Keller Research Team's ChemFate and Transport Model Evaluation

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Background

This study was designed to support and evaluate the Chemical Fate and Transport models (ChemFate) developed by Dr. Arturo A. Keller and the Keller Lab of the Bren School of Environmental Management, UCSB, California. ChemFate contains four fate and transport models: organoFate, ionOFate, metalFate, and nanoFate. This study focuses on three specific ChemFate models: a nonionizable organic chemical model (organoFate); an ionizable organic chemical model (ionOFate); and a metal based chemical model (metalFate). Operating the program to run each of the models requires at least three separate files: a region of interest file specific to the environmental region over which the chemicals will be modeled; a chemical release file which indicates on an annual basis how much of, and when, a chemical is released within a region; and, a chemical parameter file which houses characteristics specific to the chemical that is to be modeled.

In order to complete this study a global ranking of most widely used pesticides had to be developed. For each of those pesticides, a collection of toxicological endpoints, common application statistics, as well as physical and chemical characteristics then had to be developed. A regional environmental study on Salinas River Valley was undertaken and a synthesis of pesticide and regional environmental data was developed to evaluate the general use and feasibility of use of the ChemFate models by the general user, who would be evaluating the fate and transport of select pesticides. The feasibility and general use evaluation of the ChemFate models will hopefully support the rollout of ChemFate.

1. Pesticide Ranking

The most widely used pesticides on a global scale were selected from the available annual sales reports of the top four grossing worldwide pesticide producing companies:[1] Syngenta[2], Bayer AG[3], Dow and Dupont[4], and BASF[5]. All of the commercial insecticide, herbicide, rodenticide, phytohormone, fungicide and bactericide products listed in the available annual recorded sales for each company were ranked based on their sales as a percentage of each company's sales. After listing each commercial pesticide products by percentage of sales, the percent per volume of active ingredient(s) was examined for each pesticide as well. The active ingredient chemicals were then cross-referenced by volume of usage in the United States from the USGS Pesticide National Synthesis Project website[6]. Of the original researchable one-hundred-and-nine globally use pesticides from the most frequently listed categories (fungicides, herbicides and insecticides); sixteen fungicides and herbicides, and fifteen insecticides were selected. The top pesticide chemicals from each category were chosen based on how frequently the chemicals were used within the agricultural industry, the number of commercial products containing the pesticide chemical, and the overall volume of use of each chemical in the United States (*Appendix A*). That process resulted in a group of forty-seven of the most widely used pesticide chemicals being selected for further research from the original top one-hundred-and-nine chemicals found within the annual sales reports.

[1] Investopedia 2019. The Biggest Pesticide Companies in the World. https://www.investopedia.com/articles/markets-economy/082516/top-5-pesticide-companies-world-syt-dow.asp
[2] Syngenta 2018. Presentations and Publications. https://www.syngenta.com/company/presentations-and-publications
[3] Bayer 2018. Annual Report. https://www.bayer.com/
[4] Dow and Dupont 2018. https://www.annualreports.com/HostedData/AnnualReports/PDF/NYSE_DD_2017.PDF
[5] BASF 2018. Online Report 2018. https://report.basf.com/2018/en/
[6] USGS 2018. Pesticide National Synthesis Project. https://water.usgs.gov/nawqa/pnsp/usage/maps/compound_listing.php

2. Pesticide Data Collection

The ChemFate models requires a great deal of data collection to complete the files necessary to operate the program. Fortunately, the user guide provides excellent, and in some cases step-by-step, methods or references for which to collect aspects of data needed to complete the input files that are necessary to operate the program. In addition to the chemical and regional characterization and parameters data needed to operate the model programs, toxicological endpoints for each pesticide chemical were documented from scientific literature, databases, EPA references. The endpoint data collected was used to compared with the model results. The comparisons drawn could be used to, name a few examples, illustrate whether the total maximum daily load of a pesticide is met, exceeded, or appropriate for the region.

The ChemFate models requires the collection of a large amount of data to complete the files necessary to operate the program. Fortunately, the user guide also provides some methods and references from which to collect aspects of data necessary to complete the input files and operate the program. In addition to the chemical and regional characterization and parameter data need to operate the models, toxicological endpoints for each pesticide chemical were synthesized from academic and government run databases as well as scientific literature. The endpoint data collected was used for comparison with the model results. The comparisons drawn, for example, could illustrate whether the total maximum daily load of a pesticide is met, exceeded, or appropriate for the region.

2.1 Toxicological Endpoints (Ecotoxicology)

The toxicological endpoints were found for each of the selected pesticide chemicals. The endpoint parameters collected were LC50, EC50, NOAEL/NOEL, and LOAEL/LOEL for key species. The value for each endpoint parameter collected by key species was somewhat limited by the information available from listed references *(Appendix B*). The toxicological endpoints will be compared with the modeled results for a select group of pesticide chemicals in section 4.

2.2 Application

Analysis of the common volumes of usage by commercial products, crops, and regional area was document for each chemical. The data used to determine the volume per commercial product, crop, and region, together with the attached data package and the location of the data along with the resulting analytical files (chemical statistics and chemical release) can be found in Appendix B.

The annual volume used, and the frequency of use, per chemical, must be entered in the chemical release input files. Those files depend on the regional configuration data. The regional configuration data yields the application unit area conversion value for each environmental compartment indicating how much of the chemical has been released per area. In this study, the model's chemical release information was exaggerated. The chemical release file used in the model was configured to indicate a simultaneous release of the pesticide chemical over the entire landscaped urban, agricultural, and biosolid soil environmental compartments with contamination infiltrating the adjacent air, freshwater and saltwater compartments.

The California Department of Pesticide Regulation[7] database was used to process the most common products, crops, and unit volume per area associated with each pesticide chemical. The maximum and mean usage was determined in kg per meter squared units from the given data. This area was then divided by three-time usage per season or three-hundred-and-sixty-five days per year depending on seasonal or constant (i.e., daily)[8] application tests of the model. The resulting application rate was further parceled out by the percentage of chemical 0.4%, 2%, 4%, 2%, 30%, and 5% that was applied directly to or contaminated through air, freshwater, seawater, undeveloped surface soils, developed soils, and agricultural biosolid areas as well as agricultural application sites (*Appendix B)*.

2.3 Physical & Chemical Characteristics

In addition to pesticide application data, each pesticide was evaluated by its respective physical and chemical characteristics. These characteristics were detailed depending on the nature (metal, ionizable, or nonionizable) of each pesticide chemical. The characteristics or properties specific to the nature of the pesticide chemicals such as molecular weight, K partition constants, chemical speciation, and the half-life for each environmental compartment are stored in both research files as well as the chemical parameter files necessary to operate the ChemFate model (*Appendix B*).

These chemical parameter files were completed in the format provided for by ChemFate model GitHub repository and user guide[9]. They are supplied for each chemical studied for this report and supplied along with the data package. The location of those files can be found in Appendix B. The user guide suggests excellent references and models such as MINTEQ[10], Windermere Humic Aqueous Model (WHAM)[11], and Estimation Program Interface (EPI)[12], which was used in this study. These models have specific platform requirements which cannot always be met by the average use. The user guide methods should be followed to the highest extent possible for the best measure of success, however, in the event that the user cannot meet those requirements, reference materials outlined in Appendix B can also provide, at least in part, the parameter data needed to operate the ChemFate models.

3. Regional Study

A regional file is also required to run ChemFate models in accordance with the user guide. For the purposes of this study the coastal region of Salinas River Valley, California was selected to evaluate these models. The regional file created for this study is supplied, along with the data package that accompanies this study report. The location of the file is shared in Appendix C.

The Salinas River Watershed contains the Salinas River which runs the entire length of the valley on the western edge of central California. It flows from south to north from San Louis Obispo county into Monterey county, emptying into the Monterey Bay. The Salinas River Watershed has a heavy concentration of agricultural land in close proximity to the river, which is

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[7] California Department of Pesticide Regulation 2019. CalPIP Navigation Menu. https://calpip.cdpr.ca.gov/main.cfm
[8] ChemFate uses the term "constant" to indicate the daily release of pesticides. To be consistent with the ChemFate usage, "constant" is used herein to indicate the daily release of pesticides.
[9] GitHub 2020. ChemFate Repository. https://github.com/klaris-ak/ChemFate
[10] John Peter Gustafsson 2013.Visual MITEQ ver. 3.1 https://vminteq.lwr.kth.se/
[11] U Centre for Ecology and Hydrology. Windermere Humic Aqueous Model (WHAM). https://www.ceh.ac.uk/services/windermere-humic-aqueous-model-wham
[12] EPA 2017. EPI Suite™. https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface

adjacent to the coast. This region has a long agricultural history, growing a wide variety of crops on which there is a variety of pesticide chemical dependency[13].

The user guide provides an excellent step-by-step method for collecting the regional data necessary to complete the input files and operate the program. Those step-by-step methods include the use of Better Assessment Science Integrating Point and Non-point Sources (BASINS)[14] model, USGS National Land Cover Database (NLCD)[15], and STORET Data Warehouse[16] database. Processing the data from these sources requires GIS software. This study was completed without using GIS; in the event that the user is unable to access GIS, it is possible to complete the data collection using a variety of researched papers and online USDA web interface Soil Survey[17] data.

4. ChemFate Models

The ChemFate models are relatively easy to operate. The GUI is clear, concise, easy to understand, and loads on command quickly and without fail. The most complicated and time-consuming part about running the model is completing the requisite files. The data has to be collected, synthesized, and placed into the appropriate fields. Once the data collection and processing are complete, the model allows for quick and easy use.

For the purpose of this study, a subset of the researched pesticide chemicals was selected based on their unique set of inputs and a regional environmental study was performed on Salinas River Valley to complete the evaluation of the ionizable organic, nonionizable organic and metal ChemFate models. The resulting data from these models were then compared with their respective toxicological endpoints described in section 2.1.

4.1 Inputs

Of the four ChemFate models, only the metalFate, organoFate, and ionOFate chemical fate and transport models were used to evaluate ChemFate performance. Therefore, each of the forty-seven pesticide chemicals selected were determined to be either be metal (metalFate), nonionizable organic (organoFate), or ionizable organic (ionOFate) in nature. Only one metal-based pesticide chemical was commonly used enough world-wide to be selected as part of this study; the remaining pesticides selected were either ionizable or nonionizable organic pesticides. Of the remaining pesticides selected, ionizable organics chemical pesticides appear to be over two times more frequently used than the nonionizable organic counterpart chemicals.

MetalFate, organoFate, and ionOFate naturally do not have identical parameter inputs. The characteristics of each chemical type have distinctly different behaviors and require specific inputs as such. The chemical parameter file location within the data package for each model are found in Appendix D. The common components to each chemical parameter file required to operate the three models are the chemical name and molecular weight as well as the octanol/water (Kow), organic carbon/water (Koc), air/water (Kaw), and aerosol/air (Kp) partition

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[13] California Department of Pesticide Regulation 2019. CalPIP Navigation Menu. https://calpip.cdpr.ca.gov/main.cfm
[14] EPA 2019. BASINS. https://www.epa.gov/ceam/better-assessment-science-integrating-point-and-non-point-sources-basins
[15] USGS 2017. Earth Engine Data Catalog; USGS National Land Cover Database. https://developers.google.com/earth-engine/datasets/catalog/USGS_NLCD
[16] EPA 2012. STORET Data Warehouse Access. https://www3.epa.gov/storet/bck/dbtop.html
[17] USDA 2019. Web Soil Survey. https://websoilsurvey.sc.egov.usda.gov/App/WebSoilSurvey.aspx

coefficients. The ionizable and metal chemical parameter files also require the chemical formula, SMILES, CAS number, chemical type (organic acid or organic base), pKa, and enrichment factor.

All three model chemical parameter input files have sections requiring entries for stratified environmental compartments within ChemFate. Those environmental compartments are air, freshwater and sediment, saltwater and sediment, and soil compartments. The stratification of the compartments starts from top to bottom within each section except for air, which is broken down as either air or aerosol. Freshwater and saltwater compartments are broken down into pure water (freshwater or saltwater) likely found at the top of a water column, then some mixture of water and sediment, followed by solid sediment likely found at the base of the water column. The soil system is similarly stratified with the top being influenced by air, then water from the water table, then growing more solid as the soil structure become denser or clay laden, and finally the deep soils layer which would be anoxic. The soil system is further subdivided into urban, undeveloped, agricultural, and biosolid agricultural soil compartments. Each subsection of soils will represent different characteristics of permeability, water flow, biomatter, carbon content, etc. within the model.

The ionizable chemical parameter file has an entry for both neutral and ionic half-life for each parameter while the nonionizable chemical parameter file will only have the neutral half-life entry for chemical decay. The research conducted for this study did not locate any reference or literature for ionizable half-life differentiated from neutral half-life entries for any of the pesticide chemicals listed. This suggests that such a differentiation (neutral vs. ionizable) of half-life is rarely made or published. Having the same half-life value for neutral and ionic parameter entries does not appear to have impacted model's performance.

The ionizable organic and metal chemical parameter files each have a section for species fraction for all of the environmental compartment and soils subsections. It is more important to complete this section to the fullest for the metalFate model than for the ionOFate model, given that this one of the primary sections in the metal chemical parameter file. The user guide illustrates common references such as MINTEQ[18] and WHAM[19] to complete this section of the chemical parameter file. From the literature, it appears fairly common to find species fraction values for metal chemicals in environmental compartments. For ionizable organic chemical pesticides, species fraction values were less common to find in the literature, however, as a secondary characterization section, hose values are not necessary to operate the ionOFate model.

The ionizable organic chemical parameter files also contains a section for sorption partition coefficient within each environmental compartment. Values for sorption partition coefficients for ionizable pesticides were rarely found, and when located they were generally given as a range of values for soils.

4.2 Pesticide Selection for Models

A subset of thirteen pesticide chemicals were chosen to evaluate the ChemFate models from the original forty-seven researched chemicals. Six chemicals (two each of fungicide, herbicide, and insecticide) were selected for ionizable and nonionizable organic models. As noted above,

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[18] John Peter Gustafsson 2013.Visual MITEQ ver. 3.1 https://vminteq.lwr.kth.se/
[19] U Centre for Ecology and Hydrology. Windermere Humic Aqueous Model (WHAM). https://www.ceh.ac.uk/services/windermere-humic-aqueous-model-wham

only one commonly used metal based chemical pesticide had sufficiently frequent use globally to be evaluated in this study.

The selected ionizable and nonionizable organic models were based on the uniqueness of characteristics and inputs representative of each class of pesticide (*Tables 1 & 2*). The characteristics selected for include volatility, and the relative value of Kow or Koc compared with other chemicals. Additional selection criteria were based on the relative half-life value compared with other chemicals within each environmental compartment. The environmental compartments used for selection include air, freshwater and sediment, salt-water and sediment, and soil compartments as described in the previous section 4.1.

Table 1. IonOFate Pesticide Selection Table. This table represents the ionizable organic chemicals selected to study the ionOFate model performance given select unique characteristics and parameters.

IonOFate Selection							
Pesticide Chemical	**Type**	**Kow**	**Koc**	**Volatile**	**Air Half-life**	**Water Half-life**	**Soil Half-Life**
1,3-Dichloropropene	Insecticide	Medium	Low	Yes	Medium	Medium	Medium
Azoxystrobin	Fungicide	Medium	Medium		Short	Medium	Long
Chlorothalonil	Fungicide	High	High		Long	Short	Medium
Glyphosate	Herbicide	High	High		Short	Medium	Medium
L-Cyhalothrin	Insecticide	High	High	Yes	Long	Long	Long
Rimsulfuron	Herbicide	Medium	Low		Short	Medium	Medium

Table 2. OrganoFate Pesticide Selection Table. This table represents the nonionizable organic chemicals selected to study the organoFate model performance given select unique characteristics and parameters.

OrganoFate Selection							
Pesticide Chemical	**Type**	**Kow**	**Koc**	**Volatile**	**Air Half-life**	**Water Half-life**	**Soil Half-Life**
2,4-D	Herbicide	Medium	Low	Y	Medium	Medium	Medium
Fipronil	Insecticide	High	High		Short	High	Medium
Fludioxonil	Fungicide	High	High		Short	Medium	High
Mancozeb	Fungicide	Low	Medium	Y	Short	High	High
Novaluron	Insecticide	High	High		Short	Short	Medium
Paraquat Dichloride	Herbicide	High	High		Medium	High	High

Table 3. MetalFate Pesticide Selection Table. This table represents the metallic organic chemical used to study the metalFate model performance.

MetalFate					
Pesticide Chemical	**Type**	**Kaw**	**Koc**	**Volatile**	**Species Fraction**
Copper Hydroxide	Fungicide	Default	N/A	N/A	See File

4.3 Results

The ChemFate model analysis produces three files: a chemical concentration file which displays the concentration of chemical in grams per liter for each environmental compartment daily over the range of dates the user selects with through the GUI; a chemical mass file which displays the same data as the chemical concentration file in kilo-grams rather than grams per liter; and, a chemical process file which describes the transfer into and out of the environmental compartment or system via advection or degradation. The advective transport and degradation processes are described in detail in the user guide; however, the output files are not detailed in the user guide. While the concentration and mass files are easily understood, the advective and degradation process file is less clear. The file does not display units and it contains additional columns that are not described on the GitHub site or in the user guide. As a result, it is more difficult to interpret and understand this file. All of the output files are included with the data package. The locations of those files within the data package are found in Appendix D.

The model results were compared across each environmental compartment, release schema, and pesticide type. The results for all three models, including comparison tables, seasonal and constant release graphs, are also found in Appendix D. However, due to the size of the image files for the advective process and the ambiguity of the content, the advective process results are not displayed in this report.

Seasonal release of the pesticides reviewed follows a three-time release pattern for the spring growing season, while the constant (daily) release rate is self-explanatory. The release dates (February 25, March 29, and May 23) for the spring growing season were chosen by default from the ChemFate input files. It is important to note that these release dates are idealized for this study and in reality, may shift over time for any number of reasons.

For the purposes of this study, it was assumed that the pesticide in question was released consistently across all agricultural areas and cross contaminated into other environmental compartments simultaneously. Constant versus seasonal release rates will have a different volume per application rate due to the recommended usage per pesticide. For the seasonal release, the annual average use of the pesticide per unit area is divided by the three dates of the spring-time application. The chemical then disperses and degrades until the next application. The same is true for the constant application, although the annual average volume per area of pesticide is divide by 365 days instead.

4.3.1 IonOFate

Ionizable organic pesticides appear to be the most common type of pesticide chemical on the market. The ionOFate model is used to evaluate the fate and transport of ionizable organic pesticide chemicals. While the ionOFate model produces the three output files noted above, for the purposes of simplicity in evaluating the performance of the model in this study, only the concentration file results were evaluated. The model was run twice for each pesticide, once for a constant (daily) application of the chemical in question and once for a seasonal application.

The constant release rate and seasonal release rate of the ionizable pesticides are compared here (*Tables 4 & 5*). The time lag between seasonal applications allows for environmental processes to disperse or degrade the chemical. There is at least an order of magnitude difference between the maximum constant and seasonal release of pesticides within each environmental compartment with the exception of L-Cyhalothrin, which appears to have little change in value between constant release and seasonal release in the urban, agricultural and biosolid soils owing to the large Koc and long half-life soil values.

Table 4. IonOFate Constant Release Results. This table represents the order of magnitude of the maximum concentration value resulting from the ionOFate model run for each representative ionizable chemical selected.

IonOFate Constant Results									
Order of Magnitude of Background Concentration									
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
1,3-Dichloropropene	-11	-8	-8	-12	-10	-10	-6	-10	-9
Azoxystrobin	-16	-13	-13	-15	-14	-14	-11	-14	-14
Chlorothalonil	-13	-6	-7	-7	-8	-8	-5	-7	-7
Glyphosate	-19	-13	-13	-15	-14	-14	-11	-15	-14
L-Cyhalothrin	-15	-8	-7	-9	-8	-9	-5	-6	-6
Rimsulfuron	-16	-11	-12	-13	-13	-13	-9	-13	-13

Table 5. IonOFate Seasonal Release Results. This table represents the order of magnitude of the maximum concentration value resulting from the organoFate model for each representative ionizable chemical selected.

IonOFate Seasonal									
Max Order of Magnitude of Background Concentration									
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
1,3-Dichloropropene	-13	-10	-11	-13	-13	-13	-9	-11	-11
Azoxystrobin	-14	-11	-12	-13	-13	-14	-10	-12	12
Chlorothalonil	-11	-4	-5	-7	-7	-7	-4	-5	-5
Glyphosate	-17	-11	-11	-13	-13	-13	-10	-12	-12
L-Cyhalothrin	-13	-7	-7	-8	-8	-8	-5	-6	-6
Rimsulfuron	-14	-9	-10	-12	-12	-12	-9	-11	-11

Table 6. IonOFate Seasonal Persistence of Signal Results. This table represents persistence in concentration observed in the impulse of chemical delivered to the area.

IonOFate Seasonal									
Persistence of Signal	(High, Moderate, and	Low)							
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
1,3-Dichloropropene	Moderate	Moderate	Moderate	Moderate	Moderate	High	High	Moderate	Moderate
Azoxystrobin	Low	Low	Moderate	Moderate	High	High	High	Low	Low
Chlorothalonil	Moderate	Moderate	Moderate	Moderate	Moderate	High	High	Moderate	Moderate
Glyphosate	Moderate	Moderate	Moderate	Moderate	Moderate	High	High	Moderate	Moderate
L-Cyhalothrin	Moderate	Moderate	High	Moderate	High	High	High	High	High
Rimsulfuron	Moderate	Moderate	Moderate	Moderate	Moderate	High	High	Moderate	Moderate

Ecotoxicological comparison illustrates which ecological environmental compartments may be considered hazardous to key species. The threat is determined by the similar toxicological endpoint values and the order of magnitude of the concentration of chemical within the appropriate environmental compartment for a key species. For purposes of this study, the ecotoxicological comparison was made with the combination of endpoints across each environmental compartment. This admittedly is not the soundest of comparison methods when evaluating pesticide models; however, it was chosen in this instance to simplify and illustrate the change in ionOFate model results from constant to seasonal release and how that change might impact ecology.

The comparison of the ionOFate model between the constant and seasonal release indicates some shift in hazards. The ecological hazards increase with seasonal release due to the higher volume of chemical released into the environment over a short period of time. For chemicals that do not degrade or dissipate rapidly, this could increase the ecological threat to a given environmental compartment.

Table 7. IonOFate Constant Release Combined Ecotoxicological Comparisons. This table represents a simplified perspective on evaluating the ecological impacts the chemical may have from a constant release pattern.

IonOFate Constant Release Combined Ecotoxicological Comparisons									
						Caution	Warning	No Issue	
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
1,3-Dichloropropene									
Azoxystrobin									
Chlorothalonil									
Glyphosate									
L-Cyhalothrin									
Rimsulfuron									

Table 8. IonOFate Seasonal Release Combined Ecotoxicological Comparisons. This table represents a simplified perspective on evaluating the ecological impacts the chemical may have from a seasonal release pattern.

IonOFate Seasonal Release Combined Ecotoxicological Comparisons									
						Caution	Warning	No Issue	
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultura l Soils**	**Biosolid Soils**
1,3-Dichloropropene									
Azoxystrobin									
Chlorothalonil									
Glyphosate									
L-Cyhalothrin									
Rimsulfuron									

4.3.2 OrganoFate

Nonionizable organic pesticides appear to be the next most common type of pesticide chemical on the market after ionizable organic pesticides. The organoFate model is used to evaluate the fate and transport of these pesticides. The organoFate model produces the same three output files as the ionOFate model. The organoFate output was evaluated in the same fashion as ionOFate, with the concentration output files being run twice, once each for constant (daily) and seasonal application volumes.

The constant release rate and seasonal release rate of the ionizable pesticides are compared here (*Tables 9 & 10*). The time lag between seasonal applications allows for environmental processes to disperse or degrade the chemical. There is at least an order of magnitude, but more commonly two or more orders of magnitude, difference between the maximum constant and seasonal release of pesticides within each environmental compartment.

Table 9. OrganoFate Constant Release Results. This table represents the order of magnitude of the maximum concentration value resulting from the organoFate model run for each representative nonionizable chemical selected.

OrganoFate Constant Results Table									
Order of Magnitude of Background Concentration									
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
2,4-D	-14	-8	-8	-8	-8	-7	-5	-8	-8
Fipronil	-15	-8	-8	-8	-8	-7	-5	-6	-6
Fludioxonil	-15	-8	-8	-9	-8	-7	-4	-6	-6
Mancozeb	-14	-7	-8	-9	-8	-7	-3	-6	-6
Novaluron	-17	-10	-11	-11	-11	-8	-4	-9	-9
Paraquat Dichloride	-11	-7	-8	-8	-9	-9	-6	-7	-7

Table 10. OrganoFate Seasonal Release Results. This table represents the order of magnitude of the maximum concentration value resulting from the organoFate model for each representative nonionizable chemical selected.

OrganoFate Seasonal Results									
Max Order of Magnitude of Background Concentration									
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
2,4-D	-15	-13	-13	-14	-14	-12	-12	-5	-5
Fipronil	-19	-13	-13	-14	-14	-13	-13	-7	-5
Fludioxonil	-19	-13	-13	-14	-14	-13	-13	-5	-5
Mancozeb	-16	-12	-13	-14	-14	-13	-13	-4	-4
Novaluron	-23	-15	-17	-18	-19	-17	-17	-7	-6
Paraquat Dichloride	-9	-11	-12	-12	-13	-10	-10	-5	-5

The models indicate significant differences in trends between ionizable and nonionizable organic pesticides (*Table 11*). Nonionizable organic chemicals appeared more likely to migrate to deeper soils at the area of origin and dissipate more slowly over time from the place of origin; this can be better observed in the image files in Appendix D. Nonionizable organic chemicals also appear to remain in higher concentrations over time in soils. The results are intriguing enough and easy enough to derive that further exploration into the resulting model differences should be studied to compare the performance of the overall functions.

Table 11. Mean Order of Magnitude Results. This table represents the mean order of magnitude changes in concentration across all environmental compartments between constant and seasonal release patterns for both ionOFate and organoFate models.

Average Order of Magnitude by Environmental Compartment									
Model/Application	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
IonO/Constant	-15	-10	-10	-12	-11	-11	-8	-11	-11
IonO/Seasonal	-14	-9	-9	-11	-11	-11	-8	-10	-6
Difference	-1	-1	-1	-1	0	0	0	-1	-5

Organo/Constant	-14	-8	-9	-9	-9	-8	-5	-7	-7
Organo/Seasonal	-17	-13	-14	-14	-15	-13	-13	-6	-5
Difference	3	5	5	6	6	6	9	-2	-2

Ecotoxicological comparison illustrates which ecological environmental compartments may be considered hazardous to key species. The threat is determined by the similarity between toxicological endpoint values for a key species and the order of magnitude of the concentration of chemical within the appropriate environmental compartment. For the sake of simplicity in this study, the ecotoxicological comparison was made with the combination of endpoints across each environmental compartment. This admittedly is not the soundest of comparison methods when evaluating pesticide models; however, it was chosen to simplify and illustrate the change in organoFate model results from constant to seasonal release and how that change may impact ecology.

Comparing the organoFate model results for constant and seasonal releases indicates some shifts in the location where ecological threats are concentrated. The ecological threats appear to shift depending on whether application is constant or seasonal due to the persistence of the chemical released into specific environmental compartments. This would indicate that pesticide chemicals increase the ecological threat within the environmental compartment in which the chemical persists. The persistence of the chemical depends on its' characteristics. For instance, Paraquat Dichloride has a high Koc (octanol/carbon coefficient) value and half-life in soil. Under seasonal application conditions (*Table 13*), Paraquat Dichloride appears to persist in agricultural and biosolid soils. Those soils presumably have a higher degree of carbon content.

Table 12. OrganoFate Constant Release Combined Ecotoxicological Comparisons. This table represents a simplified perspective on evaluating the ecological impacts the chemical may have from a constant release pattern.

OrganoFate Constant Release Combined Ecotoxicological Comparisons									
						Caution	Warning	No Issue	
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
2,4-D									
Fipronil									
Fludioxonil									
Mancozeb									
Novaluron									
Paraquat Dichloride									

Table 13. OroganoFate Seasonal Release Combined Ecotoxicological Comparisons. This table represents a simplified perspective on evaluating the ecological impacts the chemical may have from a constant release pattern.

OrganoFate Seasonal Release Combined Ecotoxicological Comparisons									
						Caution	Warning	No Issue	
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
2,4-D									
Fipronil									
Fludioxonil									

Mancozeb	
Novaluron	
Paraquat Dichloride	

4.3.3 MetalFate

The metalFate model evaluates the fate and transport of metallic pesticide chemicals. Metallic pesticides appear to be the least common type of pesticide chemical on the global market based on the evaluation of pesticide sales and usage conducted as part of this study. Given the unfavorable results that the metalFate model showed for the pesticide evaluated, *copper hydroxide*, limited used of metallic pesticides would appear to be desirable.

The metalFate model produces the same three files as are produced in the ionOfate and organoFate model outputs. For the purposes of simplicity in evaluating the performance of this model in this study, only the concentration file results are to be evaluated here. As with the other models, the metalFate model was run twice for *copper hydroxide,* once for a constant application and once for a seasonal application.

The constant and seasonal release rate of the metallic pesticide are compared here (*Tables 14 & 15*). The time lag between seasonal applications allows for environmental processes to disperse or degrade the chemicals in the nonionizable and metallic compounds. This appears to happen at a slower rate, however, for the ionizable compounds (*Table 16*).

Copper Hydroxide appears to at least an order of magnitude lower with seasonal application in all but undeveloped soils, in which case the difference is six magnitudes. This result seems inconsistent with other results and inexplicable without further study.

Table 14. MetalFate Constant Release Results. This table represents the order of magnitude of the maximum concentration value resulting from the metalFate modeling the copper hydroxide fungicide.

MetalFate Constant Results Table									
Order of Magnitude of Background Concentration									
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
Copper Hydroxide	-10	-6	-6	-6	-5	-6	-2	-4	-4

Table 15. MetalFate Seasonal Release Results. This table represents the order of magnitude of the maximum concentration value resulting from the metalFate modeling the copper hydroxide fungicide.

MetalFate Seasonal Results									
Max Order of Magnitude of Background Concentration									
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
Copper Hydroxide	-12	-7	-7	-7	-6	0	-4	-6	-6

Table 16. Mean Order of Magnitude Results. This table represents the mean order of magnitude changes in concentration across all environmental compartments between constant and seasonal release patterns for ionOFate, organoFate, and metalFate models.

Average Order of Magnitude by Environmental Compartment									
Model/Application	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
IonO/Constant	-15	-10	-10	-12	-11	-11	-8	-11	-11
IonO/Seasonal	-14	-9	-9	-11	-11	-11	-8	-10	-6
Difference	-1	-1	-1	-1	0	0	0	-1	-5
Organo/Constant	-14	-8	-9	-9	-9	-8	-5	-7	-7
Organo/Seasonal	-17	-13	-14	-14	-15	-13	-13	-6	-5
Difference	3	5	5	6	6	6	9	-2	-2
Metal/Constant	-10	-6	-6	-6	-5	-6	-2	-4	-4
Metal/Seasonal	-12	-7	-7	-7	-6	0	-4	-6	-6
Difference	2	1	1	1	1	-6	2	2	2

Table 17. MetalFate Seasonal Release Persistence of Chemical Results. This table represents the persistence of the metalFate modeling the copper hydroxide fungicide signal resulting from a seasonal release pattern.

MetalFate Seasonal Results									
Persistence of Chemical	(High, Moderate, and Low)								
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
Copper Hydroxide	V High	V High	V High	V High	V High	V High	V High	V High	V High

MetalFate indicates that *copper hydroxide* can be very persistent in the environment. This non-scientific ecological threat evaluation increases significantly under seasonal application due to the volume and persistence of the metallic chemical compound released (*Tables 18 & 19*).

Table 18. MetalFate Constant Release Combined Ecotoxicological Comparisons. This table represents a simplified perspective on evaluating the ecological impacts that copper hydroxide may have from a constant release pattern.

MetalFate Constant Release Combined Ecotoxicological Comparisons									
						Caution	Warning	No Issue	
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
Copper Hydroxide									

Table 19. MetalFate Seasonal Release Combined Ecotoxicological Comparisons. This table represents a simplified perspective on evaluating the ecological impacts the chemical may have from a seasonal release pattern.

MetalFate Seasonal Release Combined Ecotoxicological Comparisons									
						Caution	Warning	No Issue	
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
Copper Hydroxide									

5. Conclusion

The ChemFate models indicate significant differences in trends between metallic, ionizable and nonionizable organic pesticides. The results are intriguing enough and easily enough derived to suggest that further exploration of the model differences should be made to compare the performance of the overall functions. The model comparison with toxicological endpoints indicates that ionizable organic pesticides appeared to be more toxic in freshwater environments and nonionizable organic pesticides appear to be more toxic in soils, while *copper hydroxide* was consistently more toxic under seasonal release patterns. This is not a scientifically sound analysis, however. This study was directed towards a user analysis of ChemFate. It was not intended to provide the type of thorough scientific analysis necessary to investigate the sources of the results found or their effects on the ecology.

Overall, the ChemFate models are easy to use, consistent, reliable, and quick. However, the model requires a great deal of specific information, not uncommon to most fate and transport models. Fortunately, the user guide provides either directions of how to obtain the necessary information or references to databases or models from which to obtain the information. This study recognizes, however, that not all users will be able to access the databases or models that the user guide suggests or be proficient in their usage. Some of the methods require GIS and or other specific platform requirements. This study presents alternative literature, resources or references that may be used to obtain some of the information necessary to run the models in the event that a user does not have access to or is not proficient in the methods suggested by the user guide. The alternate sources provided by this study, however, also must be used with caution. The information needed to run the models can still be somewhat difficult to find. It also may be inconsistently reported across reference platforms. Furthermore, the ability to find the information required to operate ChemFate can be further hindered by the relative newness of a particular pesticide chemical on the market and/or from a lack of available research. In addition to being difficult to find, the information that is available can be conflicting or show a wide range of uncertainty.

The process of data collection, organization, and entry will be the most time-consuming part of operating the model correctly. Some suggestions of material that could be included in the user guide to assist with the data assimilation include:

- A glossary of terms for the parameter inputs, including common aliases for those terms.
- A range of acceptable values for each chemical, environmental, and regional parameter, with the exception of site-specific data such as area.
- The program should have a process run-time catch routine which will let a user know if, and where, the values entered may be out of range, indicating a user error or possibly a problem with the source of those values.
- Values that are necessary to operate the program should be somehow indicated, either by listing or color coding them.
- The chemical parameter ‘type’ should be indicated as either organic acid or base. The parameter ‘type’ in and of itself is too ambiguous and can be interpreted in a number of different ways by the user.

The ChemFate models are easy to use and the GUI is clear, well defined, and yields good examples of how to complete the form. However, a user can only input one chemical at a time for each type of model. This ‘single use’ format can be a time-consuming hinderance for those users who intend to run the model repeatedly to compare various chemicals. One method that may improve this function would be a drop-down chemical selection menu that would allow a user to include several chemicals for each model using format specific filenames. The program could then read in a list of filenames of a specific format within the input directory and the user could select from that list. This list could include the list of prefabricated chemical parameter pesticide files that were researched and included from this study. This would make it easier for the user to both develop comparisons between input files, as well as run batch comparisons.

The ChemFate results also are relatively straight forward, well formatted, and easy to process. The content within the chemical concentration and mass files were well thought out and closely follow the input design, making them easy to interpret. The results could still use some explanation in the user guide. This is particularly the case with the process file, which is the densest and most confusing of the three resulting files. The user guide could be expanded somewhat to include information addressing the interpretation of the process file, such as the units for the file and adding information on the column headers.

Overall, the ChemFate models were well designed, readily usable and provided good information. The responsiveness of the programs makes analysis readily usable initially as well as leading the user to look forward to continuing to use them over a lengthy period of time for extended analysis of pesticide chemicals.

APPENDIX

[File Map: Report_Package/Report_Package_File_Map.txt]

A. Pesticide Ranking

[Pesticide Ranking: Report_Package/Data/Research/PesticideStudy/]

Table. Fungicide Selection Table. This table represents the top 16 fungicides studied and the selection parameters used to select them.

Index	Fungicides Active Ingredient	Top Pesticide Manufactures 2018 Research (#)	Active Products (Total #)	Active Products (# Since 2016)	Approximate 10^6 lbs in United States in 2016	2016 & 2017 CA Use	Max kg Per Acre Use in CA	Average KG Per Acre Use in CA
1	polyethylene oxide mono	3	111	30		1		
2	propiconazole	1	106	49	2.2	1	1.6136	0.1828
3	chlorothalonil	3	70	23	10.2	1	36.3429	1.8835
4	tebuconazole	2	69	45	1.7	1	36.3429	0.9864
5	azoxystrobin	3	65	41	2.05	1	10.4167	0.2023
6	fludioxonil	3	45	14	0.047	1	20.0000	0.2973
7	copper hydroxide	1	43	13	4.2	1	93.9671	2.0094
8	mancozeb	2	34	6	5.9	1	51.2000	1.6679
9	mefenoxam	3	26	7	0.27	1	30.3864	0.3928
10	thiabendazole	1	26	6	0.024	1	9.6468	4.8699
11	difenoconazole	3	21	7	0.32	1	3.641	0.0847
12	trifloxystrobin	5	20	4	0.58	1	2.0882	0.0878
13	pyraclostrobin	3	19	1	2.1	1	3.6750	0.1487
14	trinexapac-ethvl	1	10	4	0.007	1	1.0702	0.0850
15	boscalid	1	10	0	0.65	1	6.3000	0.2883
16	oxathiapiprolin	1	9	9	2.8	1	0.0157	0.0147

Table. Herbicide Selection Table. This table represents the top 16 herbicides studied and the selection parameters used to select them.

Index	Herbicides Active Ingredient	Top Pesticide Manufactures 2018 Research (#)	Active Products (Total #)	Active Products (# Since 2016)	Approximate 10^6 lbs in United States in 2016	Max KG/Acre Use in CA	Average KG/Acre Use in CA
1	glyphosate	5	186	68	290	0.0438	0.0184
2	dicamba	1	101	30	8		
3	quinclorac	1	63	26	0.55	0.75	0.4576
4	pendimethalin	4	50	5	11	68.1815	2.2571
5	2,4-Dichlorophenoxyacetic	1	33	6	44	2.4031	0.4969
6	indaziflam	2	22	8	0.055	1.4579	0.0483

7	glufosinate-ammonium	5	19	6	9.4	60.1496	0.9372
8	rimsulfuron	2	15	6	0.16	2.8056	0.047
9	penoxsulam	1	15	4	0.0016	0.4637	0.0273
10	mesotrione	6	14	8	3.4	1.9995	0.1761
11	clopyralid	3	13	2	1.6		
12	fluazifop-P-butyl	1	13	0	0.18	24.0175	0.3046
13	fluroxypyr 1-methylheptyl ester	1	11	1	1.15	6.5704	0.2944
14	*S*-metolachlor	4	10	1	58	12.8073	1.3639
15	paraquat dichloride	1	10	1	8.75	35.248	1.1282
16	bentazon	1	8	4	1.8	2.5199	1.1947

Table. Insecticides Selection Table. This table represents the top 15 insecticides studied and the selection parameters used to select them.

Index	**Insecticide** **Active Ingredient**	**Top Pesticide Manufactures 2018 Research (#)**	**Active Products (Total #)**	**Active Products (# Since 2016)**	**Approximate 10^6 lbs in United States in 2016**	**Max KG Per Acre Use in CA**	**Average KG Per Acre Use in CA**
1	imidacloprid	1	278	81	0.8	82.8	0.2755
2	fipronil	2	137	59	0.001	2.0016	0.5226
3	lambda-cyhalothrin	1	114	31	0.58	0.3134	0.0319
4	deltamethrin	1	94	40	0.018	0.0434	0.0257
5	spinosad	1	70	20	0.066	1.0743	0.1003
6	abamectin	2	61	18	0.65	93.8325	0.0237
7	clothianidin	2	43	23	0.2	2.1365	0.1095
8	chlorpyrifos	1	42	5	4	71.8309	1.6958
9	Indole-3-butyric acid (IBA)	1	28	6			
10	thiamethoxam	5	28	3	0.18	0.7032	0.0702
11	hydramethylnon	1	24	2	0.1	0.365	0.011
12	chlorantraniliprole	2	21	8	0.32	0.525	0.0716
13	difenoconazole	1	21	7	0.33	3.641	0.0847
14	1,3-dichloropropene	1	17	0	47	820.475	187.6796
15	novaluron	1	15	4	0.068	0.3959	0.0732

Table. Pesticide Selection Reference Table. This table represents the references used to select the pesticides studied.

Pesticide Ranking References		
Reference	Title	Link
Investopedia	The Biggest Pesticide Companies in the World.	1https://www.investopedia.com/articles/markets-economy/082516/top-5-pesticide-companies-world-syt-dow.asp
Syngenta	Presentations and Publications.	1https://www.syngenta.com/company/presentations-and-publications
Bayer	Annual Report	https://www.bayer.com

Dow and Dupont	Annual Report	1http://www.annualreports.com/HostedData/AnnualReports/PDF/NYSE_DD_2017.PDF
BASF	Online Report	1https://report.basf.com/2018/en/
USGS	Pesticide National Synthesis Project	1https://water.usgs.gov/nawqa/pnsp/usage/maps/compound_listing.php
CalPIP	California Department of Pesticide Regulation	1https://calpip.cdpr.ca.gov/main.cfm

B. Ecotoxicological Study

[Ecotoxicological File Results: Report_Package/Data/Research/Ecotoxicity/]

Table. LC50 Parameter Table. This table represents the LC50 parameters and species used in ecotoxicological endpoint comparison study.

LC50	
Parameters	***Species***
Concentration (uq/L)	*Pimephales promelas*
time (hr)	*Daphnia magna*
95% Confidence Limit (ug/L)	*Zebra Danio*
weight (g)	*Oncorhynchus mykiss*
T (degC)	*Lepomis macrochirus*
pH	*Cyprinodon variegatus*
Water hardness $CaCO_3$ (mg/L)	*Pseudokirchneriella subcapitata*
Alkalinity (mg/L)	*Eisenia foetida*
Conditions	*Americamysis bahia*

Table. EC50 Parameter Table. This table represents the EC50 parameters and species used in ecotoxicological endpoint comparison study.

EC50	
Parameters	***Species***
Concentration (uq/L)	*Selenastrum capricornutum*
time (hr)	Anabaena flosaquae
Effect	*Pimephales promelas*
Condition	*Zebra danio*
95% Confidence Limit (ug/L)	Daphnia magna
	Pseudokirchneriella subcapitata
	Eisenia foetida

Table. NOEAL/NOEL & LOEAL/LOEL Parameter Table. This table represents the NOEAL/NOEL & LOEAL/LOEL parameters and species used in ecotoxicological endpoint comparison study.

NOAEL/NOEL & LOAEL/LOEL	
Parameters	**Laboratory Animals**
Sex	Quail
NOAEL (mg/kg/day)	Mallard Duck
NOEL (mg/kg/day)	Chinchilla
LOAEL (mg/kg/day)	White Rabbit
LOEL (ppm)	Rabbit
Effect	Dog
	Beagle
	Mice
	Rat

Application

[Statistical Usage Files: Report_Package/Data/Research/CA_StatisticalUsage/]

Physical & Chemical Characteristics

Research:
[EPI Results Research Files: Report_Package/Data/Research/EPI_Results/]
[Chemical Parameter Research Files: Report_Package/Data/Research/ChemParam/]
[Chemical Release Research Files: Report_Package/Data/Research/ChemRelease/]

Input:
[Chemical Parameter Input Files: Report_Package/Data/Model/Input/…_ChemParam/]
[Chemical Release Input Files: Report_Package/Data/Model/Input/…_ChemRelease/]

References

Table. Pesticide Characterization and Ecotoxicological Reference Table. This table represents the references used to detail the chemical and physical characteristics as well as ecotoxicological endpoints for the pesticides studied here.

References		
Reference	**Title**	**Link**
PubMed	The National Center for Biotechnical Information	https://www.ncbi.nlm.nih.gov/pubmed/
Environmental Protection Agency	Pesticides: Registration Eligibility Decision	https://www3.epa.gov/pesticides
University of Hertfordshire	Pesticide Properties Database	https://sitem.herts.ac.uk
National Institute of Health	TOXNET	https://toxnet.nlm.nih.gov
European Food and Safety Authority (EFSA)	EFSA Publications	https://efsa.onlinelibrary.wiley.com
Cornell University	Pesticide Active Ingredient Information	http://pmep.cce.cornell.edu/profiles/

C. Regional Study

[Regional Research Files:	Report_Package/Data/Research/Region/]
[Regional Input Files:	Report_Package/Data/Model/Input/Region/]

D. Model Results

[Model Result Files:	Report_Package/Data/Model/Input/Output/
[ionOFate, metalFate, organoFate]]

IonOFate

Table. IonOFate Pesticide Selection Table. This table represents the ionizable organic chemicals selected to study the ionOFate model performance given select unique characteristics and parameters.

IonOFate Selection							
Pesticide Chemical	**Type**	**Kow**	**Koc**	**Volatile**	**Air Half-life**	**Water Half-life**	**Soil Half-Life**
1,3-Dichloropropene	Insecticide	Medium	Low	Yes	Medium	Medium	Medium
Azoxystrobin	Fungicide	Medium	Medium		Short	Medium	Long
Chlorothalonil	Fungicide	High	High		Long	Short	Medium
Glyphosate	Herbicide	High	High		Short	Medium	Medium
L-Cyhalothrin	Insecticide	High	High	Yes	Long	Long	Long
Rimsulfuron	Herbicide	Medium	Low		Short	Medium	Medium

Constant/Daily

Table. IonOFate Constant Release Results. This table represents the order of magnitude of the maximum concentration value resulting from the ionOFate model run for each representative ionizable chemical selected.

IonOFate Constant Results									
Order of Magnitude of Background Concentration									
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
1,3-Dichloropropene	-11	-8	-8	-12	-10	-10	-6	-10	-9
Azoxystrobin	-16	-13	-13	-15	-14	-14	-11	-14	-14
Chlorothalonil	-13	-6	-7	-7	-8	-8	-5	-7	-7
Glyphosate	-19	-13	-13	-15	-14	-14	-11	-15	-14
L-Cyhalothrin	-15	-8	-7	-9	-8	-9	-5	-6	-6
Rimsulfuron	-16	-11	-12	-13	-13	-13	-9	-13	-13

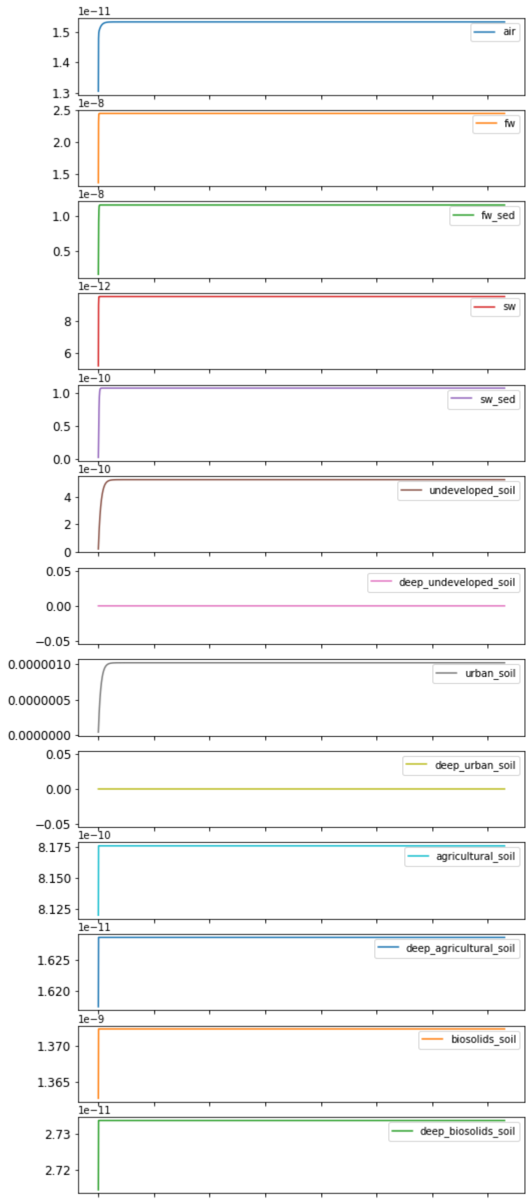
Table 7. IonOFate Constant Release Combined Ecotoxicological Comparisons. This table represents a simplified perspective on evaluating the ecological impacts the chemical may have from a constant release pattern.

IonOFate Constant Release Combined Ecotoxicological Comparisons									
						Caution	Warning	No Issue	
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**

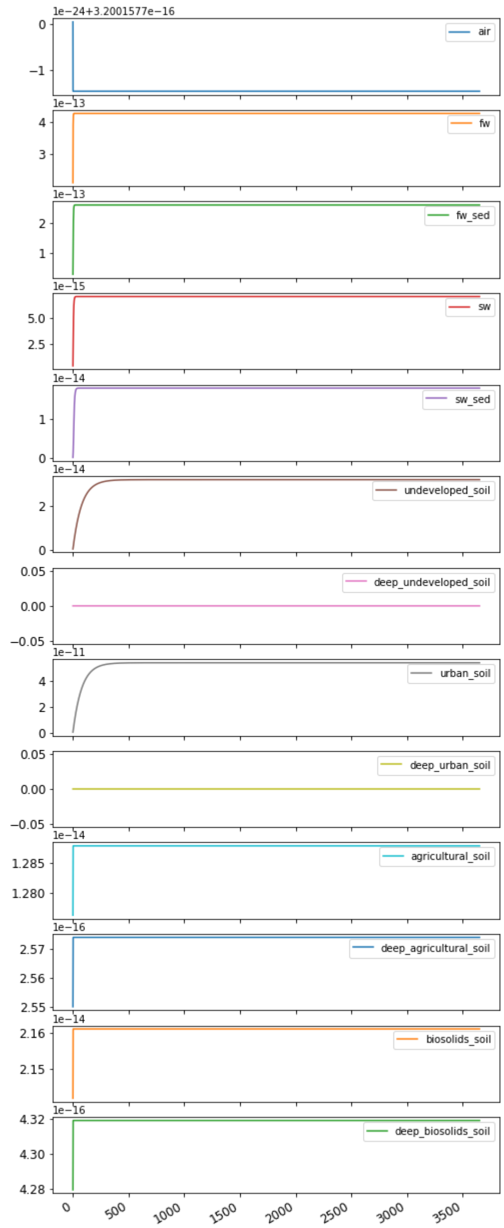
1,3-Dichloropropene	
Azoxystrobin	
Chlorothalonil	
Glyphosate	
L-Cyhalothrin	
Rimsulfuron	

Constant Release IonOFate Plot for Select Ionizable Pesticides
The following 3 pages…

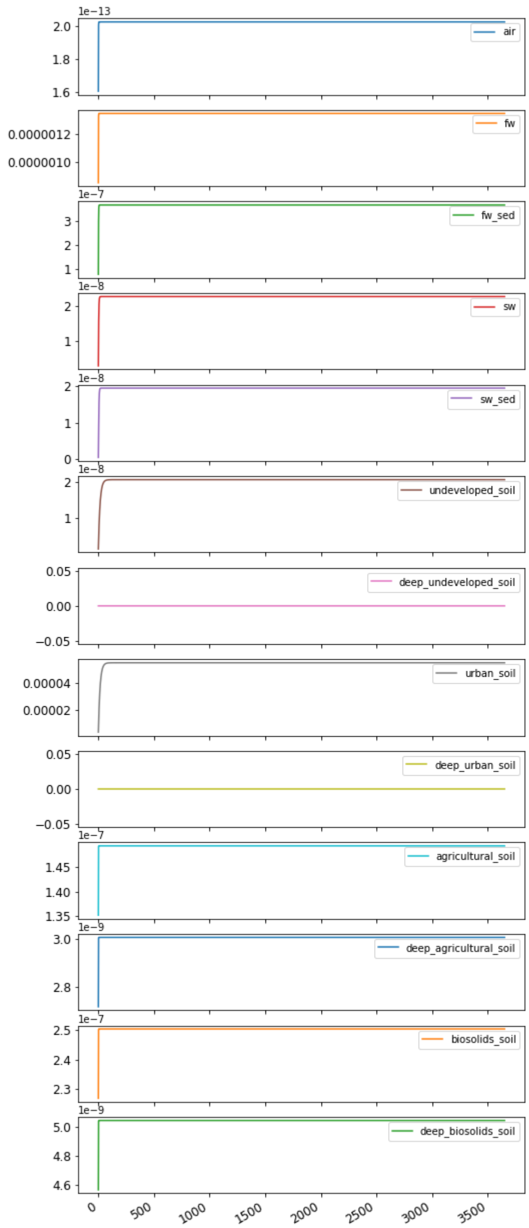
1,3Dichloropropene Pesticide ionOFate Model
Daily Release Rate for 2010-2020
in Salinas River Valley.



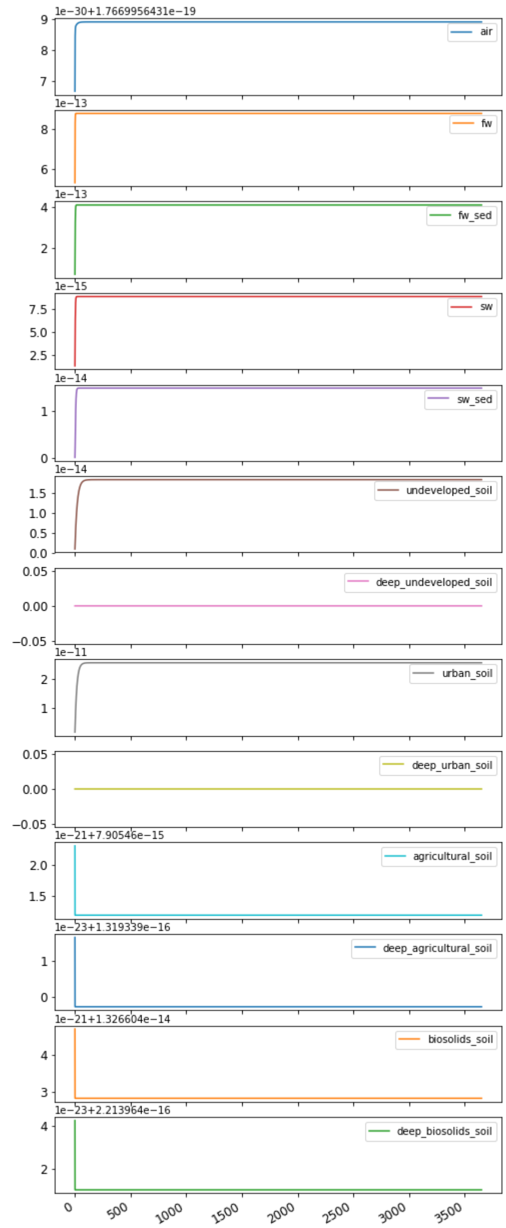
Azoxystrobin Pesticide ionOFate Model
Daily Release Rate for 2010-2020
in Salinas River Valley.

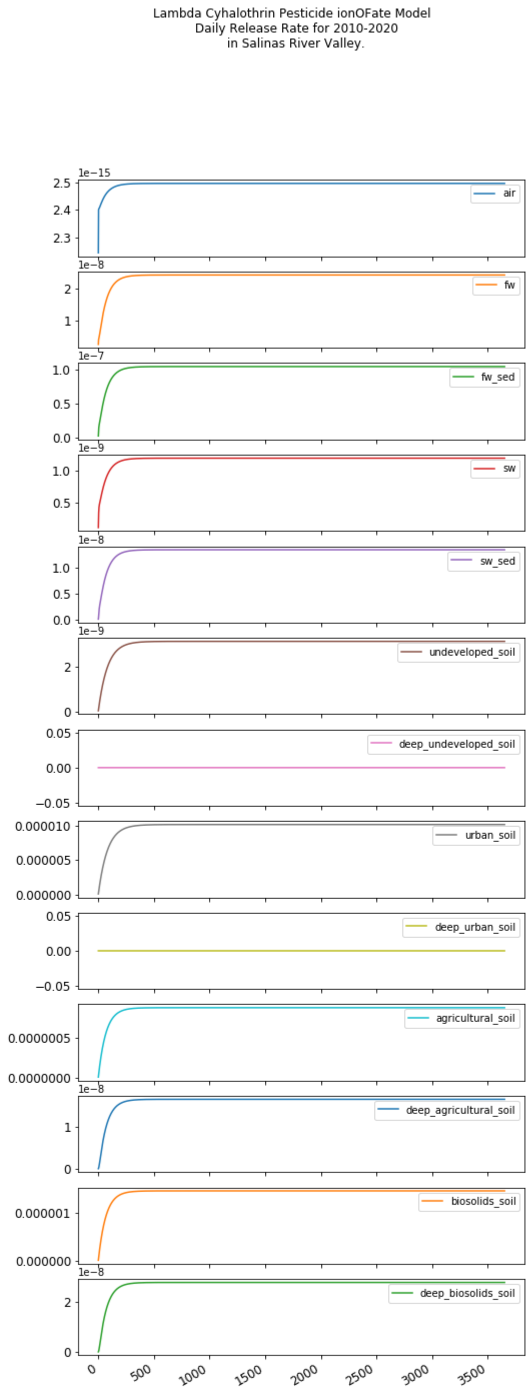


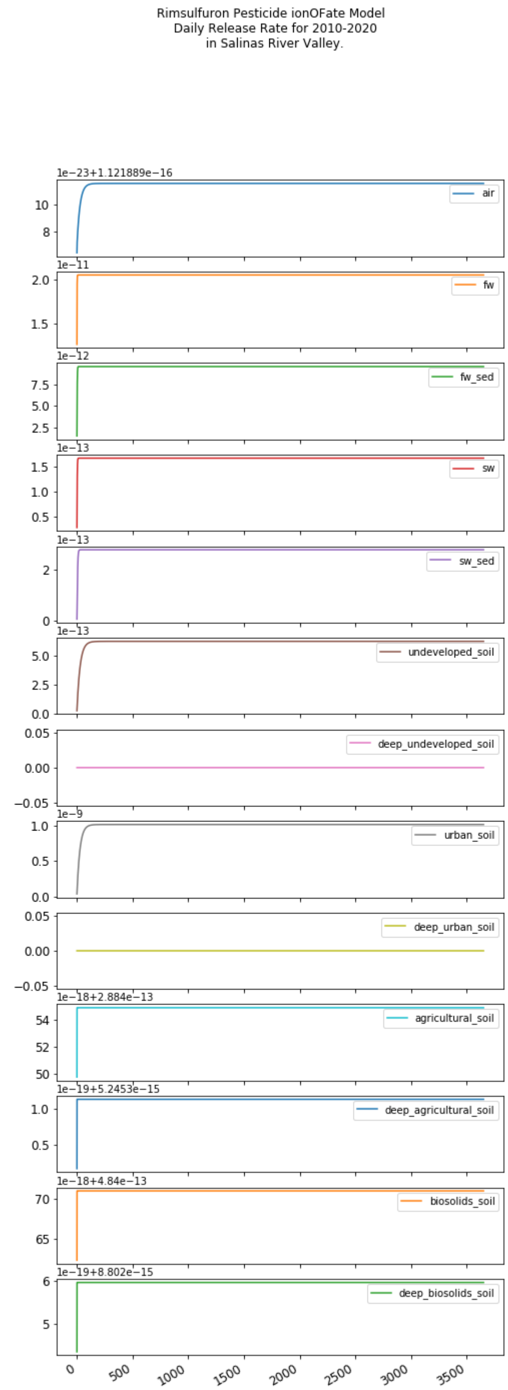
Chlorothalnil Pesticide ionOFate Model
Daily Release Rate for 2010-2020
in Salinas River Valley.



Glyphosate Pesticide ionOFate Model
Daily Release Rate for 2010-2020
in Salinas River Valley.




Lambda Cyhalothrin Pesticide ionOFate Model
Daily Release Rate for 2010-2020
in Salinas River Valley.
air
fw
fw_sed
sw
sw_sed
undeveloped_soil
deep_undeveloped_soil
urban_soil
deep_urban_soil
agricultural_soil
deep_agricultural_soil
biosolids_soil
deep_biosolids_soil


Rimsulfuron Pesticide ionOFate Model
Daily Release Rate for 2010-2020
in Salinas River Valley.
air
fw
fw_sed
sw
sw_sed
undeveloped_soil
deep_undeveloped_soil
urban_soil
deep_urban_soil
agricultural_soil
deep_agricultural_soil
biosolids_soil
deep_biosolids_soil

Seasonal

Table. IonOFate Seasonal Release Results. This table represents the order of magnitude of the maximum concentration value resulting from the organoFate model for each representative ionizable chemical selected.

IonOFate Seasonal									
Max Order of Magnitude of Background Concentration									
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
1,3-Dichloropropene	-13	-10	-11	-13	-13	-13	-9	-11	-11
Azoxystrobin	-14	-11	-12	-13	-13	-14	-10	-12	12
Chlorothalonil	-11	-4	-5	-7	-7	-7	-4	-5	-5
Glyphosate	-17	-11	-11	-13	-13	-13	-10	-12	-12
L-Cyhalothrin	-13	-7	-7	-8	-8	-8	-5	-6	-6
Rimsulfuron	-14	-9	-10	-12	-12	-12	-9	-11	-11

Table. IonOFate Seasonal Release Combined Ecotoxicological Comparisons. This table represents a simplified perspective on evaluating the ecological impacts the chemical may have from a seasonal release pattern.

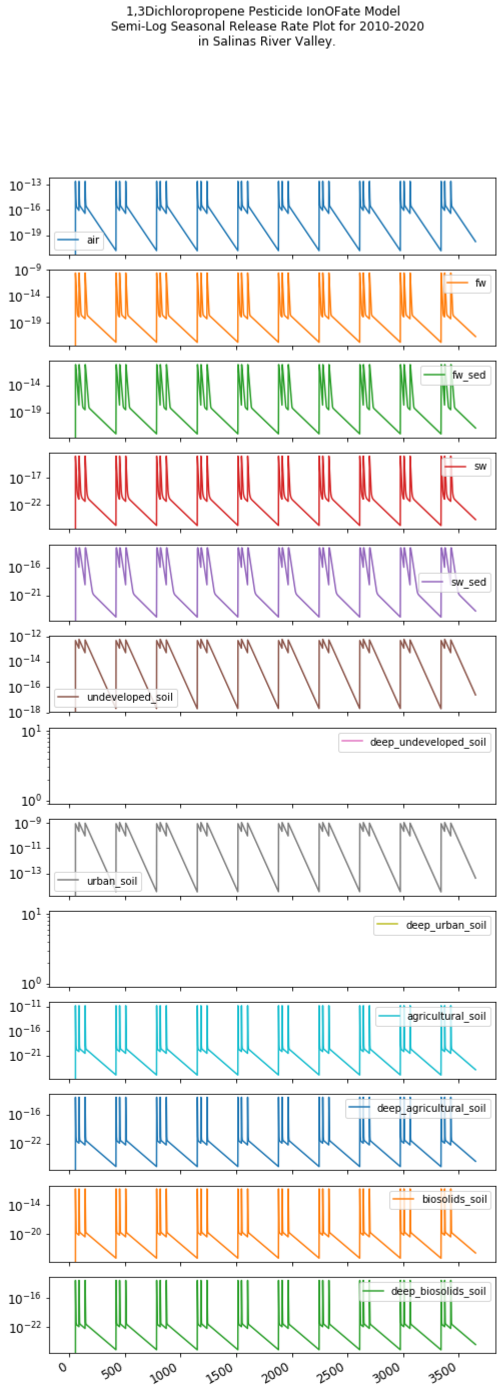
IonOFate Seasonal Release Combined Ecotoxicological Comparisons									
						Caution	Warning	No Issue	
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultura l Soils**	**Biosolid Soils**
1,3-Dichloropropene									
Azoxystrobin									
Chlorothalonil									
Glyphosate									
L-Cyhalothrin									
Rimsulfuron									

Table 6. IonOFate Seasonal Persistence of Signal Results. This table represents persistence in concentration observed in the impulse of chemical delivered to the area.

IonOFate Seasonal									
Persistence of Signal	(High, Moderate, and	Low)							
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
1,3-Dichloropropene	Moderate	Moderate	Moderate	Moderate	Moderate	High	High	Moderate	Moderate
Azoxystrobin	Low	Low	Moderate	Moderate	High	High	High	Low	Low
Chlorothalonil	Moderate	Moderate	Moderate	Moderate	Moderate	High	High	Moderate	Moderate
Glyphosate	Moderate	Moderate	Moderate	Moderate	Moderate	High	High	Moderate	Moderate
L-Cyhalothrin	Moderate	Moderate	High	Moderate	High	High	High	High	High
Rimsulfuron	Moderate	Moderate	Moderate	Moderate	Moderate	High	High	Moderate	Moderate

Semi-Log Seasonal IonOFate Plots of Select Ionizable Pesticides

The following 3 pages…


1,3Dichloropropene Pesticide IonOFate Model
Semi-Log Seasonal Release Rate Plot for 2010-2020
in Salinas River Valley.
air
fw
fw_sed
sw
sw_sed
undeveloped_soil
deep_undeveloped_soil
urban_soil
deep_urban_soil
agricultural_soil
deep_agricultural_soil
biosolids_soil
deep_biosolids_soil
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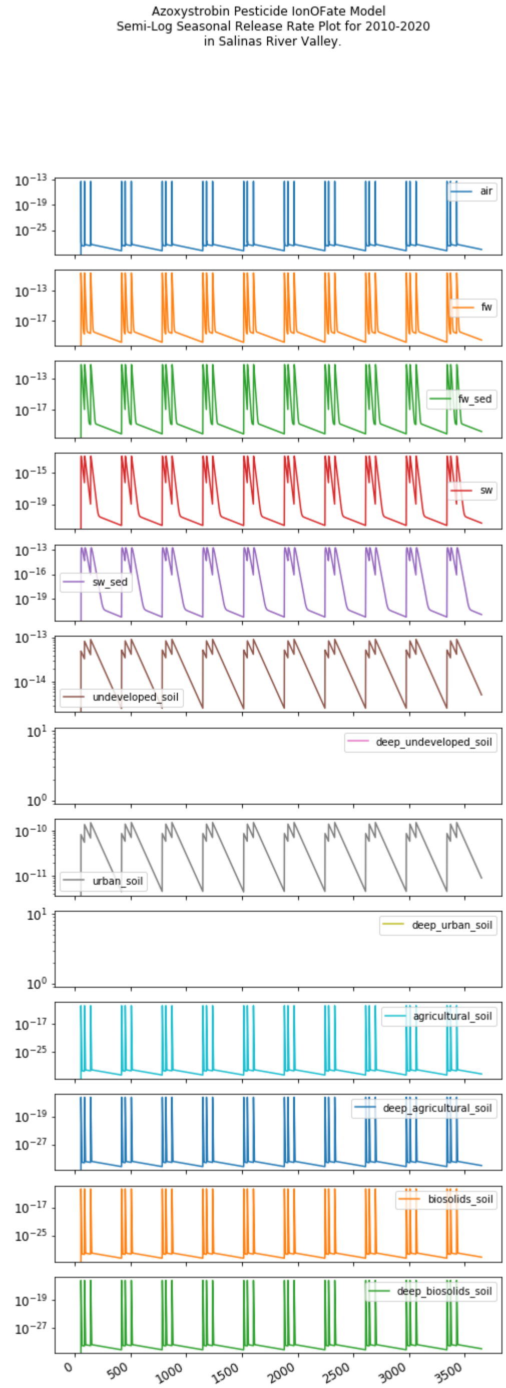
1000
1500
2000
2500
3000
3500


Azoxystrobin Pesticide IonOFate Model
Semi-Log Seasonal Release Rate Plot for 2010-2020
in Salinas River Valley.
air
fw
fw_sed
sw
sw_sed
undeveloped_soil
deep_undeveloped_soil
urban_soil
deep_urban_soil
agricultural_soil
deep_agricultural_soil
biosolids_soil
deep_biosolids_soil
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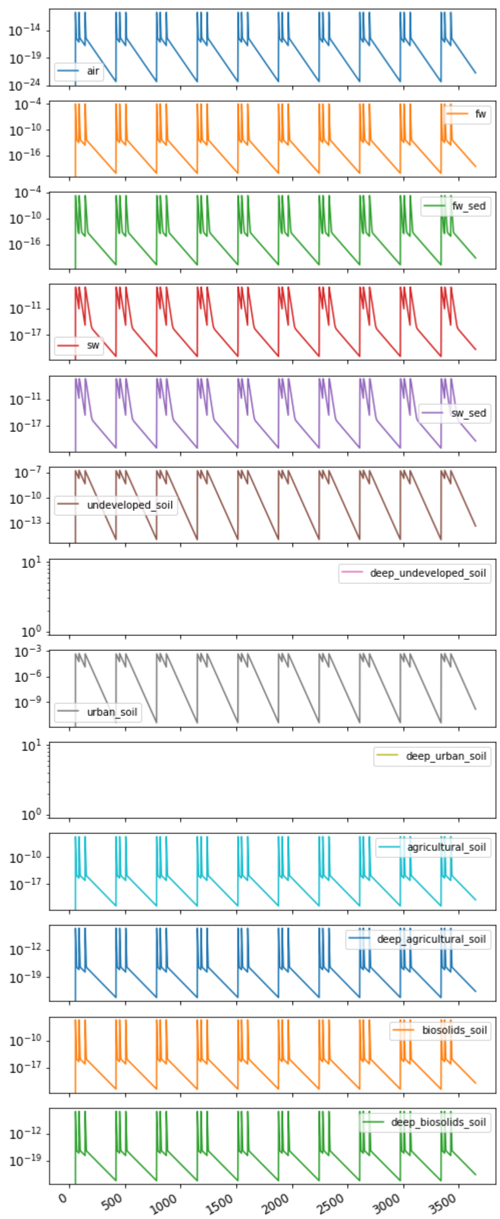
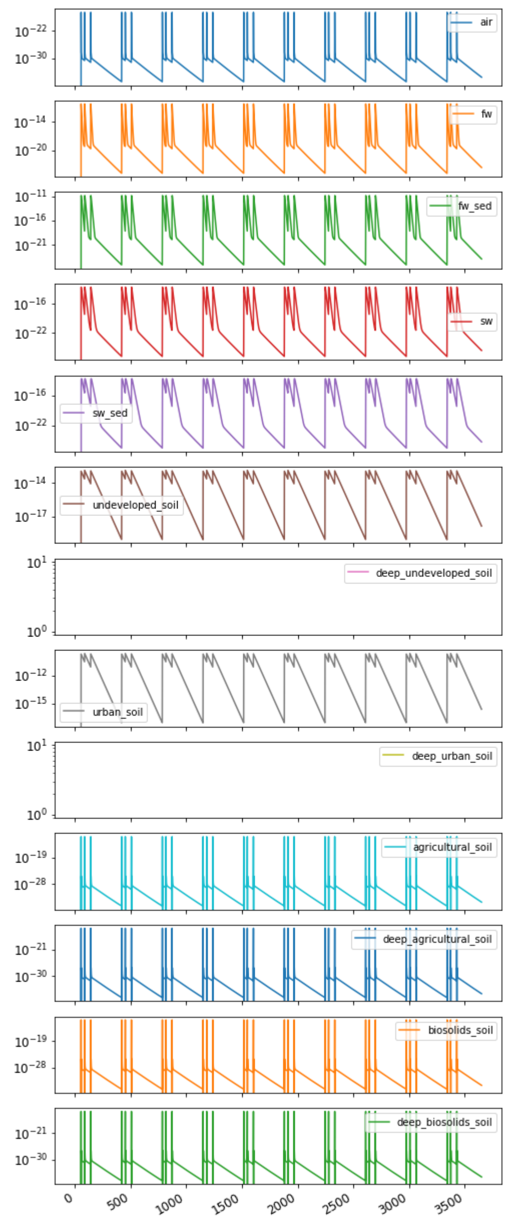
500
1000
1500
2000
2500
3000
3500

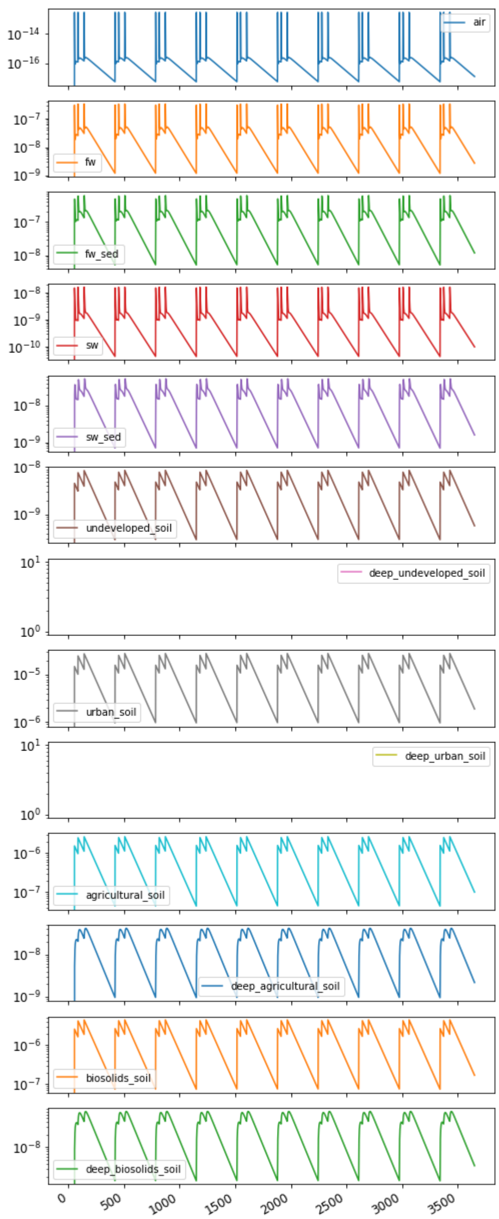
Chlorothalnil Pesticide IonOFate Model
Semi-Log Seasonal Release Rate Plot for 2010-2020
in Salinas River Valley.



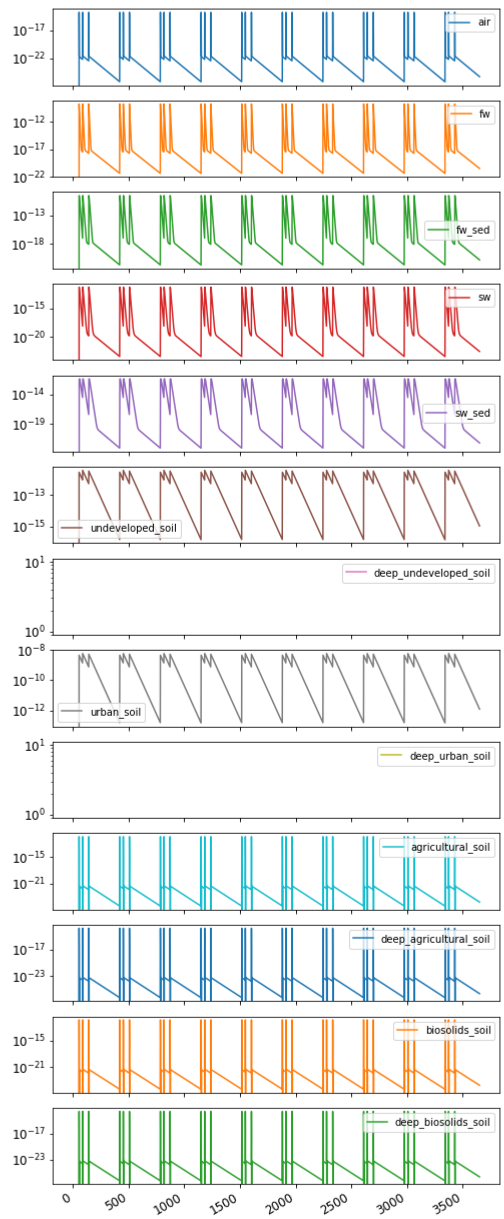
Glyphosate Pesticide IonOFate Model
Semi-Log Seasonal Release Rate Plot for 2010-2020
in Salinas River Valley.



Lambda Cyhalothrin Pesticide IonOFate Model
Semi-Log Seasonal Release Rate Plot for 2010-2020
in Salinas River Valley.



Rimsulfuron Pesticide IonOFate Model
Semi-Log Seasonal Release Rate Plot for 2010-2020
in Salinas River Valley.



OrganoFate

Table. OrganoFate Pesticide Selection Table. This table represents the nonionizable organic chemicals selected to study the organoFate model performance given select unique characteristics and parameters.

OrganoFate Selection								
Pesticide Chemical	**Type**	**Kow**	**Koc**	**Volatile**	**Air Half-life**	**Water Half-life**	**Soil Half-Life**
2,4-D	Herbicide	Medium	Low	Y	Medium	Medium	Medium
Fipronil	Insecticide	High	High		Short	High	Medium
Fludioxonil	Fungicide	High	High		Short	Medium	High
Mancozeb	Fungicide	Low	Medium	Y	Short	High	High
Novaluron	Insecticide	High	High		Short	Short	Medium
Paraquat Dichloride	Herbicide	High	High		Medium	High	High

Constant/Daily

Table 9. OrganoFate Constant Release Results. This table represents the order of magnitude of the maximum concentration value resulting from the organoFate model run for each representative nonionizable chemical selected.

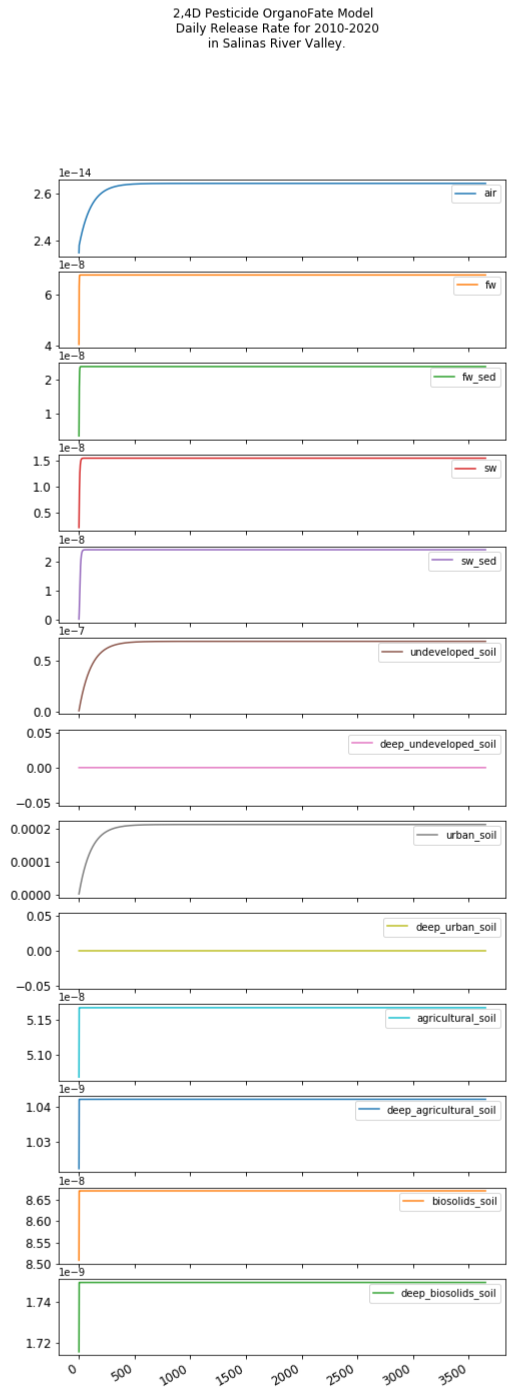
OrganoFate Constant Results Table									
Order of Magnitude of Background Concentration									
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
2,4-D	-14	-8	-8	-8	-8	-7	-5	-8	-8
Fipronil	-15	-8	-8	-8	-8	-7	-5	-6	-6
Fludioxonil	-15	-8	-8	-9	-8	-7	-4	-6	-6
Mancozeb	-14	-7	-8	-9	-8	-7	-3	-6	-6
Novaluron	-17	-10	-11	-11	-11	-8	-4	-9	-9
Paraquat Dichloride	-11	-7	-8	-8	-9	-9	-6	-7	-7

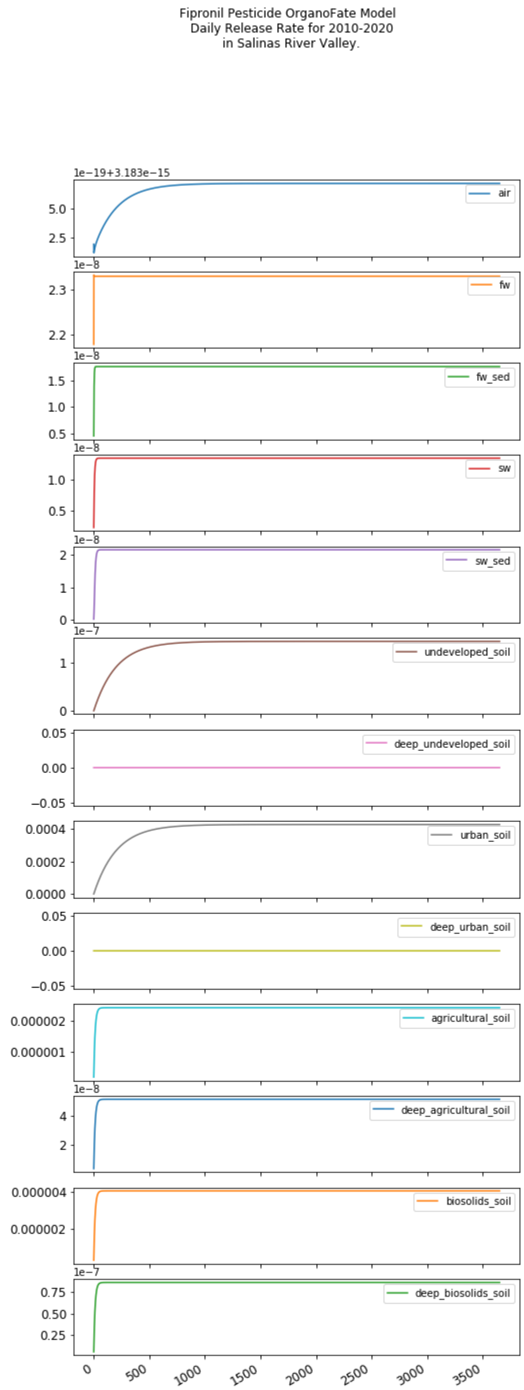
Table 12. OrganoFate Constant Release Combined Ecotoxicological Comparisons. This table represents a simplified perspective on evaluating the ecological impacts the chemical may have from a constant release pattern.

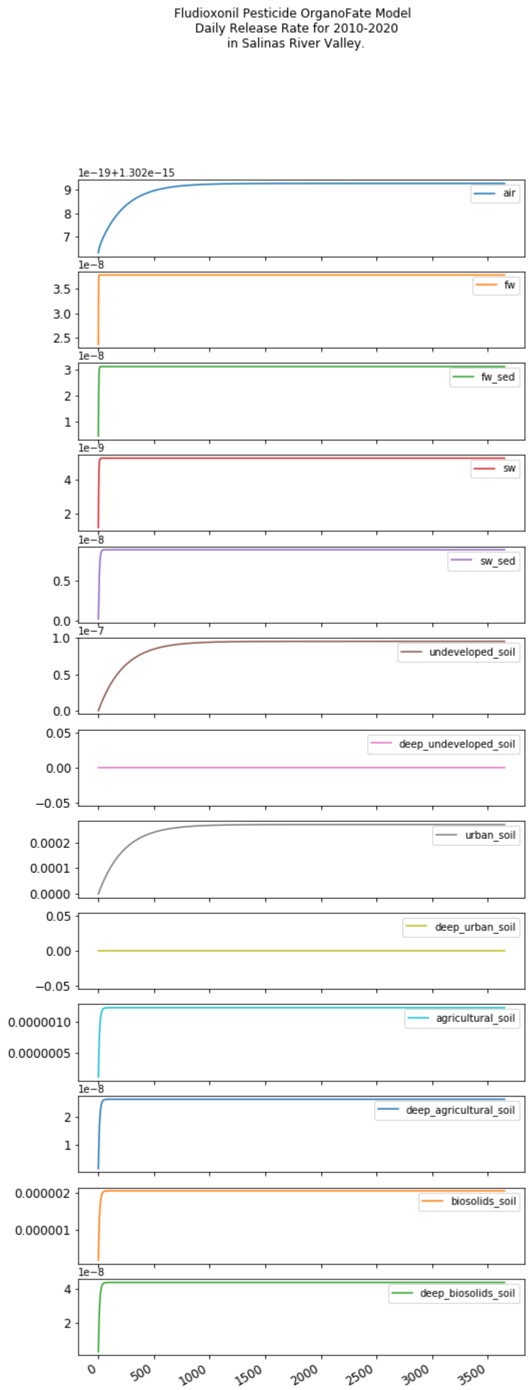
OrganoFate Constant Release Combined Ecotoxicological Comparisons									
						Caution	Warning	No Issue	
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
2,4-D									
Fipronil									
Fludioxonil									
Mancozeb									
Novaluron									
Paraquat Dichloride									

Constant OrganoFate plots of Select Non-Ionizable

The following 3 pages…


2,4D Pesticide OrganoFate Model
Daily Release Rate for 2010-2020
in Salinas River Valley.
air
fw
fw_sed
sw
sw_sed
undeveloped_soil
deep_undeveloped_soil
urban_soil
deep_urban_soil
agricultural_soil
deep_agricultural_soil
biosolids_soil
deep_biosolids_soil


Fipronil Pesticide OrganoFate Model
Daily Release Rate for 2010-2020
in Salinas River Valley.
air
fw
fw_sed
sw
sw_sed
undeveloped_soil
deep_undeveloped_soil
urban_soil
deep_urban_soil
agricultural_soil
deep_agricultural_soil
biosolids_soil
deep_biosolids_soil


Fludioxonil Pesticide OrganoFate Model
Daily Release Rate for 2010-2020
in Salinas River Valley.
1e−19+1.302e−15
air
fw
fw_sed
sw
sw_sed
undeveloped_soil
deep_undeveloped_soil
urban_soil
deep_urban_soil
agricultural_soil
deep_agricultural_soil
biosolids_soil
deep_biosolids_soil
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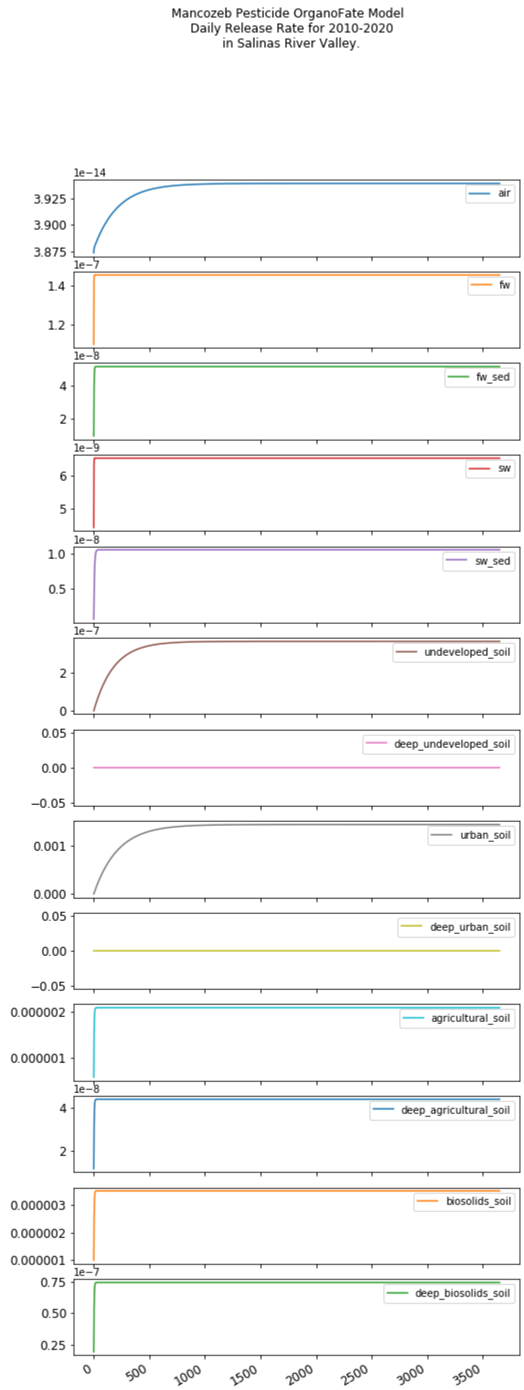
500
1000
1500
2000
2500
3000
3500


Mancozeb Pesticide OrganoFate Model
Daily Release Rate for 2010-2020
in Salinas River Valley.
1e−14
air
fw
fw_sed
sw
sw_sed
undeveloped_soil
deep_undeveloped_soil
urban_soil
deep_urban_soil
agricultural_soil
deep_agricultural_soil
biosolids_soil
deep_biosolids_soil
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2000
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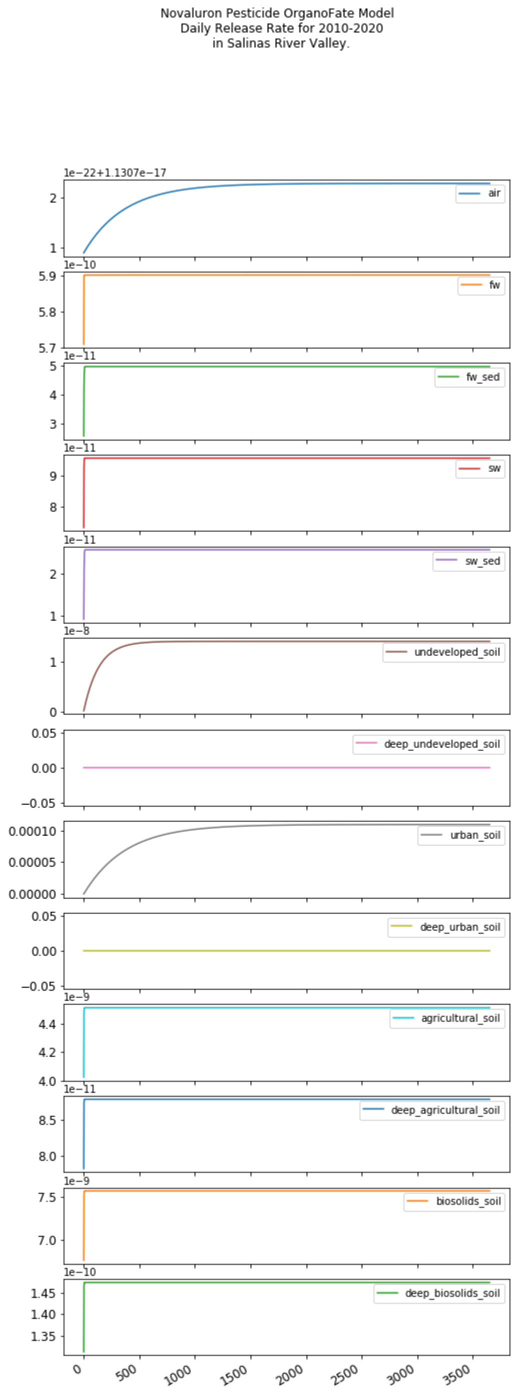
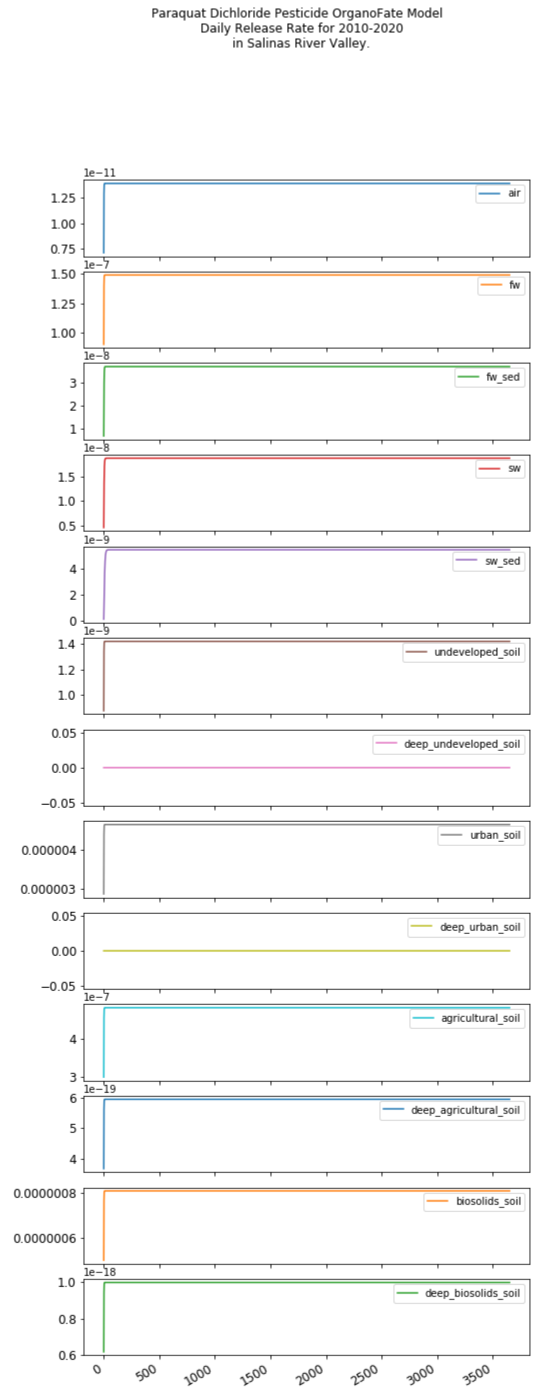
3000
3500


Novaluron Pesticide OrganoFate Model
Daily Release Rate for 2010-2020
in Salinas River Valley.
air
fw
fw_sed
sw
sw_sed
undeveloped_soil
deep_undeveloped_soil
urban_soil
deep_urban_soil
agricultural_soil
deep_agricultural_soil
biosolids_soil
deep_biosolids_soil


Paraquat Dichloride Pesticide OrganoFate Model
Daily Release Rate for 2010-2020
in Salinas River Valley.
air
fw
fw_sed
sw
sw_sed
undeveloped_soil
deep_undeveloped_soil
urban_soil
deep_urban_soil
agricultural_soil
deep_agricultural_soil
biosolids_soil
deep_biosolids_soil

Seasonal

Table. OroganoFate Seasonal Release Combined Ecotoxicological Comparisons. This table represents a simplified perspective on evaluating the ecological impacts the chemical may have from a constant release pattern.

OrganoFate Seasonal Release Combined Ecotoxicological Comparisons									
						Caution	Warning	No Issue	
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
2,4-D									
Fipronil									
Fludioxonil									
Mancozeb									
Novaluron									
Paraquat Dichloride									

Table. OrganoFate Seasonal Release Combined Ecotoxicological Comparisons. This table represents a simplified perspective on evaluating the ecological impacts the chemical may have from a seasonal release pattern.

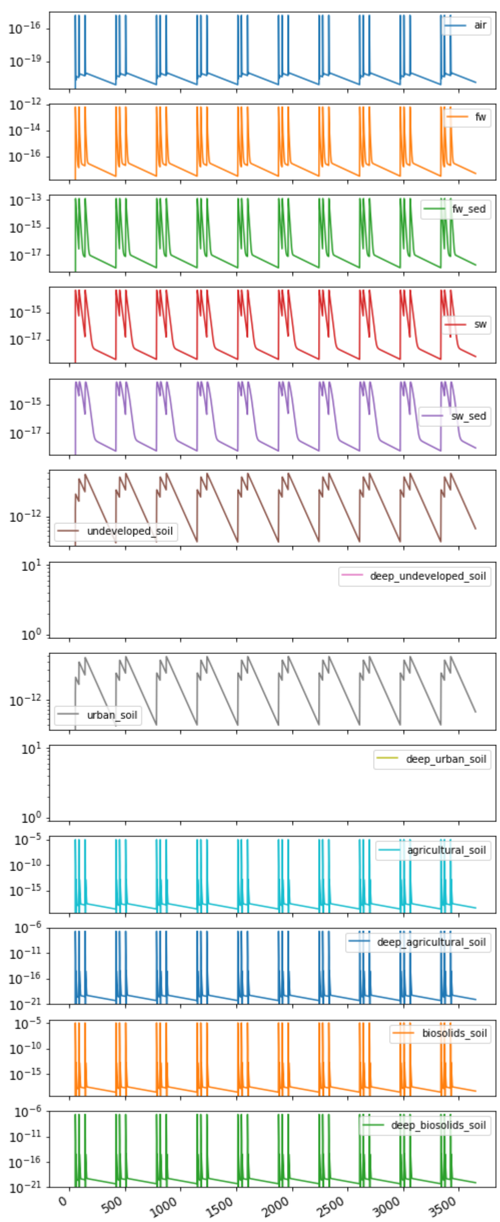
OrganoFate Seasonal Release Combined Ecotoxicological Comparisons									
						Caution	Warning	No Issue	
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
2,4-D									
Fipronil									
Fludioxonil									
Mancozeb									
Novaluron									
Paraquat Dichloride									

Table. OrganoFate Seasonal Release Persistence of Signal Results. This table represents the persistence the signal sows over time after application.

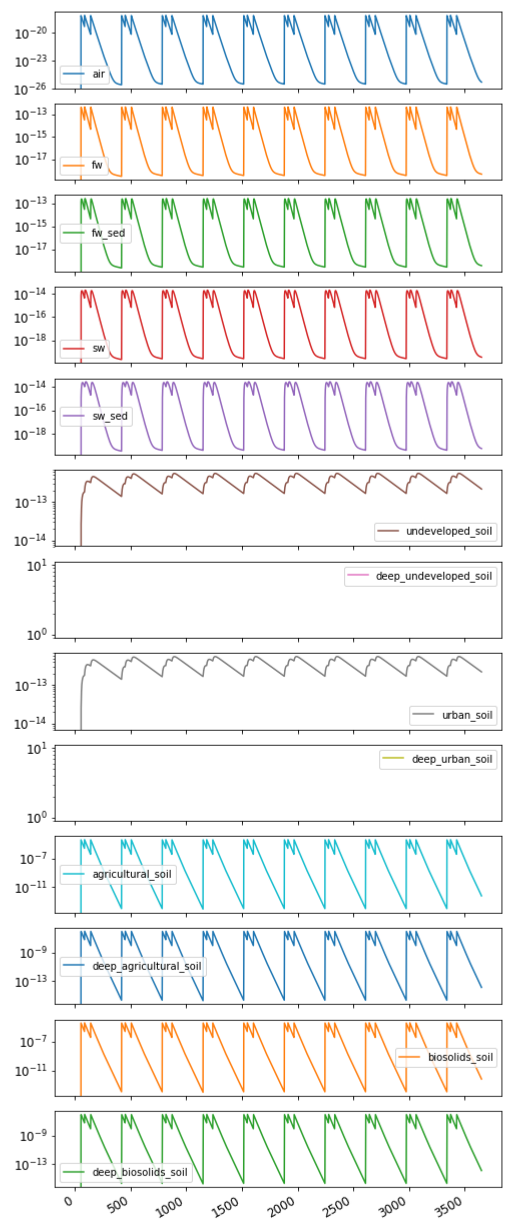
OrganoFate Seasonal Release Results									
Persistence	(High, Moderate, and Low)								
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
2,4-D	Low	Low	Low	Moderate	Moderate	High	High	Low	Low
Fipronil	High	High	High	High	High	V High	V High	High	High
Fludioxonil	High	High	High	High	High	V High	V High	High	High
Mancozeb	Moderate	Moderate	Moderate	Moderate	Moderate	V High	V High	High	High
Novaluron	Low	Low	Low	Low	Moderate	High	V High	Low	Low
Paraquat Dichloride	Moderate	Moderate	Moderate	Moderate	Moderate	Moderate	Moderate	Moderate	Moderate

Seasonal OrganoFate Semi-Log Plots of Select Non-Ionizable
The following 3 pages…

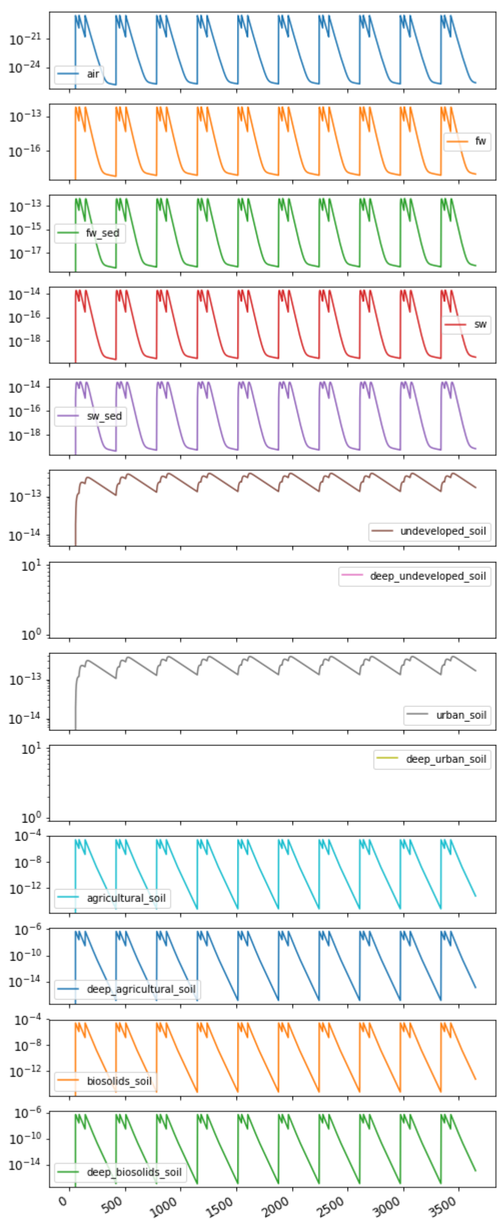
2,4D Pesticide OrganoFate Model
Semi-Log Seasonal Release Rate for 2010-2020
in Salinas River Valley.



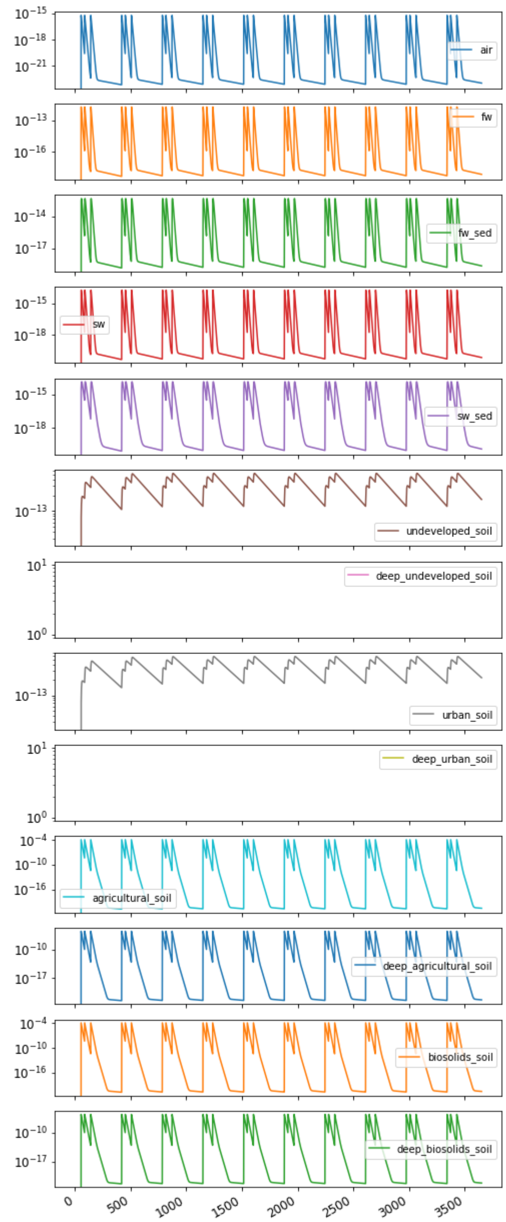
Fipronil Pesticide OrganoFate Model
Semi-Log Seasonal Release Rate for 2010-2020
in Salinas River Valley.



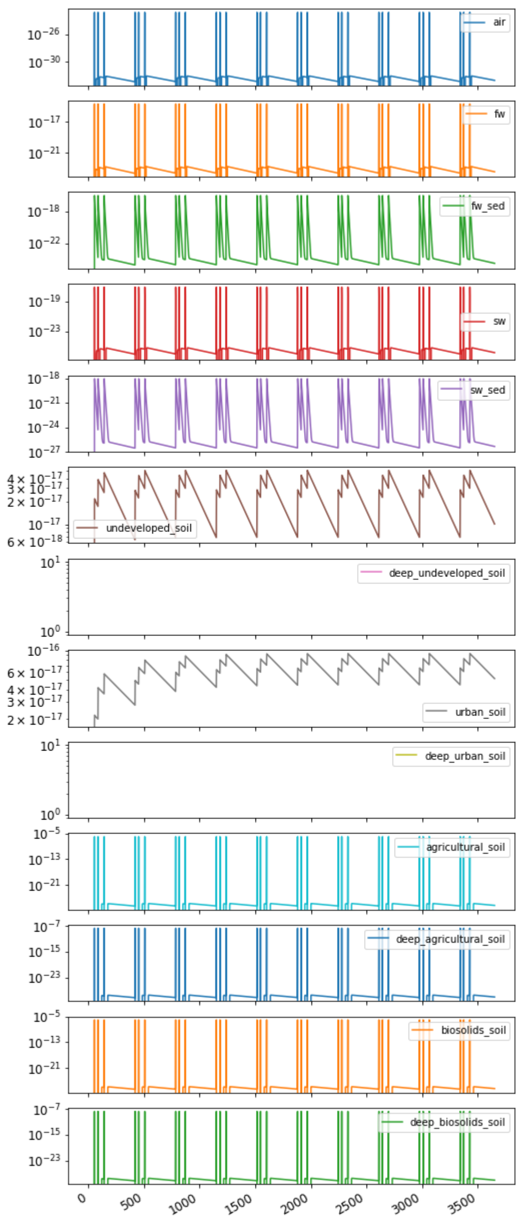
Fludioxonil Pesticide OrganoFate Model
Semi-Log Seasonal Release Rate for 2010-2020
in Salinas River Valley.



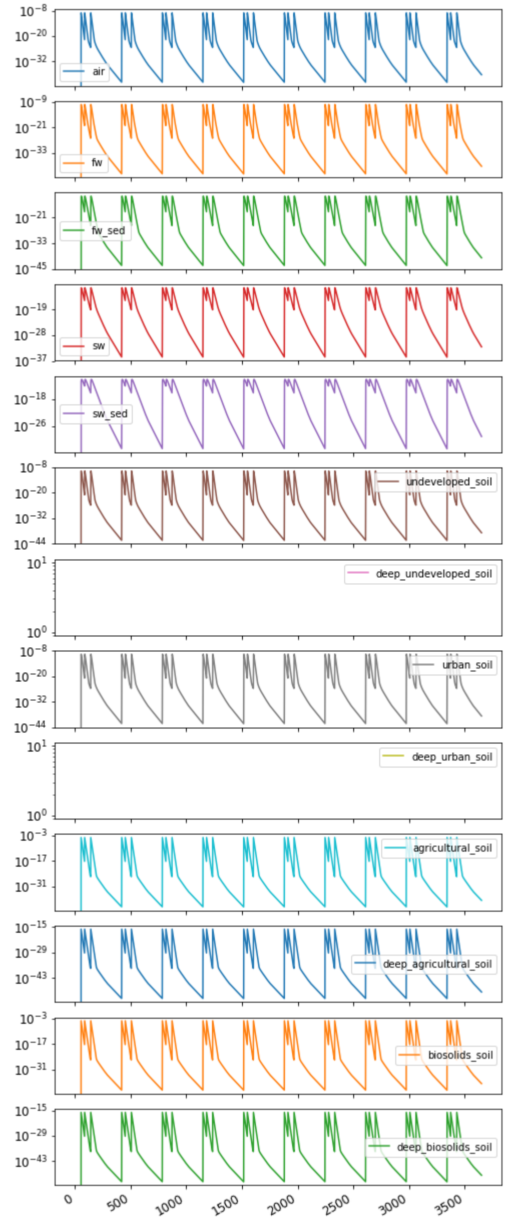
Mancozeb Pesticide OrganoFate Model
Semi-Log Seasonal Release Rate for 2010-2020
in Salinas River Valley.



Novaluron Pesticide OrganoFate Model
Semi-Log Seasonal Release Rate for 2010-2020
in Salinas River Valley.



Paraquat Dichloride Pesticide OrganoFate Model
Semi-Log Seasonal Release Rate for 2010-2020
in Salinas River Valley.



MetalFate

Table. MetalFate Pesticide Selection Table. This table represents the metallic organic chemical used to study the metalFate model performance.

MetalFate					
Pesticide Chemical	**Type**	**Kaw**	**Koc**	**Volatile**	**Species Fraction**
Copper Hydroxide	Fungicide	Default	N/A	N/A	See File

Constant/Daily

Table. MetalFate Constant Release Results. This table represents the order of magnitude of the maximum concentration value resulting from the metalFate modeling the copper hydroxide fungicide.

MetalFate Constant Results Table									
Order of Magnitude of Background Concentration									
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
Copper Hydroxide	-10	-6	-6	-6	-5	-6	-2	-4	-4

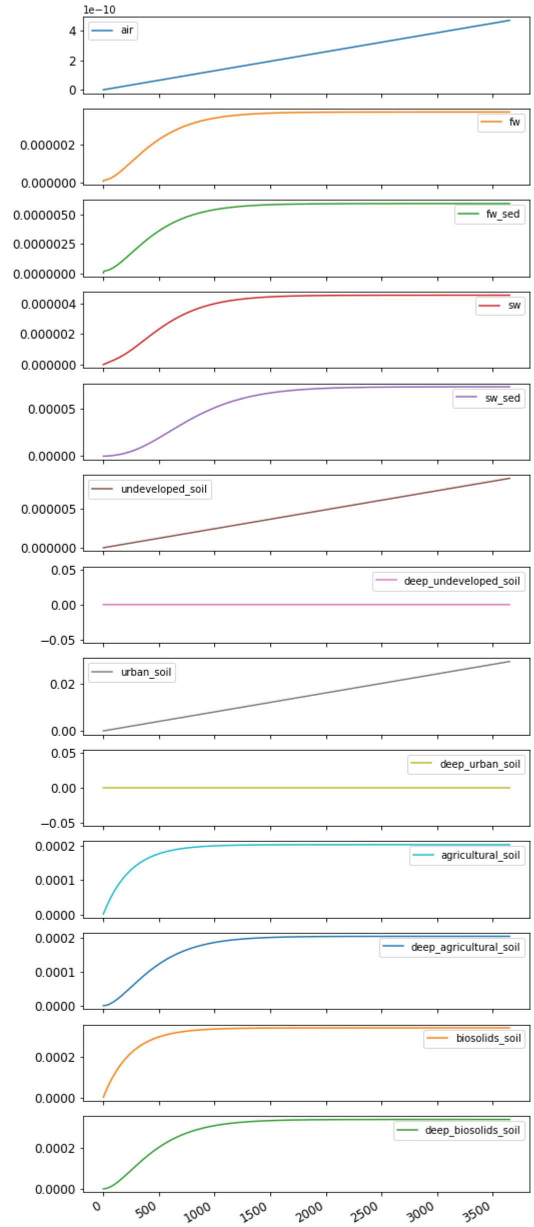
Table. MetalFate Constant Release Combined Ecotoxicological Comparisons. This table represents a simplified perspective on evaluating the ecological impacts that copper hydroxide may have from a constant release pattern.

MetalFate Constant Release Combined Ecotoxicological Comparisons									
						Caution	Warning	No Issue	
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
Copper Hydroxide									

Constant Metallic Pesticide Plot, Copper Hydroxide

The following page…

Copper Hydroxide Pesticide MetalFate Model
Daily Release Rate for 2010-2020
in Salinas River Valley.



Seasonal

Table. MetalFate Seasonal Release Results. This table represents the order of magnitude of the maximum concentration value resulting from the metalFate modeling the copper hydroxide fungicide.

MetalFate Seasonal Results									
Max Order of Magnitude of Background Concentration									
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
Copper Hydroxide	-12	-7	-7	-7	-6	0	-4	-6	-6

Table. MetalFate Seasonal Release Persistence of Chemical Results. This table represents the persistence of the metalFate modeling the copper hydroxide fungicide signal resulting from a seasonal release pattern.

MetalFate Seasonal Results									
Persistence of Chemical	(High, Moderate, and Low)								
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
Copper Hydroxide	V High	V High	V High	V High	V High	V High	V High	V High	V High

Table. MetalFate Seasonal Release Combined Ecotoxicological Comparisons. This table represents a simplified perspective on evaluating the ecological impacts the chemical may have from a seasonal release pattern.

MetalFate Seasonal Release Combined Ecotoxicological Comparisons									
						Caution	Warning	No Issue	
Pesticide Chemical	**Air**	**Fresh Water**	**FW Sediment**	**Salt-Water**	**SW Sediment**	**Undeveloped Soils**	**Urban Soils**	**Agricultural Soils**	**Biosolid Soils**
Copper Hydroxide									

Semi-Log Seasonal PNG Images of Metallic Pesticide, Copper Hydroxide

The following page…

Copper Hydroxide Pesticide MetalFate Model
Semi-Log Seasonal Release Rate for 2010-2020
in Salinas River Valley.