatmap.** Information provided by the Environmental Release Tool within the heatmap when a watershed is selected. Base map imagery is a product of OpenStreetMap [https://www.openstreetmap.org/copyright](https://www.openstreetmap.org/copyright).

When a watershed is selected in the heatmap, the additional graphical summaries will appear in the side panel. A user can view additional value-specific information for each graph by hovering over the plot. For instance, in the ‘Site Applied Toxicity’ graph for watershed HUC 18030009, it’s observable that almonds contribute 39% of watershed applied toxicity (Fig 5(a)). To save graphical summaries from the user interface, a user can hover over the summary graphic of interest, and in the top right, icons will appear. If the user selects the camera icon (Fig 5(b)), they are given the option to download the image.
**Fig E. Pesticide and site applied toxicity.** a) Example of the Environmental Release Tool graphical summary of applied toxicity from pesticide application site types and b) how hovering provides additional details. To download a graphic of interest, hover over the image. In the upper right-hand corner, select the camera icon (see red arrow) to prompt the tool to download the image.

a)

![Site Toxicity Index](image1)

b)

![Site Toxicity Index](image2)

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### 4.2 Tabular Outputs

For the web tool, users can obtain tabular data by following the data download link in the upper right of the tool window. For desktop users, the data will automatically be saved into a sub-directory named after the simulation in the ‘EnvironmentalReleaseTool/output/’ directory. For each simulation, a new sub-directory with the simulation is created in the output directory.
and is provided to the user in the format of ‘*.csv’. Each file name begins with the simulation name and ends with file name descriptors (e.g., SimulationName_Watershed.csv’).

Tabular outputs the user is provided within the ‘output/SimulationName’ include:

- ‘SimulationName_Pesticides.csv’: Applied toxicity per pesticide for the simulation period.
- ‘SimulationName_ApplicationSites.csv’: Applied toxicity per application site for the simulation period.
- ‘SimulationName_Watershed.csv’: Applied toxicity per watershed for the simulation period.
- ‘SimulationName_PesticidesPerApplicationSite.csv’: Applied toxicity for each pesticide per application site for the simulation period.
- ‘SimulationName_PesticidesPerWatershed.csv’: Applied toxicity for each pesticide per watershed for the simulation period.
- ‘SimulationName_ApplicationSitesPerWatershed.csv’: Applied toxicity for each application site per watershed for the simulation period.
- ‘SimulationName_PesticidesPerApplicationSitePerWatershed.csv’: Applied toxicity for each pesticide per application site within each watershed for the analysis period.
- ‘SimulationName_PMPM_Output_Daily_Summary.csv’: Optional output (user selects to view this output in the input file ‘Simulation_Information.csv’), which provides a daily level summary of applied toxicity by site, chemical, and watershed for the simulation period.

Fields of the output data frames include:

- **huc**: Unique hydrologic unit code watershed identifier.
- **huc_name**: Name of hydrologic unit code watershed.
- **pesticide**: Name of pesticide evaluated.
- **pmpm_id**: Unique pesticide application site type for the Environmental Release Tool (ERT) in the Pesticide Mitigation Prioritization Model (PMPM). By default, the tool simplifies 268 unique application site types in pesticide use reports to 96).
- **pesticide_kg**: The mass of pesticide applied (kg).
- **RTI**: The applied toxicity (TI/ha) weighted by the affected compartment area in a watershed, *Equation (2).*
- **NTI**: The applied toxicity (unitless) of pesticide applied weighted by the applied toxicity of a pesticide and watershed in the n\(^{th}\) percentile of applied toxicity, see *Equation (3).*
- **NTI_perc**: Percentile of pesticide applied toxicity in watersheds used to calculate the NTI, see *Equation (3).*
- **econ_score**: Score of the economic value of application sites (USD/ha).
- **econ_health_score**: Index of the economic value of an application site and its protectiveness of environmental health (USD/NTI).
- **health_score**: Index of an application site’s protectiveness of environmental health (NTI/ha).

### 5.0 Example Applications – Environmental Release Tool

This section provides examples of how users might employ the ERT to attain pesticide mitigation insights. Recall that the module does not predict exposure, enabling an evaluation of health risks (see *Section 1.0*). Instead, the ERT allows users to explore sources of applied toxicity, regional variability, and mitigation options for reducing toxicity. Similarly, economic and health indices flag high applied toxicity application sites relative to their gross economic
value. Still, they do not account for other important considerations, such as how much pesticides migrate to air and water or the costs of cultivating a crop.

5.1 Temporal Trends

The Bay Delta Watershed in California is home to a rich community of organisms, including over 90 threatened or endangered species[38–40]. Significant concerns for pesticide toxicity in waterways have been observed within the watershed.[41] In reviewing results from the ERT for sub-watersheds of the Bay Delta for 2014-2018, two sub-watersheds that contribute to high applied toxicity are the Dry Creek and the Lower Feather River. Graphical summaries provided by the ERT of temporal trends in the Dry Creek subwatershed demonstrate the applied toxicity increased from 2014-2018 (Fig 6). In the Lower Feather River Watershed, applied toxicity has remained relatively steady and decreased marginally. These insights suggest mitigation efforts should prioritize better understanding and mitigating the increased pesticide-applied toxicity in the Dry Creek Watershed, which is also higher than that of the Lower Feather River Watershed.

**Fig F. Temporal trends.** Example of temporal trends of pesticide-applied toxicity provided by the Environmental Release Tool for a) the Dry Creek subwatershed and b) the Lower Feather River subwatershed.

a) 

b)
5.2 Chemical Alternatives

From the ERT heatmap of statewide watersheds, an almond farmer observes that her Upper Poso watershed receives high applied toxicity (Fig 7). In the review of the crops contributing to toxicity in the watershed, almonds introduce over 60% of applied toxicity. Moreover, of the hundreds of different pesticide and crop treatment types in the watershed, bifenthrin on almonds accounts for 30% of all pesticide-applied toxicity. The almond farmer considers her routine use of bifenthrin to combat mites, one of the watershed's most damaging pests to almonds. Given this knowledge of the high environmental impact of bifenthrin on bees and aquatic fauna, she reviews a chemical alternatives database [42]. In the review of alternatives, she observes that bifenazate is a pesticide that targets mites and has a substantially lower toxicity profile and environmental persistence. If bifenazate were employed as an alternative to bifenthrin to treat almond mites, the applied toxicity per hectare would be reduced by 400-fold for fish and over 100,000-fold for aquatic invertebrates. For the subsequent treatment of mite pests, the farmer employs bifenazate.
Fig G. Example application – Poso Creek. Environmental Release Tool results for the Poso Creek watershed. Base map imagery is a product of OpenStreetMap
https://www.openstreetmap.org/copyright.

5.3 Prioritizing Monitoring

For pesticide use practices in California, it was observable from outputs of the ERT for 2014-2018 that of the hundreds of pesticides in use, 15 introduced 99% of environmental applied toxicity. Moreover, 80% of applied toxicity was applied to 14 different site types and 14 watersheds. Exemplary actions that may be taken from these insights include exerting more effort in the registration/re-registration process for the chemicals and sites identified as contributing the majority of applied toxicity or designing monitoring campaigns to more closely monitor high-impact chemicals and application sites.

5.4 Health and Economic Tradeoffs

The ERT provides health and economic indices of the sites to which pesticides are applied. By considering health protectiveness and the economic value of sites targeted during pesticide application, users can evaluate approaches for working with pesticide users to reduce applied toxicity in at-risk watersheds. For example, from 2014-2018 in California, cotton was observed to have a low economic value per hectare of site types with the highest applied toxicity. In high-risk watersheds, farmers may be incentivized to cultivate crops with lower applied toxicity and higher economic value (see Table 1).
6.0 Errors and Updates

The ERT was developed as a part of an ongoing PhD dissertation and has limited capacity for user assistance at the time of this guide’s publication. Accordingly, the tool was developed in one of the most widely used data science tools for which a plethora of online assistance exists for errors encountered during simulation runs. Users can explore solutions to errors encountered via googling the error codes or exploring question and answer websites such as Stack Exchange. Users troubleshooting errors should prioritize ensuring all inputs match the EXACT formatting of template files and input field formats described in Section 3.0 Parameterization. Second, a user should explore device-specific errors for running the RStudio software and packages via an internet search of the error code. Third, the user should revisit the ERT download link and look for model updates.
7.0 Acknowledgements

This project was funded by the California Sea Grant Delta Science Fellowship SEADSR4/183BCA/416701/440000.

8.0 References


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