

# **Guidance for Selecting Input Parameters for the Pesticide in Flooded Applications Model (PFAM)**

## **Including Specific Instructions for Modeling Pesticide Concentrations in Rice Growing Areas**

PFAM Version 2.0

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U.S. Environmental Protection Agency  
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### **PFAM Conceptual Model Project Team:**

Melanie L. Biscoe, Meridith Fry, James Hetrick, Ph.D., Greg Orrick, Charles Peck, PE,  
Mohammed Ruhman, Andrew Shelby, MS, Nelson Thurman, Philip Villanueva, Katrina White,  
Ph.D., Dirk Young, Ph.D.

## 1 Introduction

EPA's Office of Pesticide Programs (OPP) developed this guidance document to help model users select and prepare the appropriate input values when using the Pesticides in Flooded Applications Model (PFAM). The model has been tested for modeling exposure for pesticide uses on rice. The input guidance may be used to inform how to parameterize PFAM for simulating pesticide uses to flooded and intermittently flooded areas other than rice (*e.g.*, cranberry bogs, watercress, or direct applications to water); however, specific scenarios and conceptual models for drinking water are not available for those use patterns. Scenarios and conceptual models for use with PFAM have only been developed for rice growing areas at this time.

Implementing this guidance should improve the consistency in modeling the fate of pesticides in the environment and ultimately the overall quality of risk assessments. The primary sources of fate input parameters that are used in the model include pesticide product chemistry and labeling information, as well as, sorption coefficients and degradation rates calculated from environmental fate studies that are usually conducted or sponsored by pesticide manufacturers. Additionally, model results are sensitive to assumptions made on the timing of applications and flood releases.

If there is a need to deviate from this guidance during risk assessment, the model user should provide adequate justification for model inputs in the assessment. This guidance document reflects the current policy for modeling in the OPP.

PFAM inputs are entered by the user on different tabs of the graphical user interface. Inputs on each tab are discussed below under each tab heading.

## 2 Ecological Versus Drinking Water Assessment

For ecological risk assessment, exposure to aquatic invertebrates, and aquatic vertebrates are assessed in the rice paddy. Exposure is also characterized for aquatic animals and aquatic plants for exposure after a specified holding period in tailwater. Conceptual models for human health drinking water have been developed independently for California and Arkansas/Missouri. PFAM is run with different inputs for ecological risk assessments and human health drinking water assessments.

## 3 Summary Tables for Model Input Parameters

### 3.1 Representative Half-life Values

The PFAM degradation kinetics routines follow single first-order (SFO) kinetics. Guidance has been developed for estimating a representative SFO model input half-life (in soil and aquatic systems) for degradation curves that do not follow SFO kinetics. The following guidance document may be used to evaluate degradation curves for individual studies and to calculate representative SFO half-lives for each dataset.

- USEPA. 2015. *Standard Operating Procedure for Using the NAFTA Guidance to Calculate Representative Half-life Values and Characterizing Pesticide Degradation. Version 2.* March 23, 2015. Environmental Fate and Effects Division. Office of Pesticide Programs. U.S. Environmental Protection Agency. Available [here](#) (Accessed May 9, 2016).

## 3.2 Chemical Tab

**Table 1. Inputs on the Chemical Tab in PFAM**

Parameter	Value	Data Source	Comment, Source
Organic-carbon Normalized Distribution Coefficient (K <sub>oc</sub> )	<p>Enter the mean K<sub>OC</sub> value. The value should be in units of ml/g or L/kg.</p> <p>K<sub>d</sub> can be applied by making note of the organic carbon content (under Physical Tab) and recognizing that <math>K_d = K_{oc} \times</math> organic carbon fraction, and adjusting the K<sub>oc</sub> or mean K<sub>d</sub> as appropriate.</p>	Adsorption/desorption data (Harmonized Test Guideline 835.1230)	<p>Either the mean K<sub>d</sub> or K<sub>OC</sub>, whichever has the lowest coefficient of variation (<i>e.g.</i>, the standard deviation ÷ mean), is used to determine the model input.</p> <p>Use of K<sub>oc</sub> may not be appropriate for chemicals with sorption not associated with organic carbon content, such as those that are ionic at environmental pH values. In these cases, the model user should document the rationale for the selected model input values.</p>
Water Column Half-life and Reference Temperature	<p><b>Representative Half-Life:</b> If multiple aerobic aquatic metabolism half-life values are available, enter the 90% confidence bound on the mean half-life value for the total system (water plus sediment) (see Equation 1 in Appendix A for instructions).</p> <p>If a single aerobic aquatic metabolism half-life value is available, enter 3x the half-life value (see Equation 2 in Appendix A).</p> <p>If no aerobic aquatic metabolism data are available and the pesticide shows insignificant hydrolysis, use 2x the aerobic soil metabolism half-life input value.</p> <p>If no aerobic aquatic metabolism data are available and the pesticide shows significant hydrolysis, enter zero (0).</p> <p><b>Temperature:</b> Enter the temperature in °C corresponding to the temperature at which the aerobic aquatic metabolism studies were conducted. If the studies were conducted at multiple temperatures, use equation 3 to adjust the half-life values to the same temperature and use the adjusted values to calculate the representative half-life input and enter the temperature that corresponds to the adjusted values.</p>	Aerobic aquatic metabolism data (Harmonized Test Guideline 835.4300)	<p>When both aquatic metabolism and hydrolysis rate data are included, the metabolism rate should be corrected for the hydrolysis rate at the pH of the aquatic metabolism study. Hydrolysis correction should be performed for both aerobic aquatic metabolism and anaerobic aquatic metabolism, or for neither.</p> <p>Example for the case when no aerobic aquatic data are available and the pesticide is hydrolytically stable: For a single aerobic soil metabolism half-life of 30 days, the aerobic soil metabolism half-life input value is 90 days (30 days x 3); thus the estimated aerobic aquatic metabolism half-life input value is 180 days (90 days x 2).</p>

Parameter	Value	Data Source	Comment, Source
Benthic Compartment Half-life and Reference Temperature	<p><b>Representative Half-Life:</b> If multiple anaerobic aquatic metabolism half-life values are available, enter the 90 percent confidence bound on the mean half-life value for the total system (water plus sediment) (see Equations in Appendix A for instructions).</p> <p>If a single anaerobic aquatic metabolism half-life value is available enter 3x the half-life value (see Equations 2 and 3 in Appendix A).</p> <p>If no anaerobic aquatic metabolism data are available and the pesticide shows insignificant hydrolysis, enter 2x the half-life corresponding to the anaerobic soil metabolism rate constant input value.</p> <p>If no anaerobic aquatic metabolism data are available and the pesticide shows significant hydrolysis, assume that the compound is stable to anaerobic aquatic metabolism, i.e., enter zero (0).</p> <p><b>Temperature:</b> Enter the temperature in °C corresponding to the temperature at which the anaerobic aquatic metabolism studies were conducted. If the studies were conducted at multiple temperatures, use equation 3 to adjust the half-life values to the same temperature and use the adjusted values to calculate the representative half-life input and enter the temperature that corresponds to the adjusted values.</p>	Anaerobic aquatic metabolism data (Harmonized Test Guideline 835.4400)	When both aquatic metabolism and hydrolysis rate data are included, the metabolism rate needs to be corrected for the hydrolysis rate at the pH of the aquatic metabolism study.

Parameter	Value	Data Source	Comment, Source
Unflooded Soil Half-life and Reference Temperature	<p><b>Representative Half-life:</b> If multiple aerobic soil metabolism half-life values are available, enter the 90 percent confidence bound on the mean of the half-lives (see Equation 1 in Appendix A for instructions).</p> <p>If a single aerobic soil metabolism half-life value is available, enter 3x the half-life value (see Equation 2 in Appendix A).</p> <p>If no aerobic soil metabolism data are available, assume that the compound is stable to biodegradation under these conditions, i.e., enter zero (0).</p> <p><b>Temperature:</b> Enter the temperature in °C corresponding to the temperature at which the anaerobic aquatic metabolism studies were conducted. If the studies were conducted at multiple temperatures, use equation 3 to adjust the half-life values to the same temperature, use the adjusted values to calculate the representative half-life input, and enter the temperature that corresponds to the adjusted values.</p>	Aerobic soil metabolism data (OPPTS Guideline 835.4100)	--
Near-Surface Photolysis Half-life and Reference Latitude	<p>Enter the maximum dark-control corrected environmental aqueous phototransformation half-life value. If no aqueous photolysis data are available or if there is no evidence of photolysis, enter zero (0).</p> <p><b>Degrees Latitude:</b> Enter the degrees latitude that the representative half-life value simulated. Typically, this is 40°N.</p>	Aqueous photolysis data (Harmonized Test Guideline 835.2240)	--

Parameter	Value	Data Source	Comment, Source
Hydrolysis Half-life	<p>If the chemical undergoes both aerobic aquatic or anaerobic aquatic metabolism and hydrolysis and the aquatic metabolism inputs are corrected for hydrolysis, enter the hydrolysis half-life at pH 7.</p> <p>If the chemical undergoes both aquatic metabolism and hydrolysis and the aerobic aquatic and anaerobic aquatic metabolism inputs are not corrected for hydrolysis, enter zero as the hydrolysis input.</p> <p>If no hydrolysis data are available, assume that the compound is stable, <i>i.e.</i>, enter zero (0).</p>	Hydrolysis data (Harmonized Test Guideline 835.2120)	--
Molecular Weight	Enter the value for the modeled pesticide in g/mole	Product chemistry	--
Vapor Pressure	Enter the maximum value in torr from product chemistry data for the temperature of the modeled water body	Product chemistry	If you desire to use a measured Henry's law constant, then enter vapor pressure and solubility that will give you the desired Henry's law constant. Henry's Law Constant = (Vapor Pressure in Torr/760)/(Solubility in mg L <sup>-1</sup> /Molecular Weight in g mole <sup>-1</sup> )
Solubility	Enter the maximum water solubility of the modeled pesticide at 20- 25° C.	Product chemistry	--
Heat of Henry	Enter the Heat of Henry of the modeled pesticide. Instructions on calculating the Heat of Henry are described in Appendix B.	Calculated using EPIWEB	
Henry Reference Temperature	Enter the temperature at which the vapor pressure and solubility were measured. These values are used for Henry's law constant.	Product chemistry	

### 3.3 Applications Tab

**Table 7A and 7B** describe the inputs for the 'Applications' tab for both ecological risk assessments and drinking water assessments. Additional information on ecological and drinking water assessments is also discussed in this section.

#### Ecological Risk Assessment: Number of Applications, Application Rate, and Dates of Application

For ecological risk assessment, risk is evaluated in the rice paddy. The Applications tab and use of application rates and dates of applications are consistent with how EFED typically uses these parameters. The number of applications and the application rate are specified on the product

label. Choose ‘Apply Pesticide on Specific Days’ on the applications tab for ecological risk assessment. Application dates are based on the timing recommended on the label, typical agronomic practices, and timing of when water or the crop is on the field from the Floods and Crop tabs. Typical flood patterns for a single paddy are reflected in the scenario metadata chapter (*Metadata for Pesticides in Flooded Applications Model Scenarios for Simulating Pesticide Applications to Rice Paddies Version 1.0*) and can be loaded by loading a scenario for ecological risk assessment. The flooding patterns may also be viewed in the Graphical User Interface (GUI) of PFAM on the floods tab by loading a scenario. Example application inputs for a pesticide applied at 4.5 kg/ha, 2 times, with a five day minimum retreatment interval are provided in **Table 2**.

**Table 2. Example Application Tab Parameters for Ecological Risk Assessment (Application Tab)**

Parameter	Value	Comment, Source
Apply Pesticide Over Specific Days or a Distribution of Days	Specific Days	Choose for ecological risk assessment
Month, Day	5/4 5/9	Dependent on pesticide, pre-emergence vs post-emergence, pre-flood or post-flood
Mass Applied in kg/ha	4.5 4.5	
Slow Release (1/day)	0	This is used if the formulation slowly releases the pesticide over time.
Drift Factor	0	

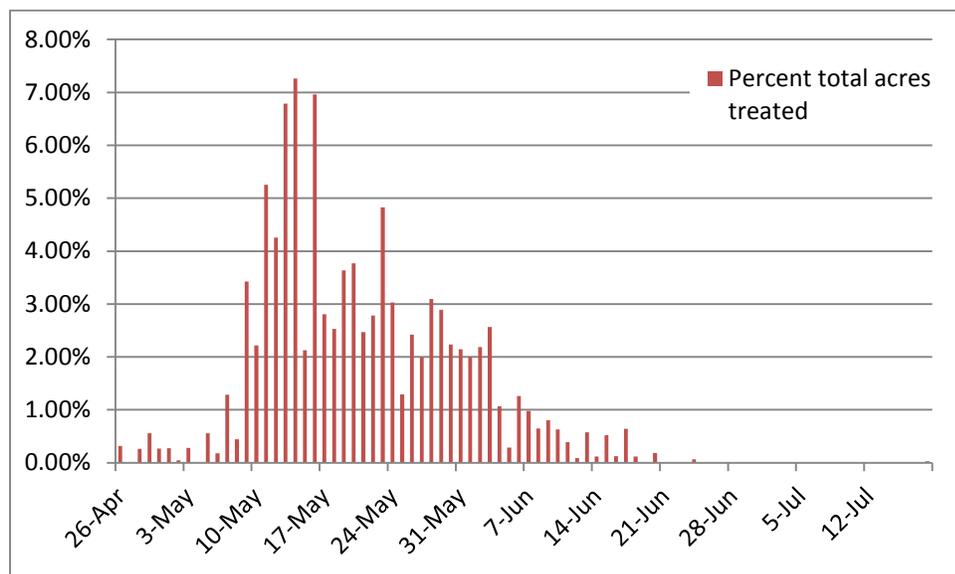
As exposure is estimated in the rice paddy for ecological risk assessment, releases of water after an application could reduce estimated exposure in the paddy, leading one to erroneously conclude that risk could be reduced by early paddy releases. The risk, however, would move with the residues in the water after they left the paddy, and it is uncertain to what extent residues in the water would be diluted after the water left the rice paddy as some canals that water will flow into may not have much water in them or the water may be coming from releases from rice paddies upstream. Therefore, to follow the residues in the water and to fully capture the potential for risk for ecological organisms, water should be held on the rice paddy after the application and until harvest. Reports of individuals using the canals right next to rice paddies for fishing are common, and the canals are often promoted to be a resource for wildlife.

### Drinking Water Assessment: Number of Applications, Application Rate, and Dates of Application

Estimating application parameters for human health drinking water assessments using PFAM differs from the method used for ecological risk assessment and the methods used for the USEPA standard index reservoir or farm pond. The conceptual models for the index reservoir and farm pond are on a smaller spatial scale than the conceptual model for rice. For drinking water assessments, the number of applications, application rate, and dates of application are approached differently because the number of the acres treated is very large (511,824 acres in California and 102,345 acres in Arkansas/Missouri). Not all of the acreage is expected to be

treated on one day. However, PFAM does not automatically adjust for the number of acres treated per day if you select “Apply Pesticide on Specific Days”. It assumes that all acres are treated with the application rate provided on the Applications tab.

Thiobencarb is an herbicide that is typically applied early in the rice season once per year. Based on usage data in the California Department of Pesticide Regulations (CADPR) Pesticide Use Database<sup>1</sup> in 2009, 87% of the acres treated were treated between May 9 and June 3 (26 days). The most intensive treatment days were May 11, 13, 14, and 16 where 5 to 7 percent of the acres were treated. On the other days, less than 3% of the acres were treated on a single day. **Figure 1** shows the distribution of rice acres treated in California with thiobencarb in 2009.



**Figure 1. Percent total acres of rice treated with thiobencarb in California in 2009**

Several usage pattern scenarios were developed to represent typical applications for the California rice growing area, based on observed typical usage for different pesticides.

For drinking water assessments, PFAM has been updated to allow the user to distribute applications over a given time period. **Figure 2** provides a screen shot of the PFAM Applications tab. The screen depicts an example where applications are being distributed throughout the watershed from May 7 to June 23, where a total of 4 lbs a.i./A/year (4.48 kg a.i./ha/year) is applied. The drift factor is the result of an aerial application using medium to coarse nozzles (see **Table 2** below). The selections to the far right allow the user to distribute the application across all of the watershed uniformly ( $\square$ ) or using a triangular distribution ( $\wedge$ ), where applications start low at the start date, peak at the midpoint of the application period, then taper off at the end date. The scenario metadata document provides guidance on recommended application dates for different modeling runs, and those inputs are also provided below for

<sup>1</sup> [California Department of Pesticide Regulations \(CADPR\) Pesticide Use Database](http://www.cdpr.ca.gov/docs/pur/purmain.htm) (accessed January 31, 2014)

specific scenarios. For drinking water assessments, it is recommended that pesticide applications be spread out over 46 days.

Because of the large area of rice simulated, it is not expected that all acres of rice would be treated with a single pesticide. Therefore, a percent crop treated (PCT) may be used to refine a drinking water estimate of exposure. In the first tier, a maximum five-year average PCT for the pesticide type (*e.g.*, insecticide, herbicide, fungicide) specific to the state being simulated is used. Then the application rate is multiplied by the PCT as a decimal<sup>2</sup>. The maximum five year average PCTs are available in *Percent Crop Treated Values for Active Ingredients with Reported Use on Rice* (USEPA, 2016) and in **Table 3**. For the Arkansas, Missouri conceptual model, the state with the highest PCT is used. For example, for fungicides the Arkansas/Missouri PCT of 47% (for Arkansas) is applied to the application rate, and for herbicides the PCT applied to the application rate is 88% (for Missouri).

One common mistake is to switch the month and day input on the application dates and flood dates. On the ‘applications’ tab, the date is entered in the order of month then day. On the ‘floods’ tab the ‘reference date’ is entered as day followed by month. PFAM has a feature on the ‘floods’ tab to graphically plot the application and flood events so the user can visually see when events are occurring across the year. This feature can be very helpful when evaluating application timing with regards to the timing of the flood events.

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<sup>2</sup> For an herbicide simulated in California with a maximum annual application rate of 1 kg/ha, the application rate would be adjusted to 0.80 kg/ha using the 80% PCT.

**Table 3. State-Level Five-year Average Annual Percent Cropped for Rice Treated by Pesticide Type Between 2010 – 2014**

**(a) Fungicide**

State	Active Ingredient	Percent Crop Treated (5-yr annual average)
<b>Arkansas</b>	<b>Propiconazole</b>	<b>47%</b>
<b>California</b>	<b>Azoxystrobin</b>	<b>47%</b>
Louisiana	Propiconazole	81%
Mississippi	Azoxystrobin	49%
Missouri	Propiconazole	35%
Texas	Propiconazole	72%

**(b) Herbicide**

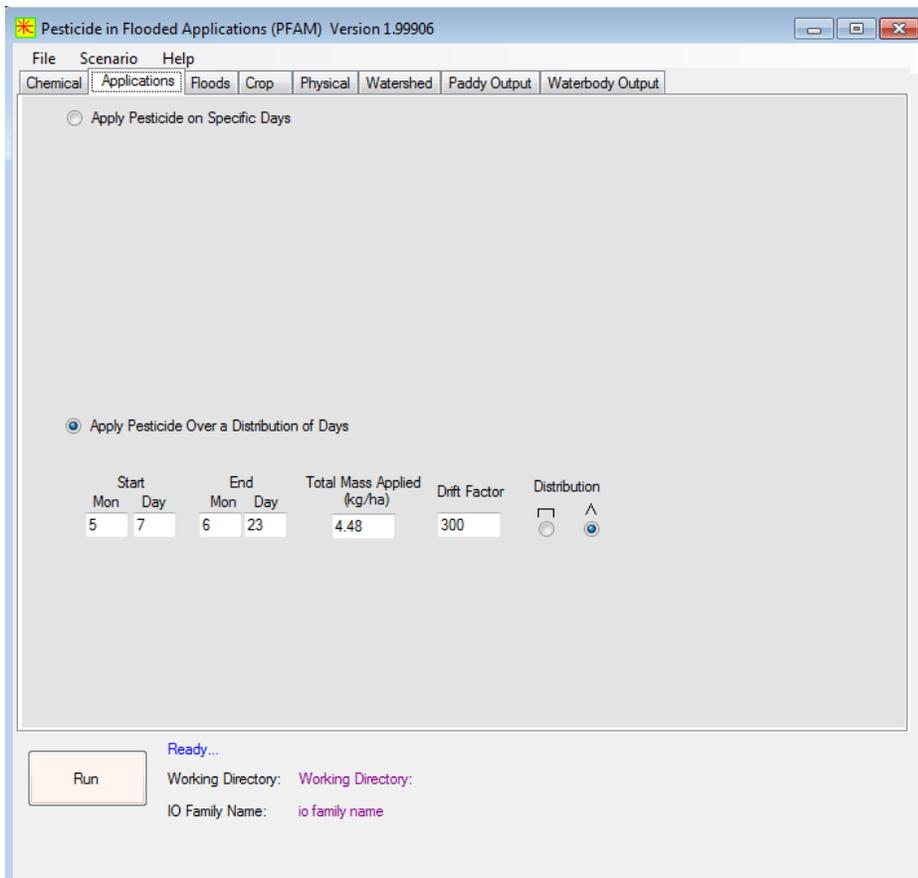
State	Active Ingredient	Percent Crop Treated (5-yr annual average)
Arkansas	Clomazone	77%
<b>California</b>	<b>Propanil</b>	<b>80%</b>
Louisiana	Imazethapyr	75%
Mississippi	Quinclorac	65%
<b>Missouri</b>	<b>Clomazone</b>	<b>88%</b>
Texas	Glyphosate	47%

**(c) Insecticide**

State	Active Ingredient	Percent Crop Treated (5-yr annual average)
<b>Arkansas</b>	<b>Cyhalothrin-Lambda</b>	<b>33%</b>
<b>California</b>	<b>Cyhalothrin-Lambda</b>	<b>29%</b>
Louisiana	Cyhalothrin-Lambda	32%
Mississippi	Cyhalothrin-Lambda	56%
Missouri	Cyhalothrin-Lambda	23%
Texas	Zeta-Cypermethrin	43%

Source: Market Research Data, 2010-2014

Bolded values are the PCTs that are used in drinking water assessments.



**Figure 2. Distribution of applications for drinking water assessments (Applications Tab)**

**Table 4. Example application input parameters for a drinking water assessment (Application Tab)**

Parameter	Value	Comment, Source
Apply Pesticide Over a Distribution of Days	Yes	Choose for a drinking water assessment
First Day of Application	May 7	Based on CA PUR data, herbicides are commonly applied within a 30- to 60-day time window with a peak application period. Conceptual models for drinking water were developed with applications spread over a 46-day period.
Last Day of Application	June 23	Based on CA PUR data, herbicides are commonly applied within a 30- to 60-day time window with a peak application period. Conceptual models for drinking water were developed with applications spread over a 46-day period.
Total Mass Applied in kg/ha	Enter the total kg/ha allowed on the label over the entire year.	This value may be refined by multiplying by the maximum percent use area for the pesticide class ( <i>e.g.</i> , herbicide, fungicide, insecticide).
Drift Factor	Enter the spray drift factor based on label recommendations	Determined by label recommendations and corresponding spray drift factor
Distribution	^	Based on CA PUR data.

**Table 5. Specific Application date ranges for the drinking water scenarios<sup>1</sup>**

Scenario	First Day of Application (Month, Day)	Last Day of Application (Month, day)
DW CA Mixed noHold.PFS	May 7	June 23
DW CA Preflood noHold.PFS	April 6	May 22
CA Postflood noHold.PFS	May 23	July 8
DW MO Mixed Winter noHold.PFS	April 25	June 10
DW MO Mixed noWinter noHold.PFS	April 25	June 10
DW MO Preflood noWinter noHold.PFS	March 15	April 30
DW MO Postflood noWinter noHold.PFS	April 30	June 15

<sup>1</sup> Pre-flood scenarios are used when applications occur before flood. Post-flood scenarios are used for applications that occur post-flood. Mixed scenarios are used when applications may occur pre- and post-flood.

### Spray Drift Factor

The approach for estimating spray drift to canals and other water bodies surrounding rice paddies differs from the estimation of spray drift to the USEPA standard index reservoir or farm pond. Aquatic spray drift exposures from the index reservoir and farm pond integrate spray drift from a single field application to a single body of water. The conceptual model for rice includes the watershed relevant to the drinking water intake of concern and all rice paddies within that watershed. Spray drift to the canals that are proximate to the rice paddies receive more or less drift depending on their distance to a rice paddy and their particular width. The fraction of the mass applied to all paddies that will enter canals, streams, and rivers by spray drift is estimated according to the Chapter 5 in the *Development of a Conceptual Model to Estimate Pesticide Concentrations in Ecological Risk Assessments and Human Health Drinking Water Using the*

*Pesticides in Flooded Applications Model.* Default values for use in DWAs using PFAM are provided in **Table 6.**

**Table 6. Spray drift factor for use in PFAM for estimating human health drinking water\***

(a) Aerial Applications

Spray drift release and droplet size distribution	Very Fine to Fine	Fine to Medium	Medium to Coarse	Coarse to Very Coarse
California spray drift factor	927	<b>404</b>	300	214
Delta spray drift factor	198	<b>86</b>	64	46

(b) Ground Applications

Spray drift release and droplet size distribution	Low Boom - Fine to Medium/Coarse	Low Boom - Fine/Very Fine	High Boom- Fine to Medium/Coarse	High Boom- Fine/ Very Fine
California spray drift factor	343	559	566	<b>941</b>
Delta spray drift factor	73	119	121	<b>201</b>

\*Bold values show the default assumption for spray drift.

**Table 7A. Summary of Inputs on the Applications Tab in PFAM: Apply Pesticide On Specific Days (EcoRA)**

Parameter	Input Value	Data Source	Notes
Number of Applications	Enter the number of applications.	Label	The maximum is 30 applications.
Mon	Enter the month of application	Label	
Day	Enter the Calendar day of application	Label	
Mass applied (kg/ha)	EcoRA: Enter the application rate in kg/ha	Label	
Slow Release	If data are available indicating a pesticide is slowly released over time, calculate a rate constant on the rate of release and enter the value.  If data are not available indicating a pesticide is slowly released over time, enter 0.		Specifies whether the pesticide is designed as a slow-release agent. The release rate is first order with the mass of pesticide remaining after time t equal to $M_0 \exp(-kt)$ , where k is the user specified release rate (per day), $M_0$ is the <i>Applied Mass</i> (see above), and t is time in days. A slow release of zero by convention means that there is an instantaneous full release. As a reference, a Slow Release rate of 0.6 per day will result in 95% of the pesticide released in 5 days.
Drift Application (Fraction)	Enter zero		

Abbreviation: EcoRA=ecological risk assessment; DWA=drinking water assessment

**Table 7B: Summary of Inputs on the Applications Tab in PFAM: Apply pesticide over a distribution of days (DWA)**

Parameter	Input Value	Data Source	Notes
Start Mon and Day	Enter the calendar month and day for the start of applications	Label	See scenario metadata for suggested start dates
End Mon and Day	Enter the calendar month and day for the end of applications	Label	See scenario metadata for suggested end dates
Total Mass Applied (kg/ha)	Enter the total annual application rate in kg/ha	Label	Total mass applied may be refined by multiplying by the maximum percent crop treated for the pesticide type (e.g., herbicide, fungicide, insecticide) for the state(s) being simulated.
Drift Factor (unitless)	See Table 2 for spray drift factors		
Distribution	^		A triangular distribution is default

### 3.4 Floods Tab

For both the ecological risk and drinking water assessments, the metadata files provide examples of typical flooding dates. Metadata and scenarios were developed for the ‘Floods’ tab. To load the appropriate data for an area of the country or conceptual model, load the scenario for that area. Additionally, Chapter 2 of *Development of a Conceptual Model to Estimate Pesticide Concentrations in Ecological Risk Assessments and Human Health Drinking Water Using the Pesticides in Flooded Applications Model*, describes typical agronomic practices for growing rice in different geographic areas.

Prior to Event 1, the weir height, fill height, minimum level, and turnover are set to 0 by default. The ‘Fill’ level is the level that the water is refilled to once the level falls below the minimum level. The ‘Weir’ level is the maximum level that water may rise to before a release occurs; in reality, the weir level represents a physical structure (weir) that should not change substantially across events unless the water level is intentionally being changed. The user can specify the weir level as greater than the Fill level if appropriate in the conceptual model, though the Weir and Fill levels are often equal. The ‘Min’ level is the water level that the water body can be reduced to by evaporation or leakage before the level is returned to the Fill level. When maintaining the water level, the Fill level and Min level may be equal; the Weir level is usually set a couple of cm higher. Water removed from the rice paddy via evaporation is based on the PAN evaporation factor. The PAN factor (cm per day) is an input from the meteorological file (second column). In the California meteorological file, PAN evaporation factors range from 0 to 1.48, with most values less than 1 cm.

Weir leakage is considered rare, but is handled the same as a manual release, reducing the daily water level in the rice paddy by a set amount (defined in meters per day on the Physical tab). Turnover represents the daily washout rate due to flow through the rice paddy (in the absence of a holding period), and can be specified for each flood event (in units of per day) on the Floods tab. The total washout rate, used to ultimately calculate the pesticide mass transported from the rice paddy to a receiving stream, river, or canal, is the sum of the rice paddy’s turnover rate and

the daily washout rate due to releases and precipitation. Both precipitation and irrigation both add to the overall water level; in some cases, they contribute to releases when the daily water level exceeds the Weir level. Pesticide mass can also be lost via benthic leakage (specified in meters per day on the Physical tab), independent of any water level changes, but this is usually assumed to be 0.

The user has the ability to model the changes in flooding events using a ‘Sharp Transition’ or ‘Gradual Transition’ selection. If the user selects to use a ‘Sharp Transition,’ then water levels will increase and decrease instantaneously on the day of the flood event. If the user selects ‘Gradual Transition,’ then water levels will increase and decrease linearly between flood events. The default value for ecological risk assessments is ‘Sharp Transition’ while the default value for human health drinking water assessments is ‘Gradual Transition.’

PFAM also has a feature to graphically plot the application and flood events so the user can visually see when events are occurring across the year. This feature can be very helpful when evaluating application timing with regards to the timing of the flood events.



**Figure 3. Example Floods Tab for a Human Health Drinking Water Assessment**

**Table 8. Inputs on the Floods Tab in PFAM**

Parameter	Input Value	Notes
Show More Events	Enter the number of flood events	--
Reference Date Day and Month	Enter the calendar day of the first flood event	--
Days and Fill level (m)	Enter days after the reference date of the event and the fill level. See the metadata for the scenarios for typical flood assumptions for different scenarios.	Level that water is filled to for a refilling event.
Days and Weir Height (m)	Enter the days after the reference date of the event and level of the weir in meters. This is normally the same value as the fill level.  Standard EFED risk assessments: same input as fill level.	This is the level that water may rise over the fill level, before it will release into the mixing cell. Generally, this parameter is the maximum water level in the paddy. In California, the weir level is not typically kept above the fill level.
Days and Min level (m)	Enter days after the reference date of the event and the minimum level of the water body in meters, below which the level is refilled to the fill level.  Standard EFED risk assessments: same input as fill level	Represents the water level that the water body can be reduced to (by evaporation or leakage) before the level is returned to the fill level by refill. Generally, this level is set to a lower value than the weir height and fill level.
Days and Turn Over (1/day)	Enter a turnover rate of 0.017 (1/60) when there is no holding period. Enter a turnover rate of 0 during a holding period.	In California, a low level flow is maintained to prevent algae growth. Releases are prohibited during a required water holding period.

### 3.5 Crop, Physical, and Watershed Tab

Metadata and scenarios were developed for the Crop, Physical, and Watershed tabs. See the metadata for a description of specific inputs for the conceptual models. To load the appropriate data for an area of the country, load the scenario for that area. To calculate a downstream water body concentration, the box for “Calculate downstream water body concentration’ must be selected.

### 3.6 Paddy and Waterbody Output Tabs

The Paddy and Watershed Output tabs summarize the results of the modeling run and provide the 1-in-10 year peak in the rice paddy or daily average in the receiving water body, 4-day, 21-day, 60-day, 90-day, and annual average concentrations for the water column and benthic pore water and sediment in both the paddy and the receiving water body (DWAs only). The Paddy Output tab also contains the highest concentration in the released water, as well as the ability to estimate holding times. The user needs to specify the Number of Days After the Last Application (*i.e.*, holding period) and PFAM estimates the highest, 90<sup>th</sup> percentile, and average concentration in the release water for the given holding period over the 30 years of simulation.

The Waterbody Output tab provides the Drift Contribution Fraction to the EECs as well as the Drift Fraction to the Total Applied.

### 3.7 Results/Output Files

After running PFAM, the following files will be created.

**Table 9. Summary of Files Generated with a PFAM Simulation**

File Name	Description
XXX.PFA	PFAM Input file
XXX_paddy.raw	Fixed width text file with daily results of paddy values from PFAM run
XXX_paddy_AncillaryInfo.txt	Text file with effective half-life values from PFAM run
XXX_paddy_1-in-10.txt	Text file with summary statistics for paddy water column concentrations, benthic pore water concentrations, and benthic total concentrations
XXX_paddy_DailyRecord.txt	Text file with daily values for paddy water column concentrations, benthic pore water concentrations, and benthic total concentrations
XXX_Waterbody_Benthic_daily.txt	Text file with daily values for water body benthic pore water concentrations
XXX_Waterbody_Benthic_SummaryStats.txt	Text file with summary statistics for water body benthic pore water concentrations
XXX_Waterbody_ daily.txt	Text file with daily values for water body water column concentrations
XXX_Waterbody_ SummaryStats.txt	Text file with summary statistics for water body water column concentrations

## 4 Literature Cited

USEPA. 2016. *Percent Crop Treated Values for Active Ingredients with Reported Use on Rice*. May 0216. Biological Analysis Branch. Science Information and Analysis Branch. Office of Chemical Safety and Pollution Prevention. U.S. Environmental Protection Agency.

## Appendix A. Equations

### Calculating the 90<sup>th</sup> percentile confidence bound on the mean half-life value.

- If more than one half-life value is available, use Equation 2 to calculate the 90<sup>th</sup> percentile confidence bound on the mean half-life value:

$$t_{\text{input}} = \bar{t}_{1/2} + \frac{t_{90,n-1}S}{\sqrt{n}} \quad \text{Equation 2}$$

where,

$t_{\text{input}}$  = half-life input value (*time*)

$\bar{t}_{1/2}$  = mean of sample half-lives (*time*)

s = sample standard deviation (*time*)

n = number of half-lives available (-)

$t_{90,n-1}$  = one-sided Student's t value at  $\alpha = 0.1$  (*i.e.*, 1.0-0.9) (-)

This equation does not calculate the 90<sup>th</sup> percentile of the distribution of half-life values.

Some Student's t values include:

n-1	1	2	3	4	5	6	7	8	9	10	11	12	$\infty$
$t_{90}$	3.078	1.886	1.638	1.533	1.476	1.440	1.415	1.397	1.383	1.372	1.363	1.356	1.282

Student's t values can also be calculated with statistical packages or function, *e.g.* the Excel TINV function (TINV(0.2, n-2) is equivalent to  $t_{90,n-1}$ ) or the R qt function.

- If only one half-life value is available, multiply the value by 3 (Equation 3) instead of using Equation 2. This is to account for uncertainty in the environmental variability:

$$t_{\text{input}} = 3 t_{1/2} \quad \text{Equation 2}$$

### Calculating the temperature-adjusted degradation half-life

- Prior to using Equations 2 and 3 below, adjust half-lives from studies conducted at temperatures other than 25°C to values at 25°C using Equation 1.

$$t_{\text{adjusted}} = \frac{t_{\text{measured}}}{Q_{10}^{\left(\frac{T-T_{\text{ref}}}{10}\right)}} \quad \text{Equation 3}$$

where

$t_{\text{adjusted}}$  = half-life adjusted to 25°C [*time*]

$t_{\text{measured}}$  = laboratory measured aerobic soil metabolism half-life [*time*]

$Q_{10}$  = factor by which degradation increases for a 10°C temperature rise (use a  $Q_{10}$  of 2)

$T$  = temperature of modeled water body [°C] (use a  $T$  of 25°C (temperature assumed by PRZM))

$T_{\text{ref}}$  = temperature of the laboratory study [°C]

## Appendix B. Determining the Heat of Henry

**Heat of Henry** is the enthalpy of phase change from aqueous solution to air solution (Joules/mole). This enthalpy can be approximated from the enthalpy of vaporization (Schwarzenbach et al., 1993), which can be obtained from EPISuite<sup>3</sup> among other sources. Enthalpy for pesticides obtained in a literature review ranged from 20,000 to 100,000 J/mol (average 59,000 J/mol). Some example enthalpies for pesticides are

Metalochlor	84,000	Feigenbrugel et al. 2004
Diazonon	98,000	Feigenbrugel et al. 2004
Alachlor	76,000	Gautier et al., 2003
Dichlorvos	95,000	Gautier et al., 2003
Mirex	91,000	Yin and Hassett, 1986
Lindane	43,000	Staudinger et al. (2000)
EPTC	37,000	Staudinger et al. (2000)
Molinate	58,000	Staudinger et al. (2000)
Chlorpyrifos	17,000	Staudinger et al. (2000)

Enthalpies can also be estimated by the US EPA EPI Suite software. Open the software, then select the HENRYWIN subprogram on the left of the EPI Suite screen. On the top menu of the HENRYWIN window item, select *Show Options*, then select *Show Temperature Variation with Results*. Enter the chemical name of interest and then push the *Calculate* button. EPI Suite will give the temperature variation results in the form of an equation:  $HLC \text{ (atm}\cdot\text{m}^3\text{/mole)} = \exp(A - (B/T)) \{T \text{ in K}\}$ . The enthalpy of solvation in Joules/mol is equal to  $8.314 \cdot B$ . Example enthalpies from EPI Suite are:

Pendamethalin	62,000 J/mol
Carbaryl	58,000 J/mol
Carbofuran	54,000 J/mol
Molinate	54,000 J/mol
Endosulfan	37,000 J/mol

Below is the output for carbaryl from the HENRYWIN program with the equation highlighted in red. The Carbaryl Heat of Henry is calculated as 7,000 times 8.13.

### Example Output from HENRYWIN for Carbaryl

Bond Est : 3.14E-009 atm-m<sup>3</sup>/mole (3.18E-004 Pa-m<sup>3</sup>/mole)  
Group Est: Incomplete

SMILES : O=C(Oc(c(c(ccc1)cc2)c1)c2)NC  
CHEM : 1-Naphthalenol, methylcarbamate

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<sup>3</sup> EpiSuite™ is available at [here](#) (accessed May 21, 2016).

MOL FOR: C12 H11 N1 O2

MOL WT : 201.23

----- HENRYWIN v3.20 Results -----

Experimental Database Structure Match:

Name : 1-NAPHTHYL-N-METHYLCARBAMATE

CAS Num : 000063-25-2

Exp HLC : 3.27E-09 atm-m3/mole (0.000331 Pa-m3/mole)

Temper : 25 deg C

Exp Ref : VP/WSOL

Henry LC Temperature Variation:

Source: Carbamate slope analogy

HLC (atm-m3/mole) =  $\exp(3.9389 - (7000/T))$  {T in deg K}

Temp (C) atm-m3/mole unitless Pa-m3/mole

Temp (C)	atm-m3/mole	unitless	Pa-m3/mole
0	3.81E-010	1.7E-008	3.86E-005
5	6.05E-010	2.65E-008	6.13E-005
10	9.43E-010	4.06E-008	9.55E-005
15	1.45E-009	6.12E-008	0.000147
20	2.19E-009	9.11E-008	0.000222
25	3.27E-009	1.34E-007	0.000331
30	4.82E-009	1.94E-007	0.000488
35	7.01E-009	2.77E-007	0.00071
40	1.01E-008	3.92E-007	0.00102
45	1.43E-008	5.48E-007	0.00145
50	2.01E-008	7.58E-007	0.00204

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	3 Hydrogen to Carbon (aliphatic) Bonds		-0.3590
HYDROGEN	7 Hydrogen to Carbon (aromatic) Bonds		-1.0801
HYDROGEN	1 Hydrogen to Nitrogen Bonds		1.2835
FRAGMENT	1 C-N		1.3010
FRAGMENT	11 Car-Car		2.9019
FRAGMENT	1 CO-O		0.0714
FRAGMENT	1 CO-N		2.4261
FRAGMENT	1 Car-O		0.3473

RESULT | BOND ESTIMATION METHOD for LWAPC VALUE | TOTAL | 6.892

HENRYs LAW CONSTANT at 25 deg C = 3.14E-009 atm-m3/mole

= 1.28E-007 unitless

= 3.18E-004 Pa-m3/mole

GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
1 CH3 (X)		-0.62
7 Car-H (Car)(Car)		0.77
2 Car (Car)(Car)(Car) fused		0.94
1 Car (Car)(Car)(O)		-0.43
MISSING Value for: CO (O)(N)		
MISSING Value for: O (Car)(CO)		
MISSING Value for: NH (C)(CO)		
RESULT   GROUP ESTIMATION METHOD for LOG GAMMA VALUE	INCOMPLETE	0.66