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Pesticide Registration Evaluation Model (PREM) User's Manual (Version 6.0)

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4/10/2024

1 Overview

The Surface Water Protection Program (SWPP) of the California Department of Pesticide Regulation (CDPR) has been developing the Pesticide Registration Evaluation Model (PREM) to provide a consistent and transparent evaluation of registration packages routed to SWPP. There is an ongoing effort to expand the types of modeling scenarios and management practices that the model is capable of simulating. Details for the original model development and later improvement have been documented in the technical reports (Luo and Deng, 2012a, b; Luo, 2014; Luo et al., 2016; Xie and Luo, 2016; Luo, 2017a; Luo et al., 2024). A computer program has been developed to implement the model with a graphical user interface (GUI). The purpose of this document is to provide instructions to use the latest version PREM6. The model versions will change over time. Be sure to use the manual that corresponds to the PREM version being used.

Proposed use patterns of a pesticide product should be determined from its label before the model-based evaluation. Currently, the model is capable of evaluating aquatic uses, applications to terrestrial and submerged agricultural fields, urban outdoor uses, and down-the-drain products, but not capable of evaluating other pesticide use patterns such as marine antifouling paint products. Although the interface has been revised in this version, PREM6 generally shares the same modeling procedures and provides backward compatibility to the previous versions.

2 Installation

The package of PREM6 can be downloaded as a .ZIP compressed file from the CDPR webpage of "Surface Water Models" (cdpr.ca.gov/docs/emon/surfwtr/sw_models.htm) for external users, or the SWPP's network drive for CDPR internal users. Unzip the .ZIP file and extract its contents into a local hard disk of your computer. No spaces are allowed in the directory path of the installation folder. Figure 1 shows an example of the model package extracted in D:\models\PREM6\. The package includes the executable file ("PREM.exe"), supporting data and programs (in the sub-folder of "bin"), and user's manual (this document). Double click "PREM.exe" to start the model.

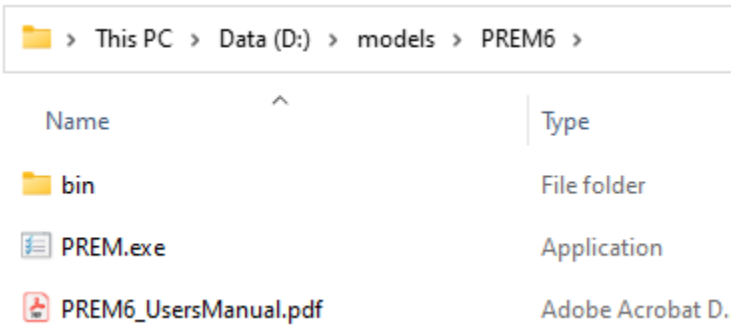


Figure 1. The PREM6 package in a local computer

3 (For external users only) Configurations for user-provided models

Some modeling functions in PREM6 require additional programs to be installed by a user (Table 1). For CDPR internal users, these models have been pre-installed.

Table 1. PREM6 functions and required external models

PREM6 functions	Required models
Evaluation of copper in freshwater based on a Biotic Ligand Model	Biotic Ligand Model
Estimation of WWTP (wastewater treatment plant) delivery factor for a DtD (down-the-drain) product	EPI Suite
Prediction of the mitigation effectiveness by vegetative filter strip (VFS)	VFSMOD

External users should download the installation packages from the official websites and install them in your computer. During the installation, please write down the program path for each model. A program path refers to the directory where the executable files for the model are located. For example, if the program path for VFSMOD is "C:\Program Files\VFSMOD", you will find the required executable file "vfsm.exe" and other supporting data for VFSMOD in this folder.

In PREM6, use the "About" dialog to configure the user-installed models. In the tab for "Other models", check the available models and specify their program path (Figure 2). There are multiple options for doing this: manually input, copy and paste, or use the small buttons next to the text box to open a folder browser.

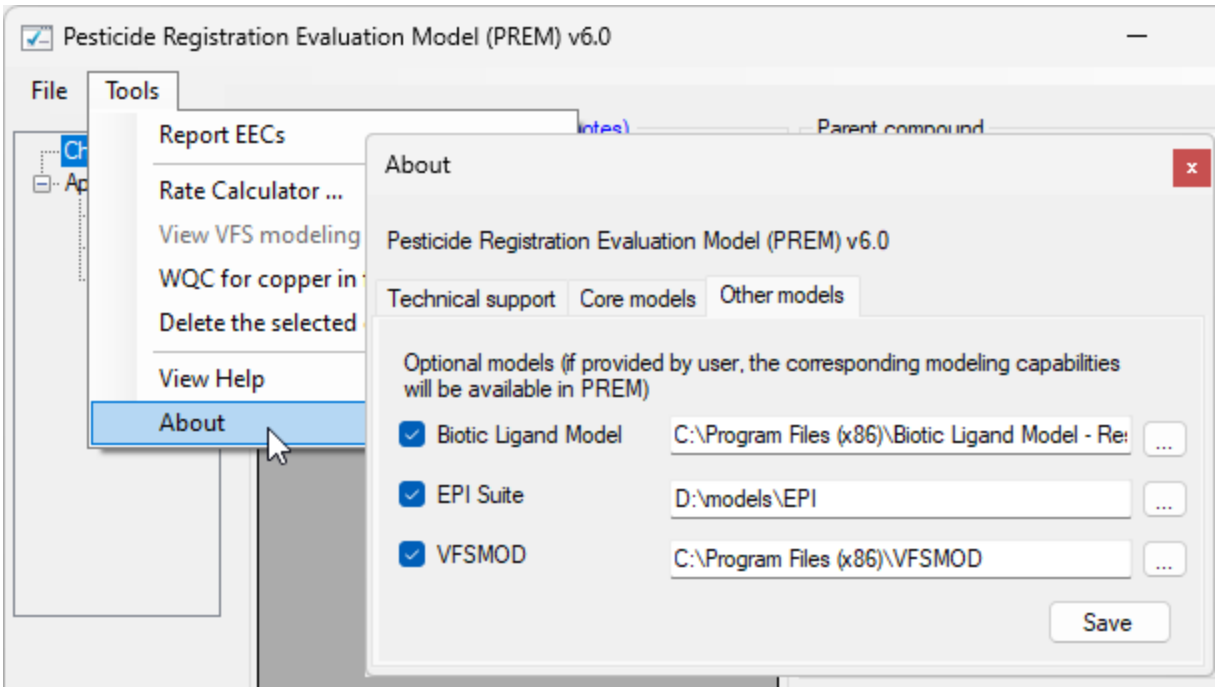


Figure 2. Configuring external models for PREM6

Note that a user does not have to install all of the models (Table 1), but just those related to the functions to be used in the evaluation. If a model is not installed and configured, the associated functions in PREM6 will be disabled.

4 The menus and navigation panel

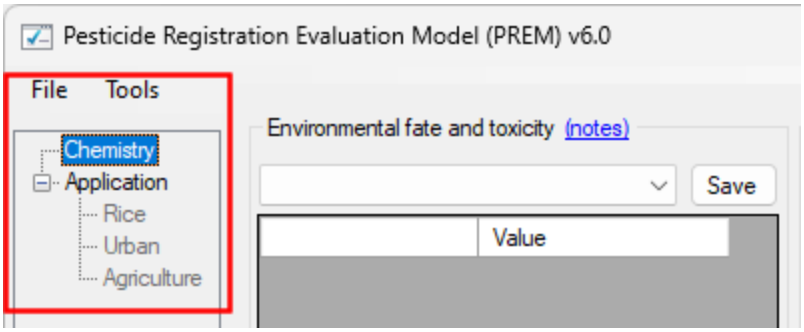


Figure 3. The menus and navigation panel in PREM6

4.1 "File" menu

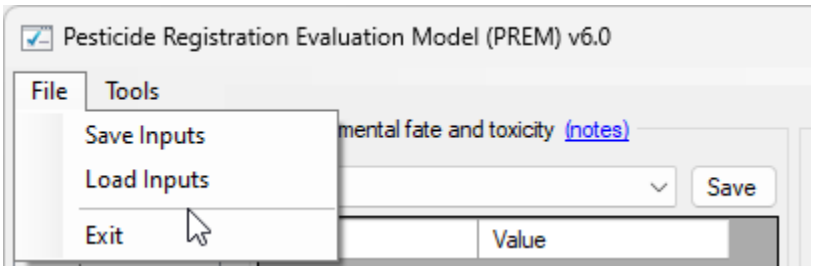


Figure 4. "File" menu in PREM6

There are three functions available under the "File" menu:

1) "Save Inputs": after a successful model simulation, the model inputs and settings can be saved as a project file with an extension of ".PREM".
2) "Load Inputs": the previously saved project file can be imported into PREM6. After loading a project, carefully check the parameters and options and make sure they are as expected.
3) "Exit": exit the program.

4.2 "Tools" menu

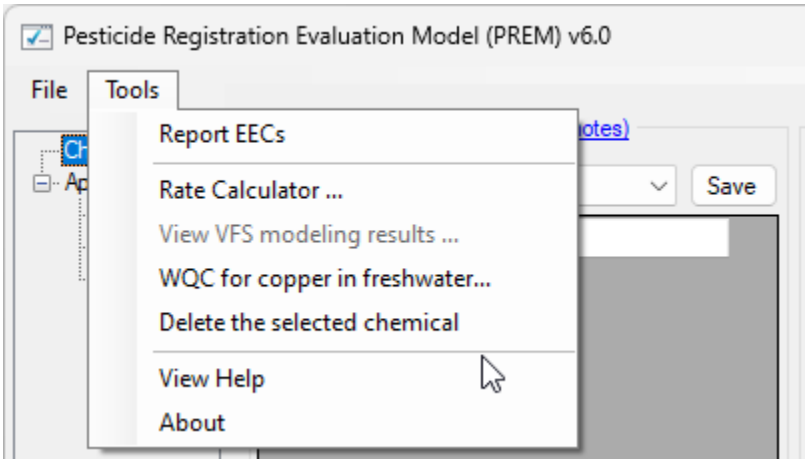


Figure 5. "Tools" menu in PREM6

The following functions and options are provided under the "Tools" menu:

1) "Report EECs": this is an option to report the estimated environmental concentrations (EECs) instead of the standard modeling results of risk quotients (RQs) and registration recommendations. After checking this option, a user is asked to provide a list of time periods (days, as comma-separated values) for calculating the moving averages of EECs. For example, with the input of "1,4,21", PREM6 will report the 1-d (i.e., daily), 4-d, and 21-d average EECs. Two special averaging periods are designated as "365" for annual

average (regardless of the actual days in a year) and "-1" for overall average during the entire modeling period. The default list of averaging periods is "1,4,21,60,365,-1" (Figure 6) following USEPA's PWC model.

2) "Rate Calculator": this tool calculates the label application rate for modeling (in the unit of kg/ha) based on the information conventionally provided on a pesticide product label. Figure 7 shows an example of the calculation based on the same input data as previously demonstrated in the PREM5 user's manual (Luo et al., 2019).
3) "View VFS modeling results": this function is only enabled after a successful model simulation with a vegetative filter strip (VFS). See Section 11.3 for more information.
4) "WQC for copper in freshwater": this function calculates the water quality criteria (WQC) for copper in freshwater based on user-specified characteristics in a water body (Figure 8).
5) "Delete the selected chemical": delete the user-selected chemical from the model database.
6) "View Help": open the user's manual (this document) in a PDF reader.
7) "About": display general information of this model and included USEPA models. This tool is also used to setup additional models for external users (See Section 3 for more information).

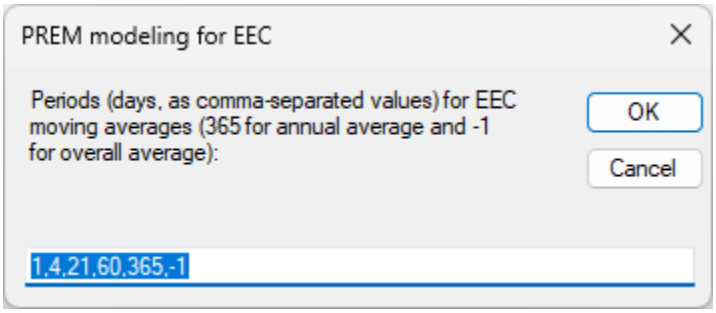


Figure 6. Moving average periods for EECs

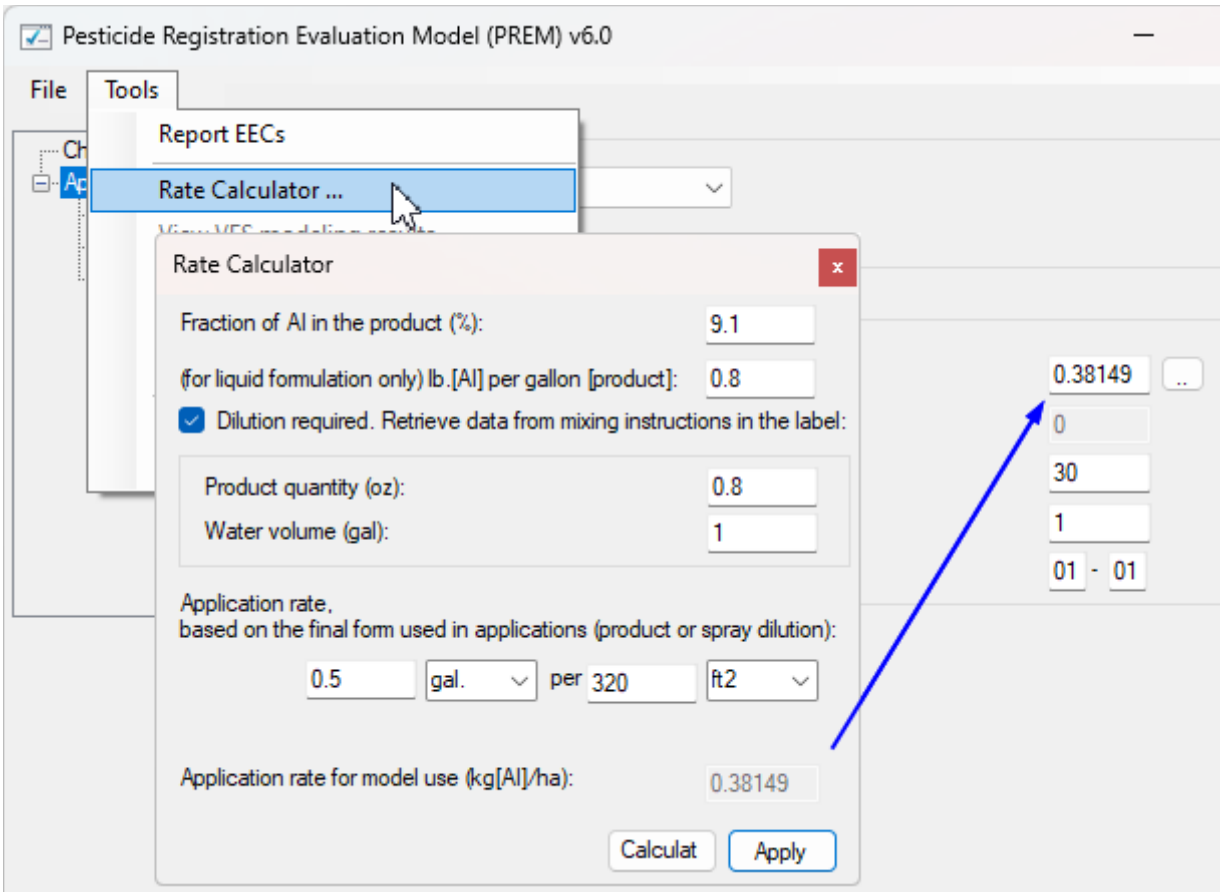


Figure 7. Application rate calculator in PREM

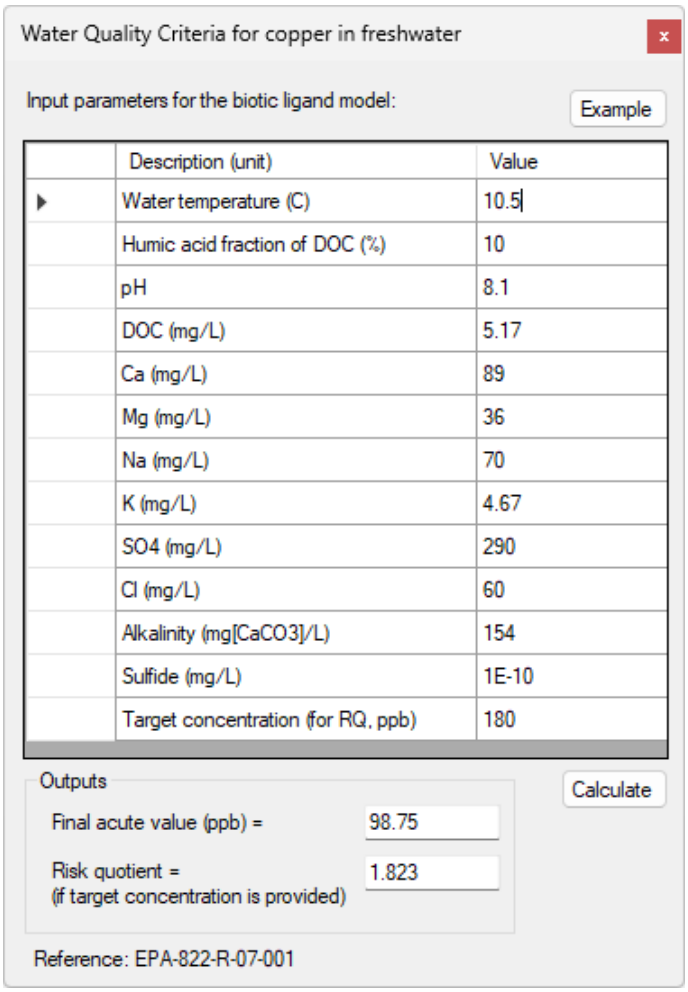


Figure 8. PREM6 function for water quality criteria for copper in freshwater

4.3 Navigation panel

Model input data and settings are grouped by tabs which can be navigated by selecting the corresponding menus on the left panel (Figure 3). When the program is initiated, only two tabs of "Chemistry" and "Application" are available. Other tabs will be activated by user-selected model options. For example, if a user selects "urban outdoor use" as the use pattern, the "Urban" panel will be become available for additional input data for the urban outdoor uses.

Table 2. Summary of the tabs for model inputs and options in PREM6

Tab	Description	Availability	Details in
Chemistry	Physicochemical properties, toxicity data, parent and degradates for modeling	Always enabled	Sections 5 to 7
Application	Pesticide use pattern, application data (rate, timing, frequency, etc.)	Always enabled	Section 8
Rice	Additional parameters for rice pesticides	Rice pesticides	Section 9
Urban	Additional parameters for urban outdoor uses	Urban outdoor uses	Section 10
Agriculture	Additional parameters for agricultural applications	Terrestrial crops	Section 11

5 Environmental fate and toxicity data ("Chemistry" tab)

The viewer/editor (Figure 9) for pesticide environmental fate and toxicity data is developed for two purposes: [1] to edit model input data for the chemicals under evaluation, including the active ingredient (AI) and its degradates; and [2] to set the parent compound for evaluation (the chemical shown in the pull-down menu before a model run is considered as the parent compound).

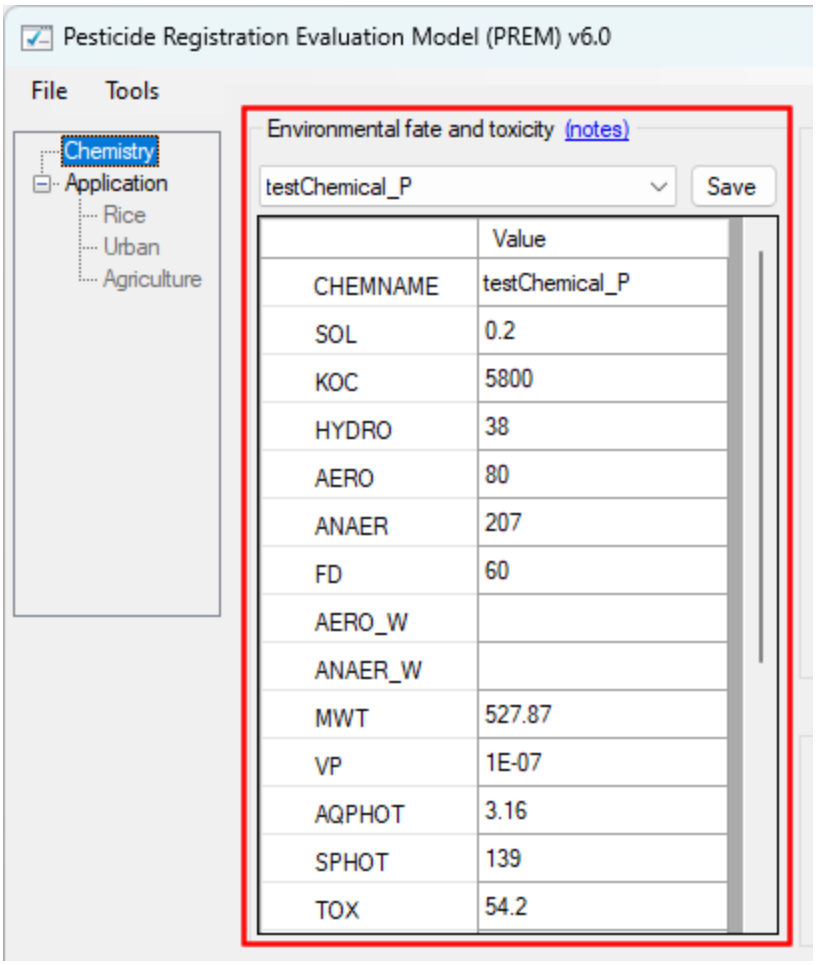


Figure 9. Editor for physicochemical properties and toxicity data of pesticides

Table 3 summarizes the input parameters, descriptions, and units required by PREM6 for physicochemical properties and toxicity data. The same information is also available by clicking the text "notes" on the program (Figure 10). A user is asked to prepare representative values for the parameters based on the data submitted by registrants and reviewed by CDPR's Pesticide Registration Branch. Detailed instructions are provided in the Section 13 "*Guideline for physicochemical and toxicological data preparation*". Care must be taken when selecting input values including their units.

Table 3. Model input parameters for physicochemical properties and toxicity of pesticide

Input parameter	Description	Unit
CHEMNAME	chemical name	-
SOL	water solubility	ppm
KOC	organic carbon (OC)-normalized soil adsorption coefficient	L/kg[OC]
HYDRO	hydrolysis half-life	day
AERO	aerobic soil metabolism half-life	day
ANAER	anaerobic soil metabolism half-life	day
FD	field dissipation	day
AERO_W	aerobic aquatic metabolism half-life	day
ANAER_W	anaerobic aquatic metabolism half-life	day
MWT	molecular weight	g/mol
VP	vapor pressure	torr
AQPHOT	aqueous photolysis half-life	day
SPHOT	(*only needed for urban outdoor uses*) soil photolysis half-life	day
TOX	the lowest acute toxicity value in water	ppb
TOXSED	the lowest toxicity value in sediment or pore water	see below
TOXSED_UNIT	index for the unit of sediment toxicity data: 1=µg/kg[dry mass of sediment]; 2=µg/L[pore water]; and 3= µg/g[OC]	-
DK's	(*only needed for degradates*) molar formation fraction, by parent degradation pathways: water column degradation (DKW), benthic degradation (BKD), aqueous photolysis (DKP), hydrolysis (DKH), soil degradation including metabolism and photolysis in the soils (DKS), and foliar degradation (DKF)	-

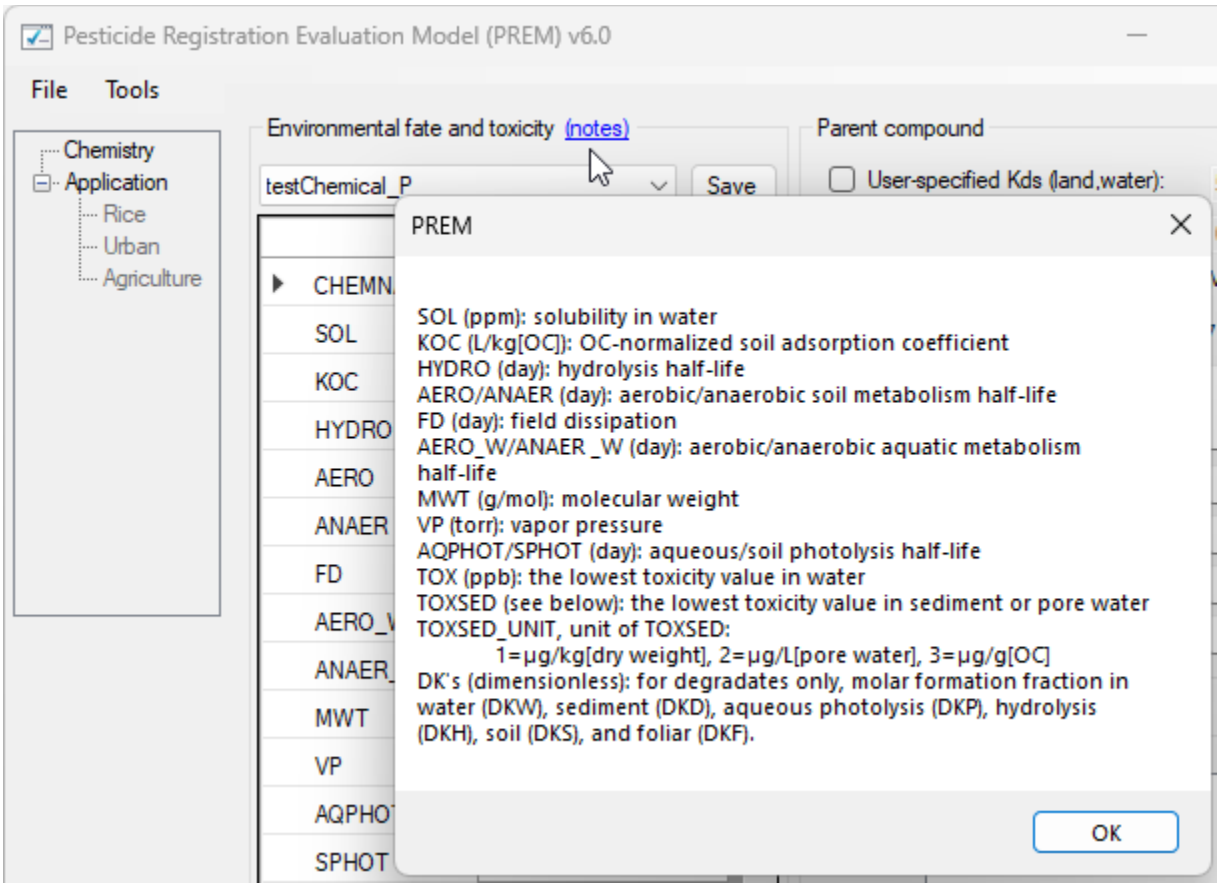


Figure 10. Descriptions of the model input parameters

5.1 View and edit data for an existing chemical in the database

Use the pull-down menu to show the chemicals with data available in the model database (Figure 9). Data can be retrieved by selecting the chemical name in the list. Except for the chemical name, all data cells are editable. Blank cells are acceptable for half-lives, indicating that the half-life value is not available or stable. This will be numerically modeled by PREM6 with a large number of 99,995 days (Section 13.4 "*Missing data handling*"). Scientific notation is allowed in the data viewer/editor, and encouraged for smaller values, e.g., "1e-4" or "1E-4" for "0.0001".

It is critical that the users verify the data values and make changes as needed before the model simulations. After all changes have been made, confirm the changes by clicking "Save" (Figure 9). If unsaved changes are detected, the model will show a warning message.

5.2 Delete a chemical from the database

Select a chemical from the pull-down menu and use the "Delete a chemical" in the "Tools" menu (Figure 5) to delete it from the database.

5.3 Add a new chemical to the database

If the chemical (parent AI or degradate) to be evaluated is not in the database, a user can create a new data entry (Figure 11). The chemical name should be unique in the database. The chemical name is not used in the model simulation but as an index for data management and model results reporting. In PREM6, a chemical name is not case-sensitive. Space and comma are not allowed in the chemical name (those characters are commonly used as a text delimiter). Renaming a chemical is not allowed. Instead, a user could add a new chemical with the preferred name.

After the new chemical has been assigned a name, a new data entry is created and users can type in values for the input parameters. Refer to Section 5.1 for editing and saving the data.

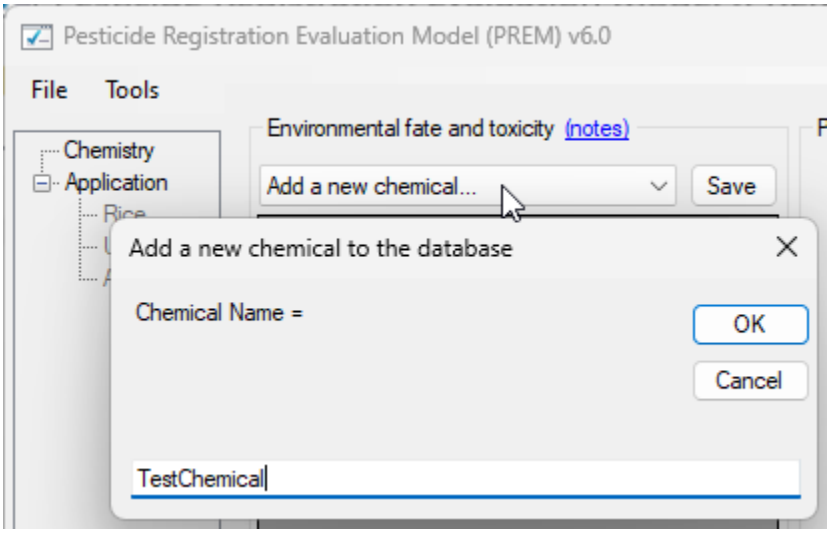


Figure 11. Create a data entry for a new chemical in the database

6 Additional chemistry data and options ("Chemistry" tab)

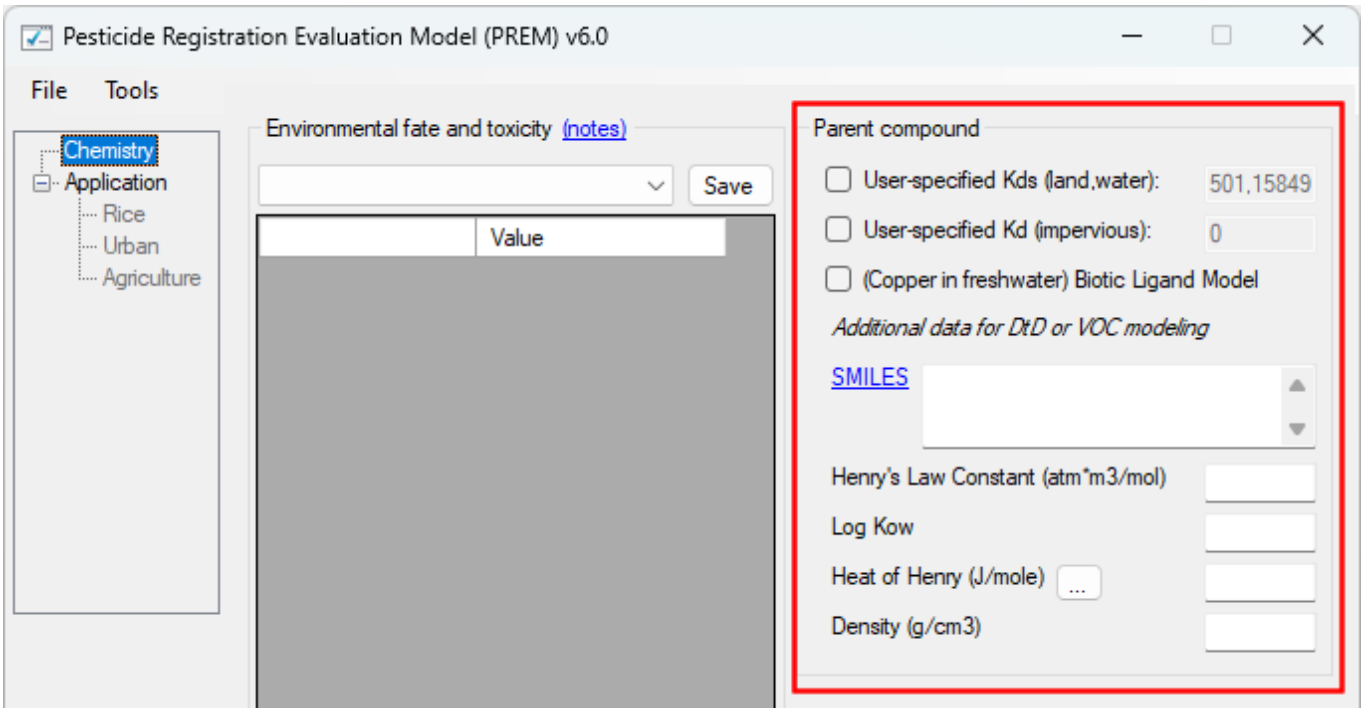


Figure 12. Advanced modeling options and additional input data for the parent compound

PREM6 allows advanced modeling options and additional chemistry input data which can be used to refine the evaluations on some pesticide products:

1) User-specified partition coefficients (Kds) for land and water. These parameters are used for metals (copper, silver, etc.) and other pesticides for which the partition coefficient is only reported as Kd or the adsorption process better represented by Kd compared to KOC value. Use a comma to separate the input values for land and water. For example, the input string "501,15849" (suggested input for copper) indicates Kd=501 L/kg for landscape simulations and 15,849 in receiving waterbody (Allison and Allison, 2005).
2) User-specified Kd for impervious surfaces. This parameter is used for pesticides with effective partition coefficient on impervious surfaces determined from field experiments. The default value of this parameter is set to be zero in PREM6, and could be refined with a user-specified input by using this option.
3) Biotic Ligand Model for copper in freshwater. With this option, PREM6 will adjust copper toxicity to freshwater aquatic organisms according to site-specific chemical constituents that can limit bioavailability of copper by either complexing or competing with copper. The EECs of copper will be compared to the adjusted copper toxicity, rather than the user-specified value (TOX in Table 3).
4) SMILES (simplified molecular-input line-entry system) is a specification in the form of a line notation for describing the structure of chemical species. In PREM6, SMILES is used for estimating the pesticide removal efficiency through a wastewater treatment plant (WWTP) in the evaluation of DtD products. Based on the PubChem web services,

PREM6 will automatically retrieve the SMILES of a pesticide according to its name specified on the interface (Figure 9). Users could also manually input the SMILES.

5) Henry's Law Constant (HLC, atm×m^3/mol) and $LogK_{OW}$ are optional but recommended parameters for estimating WWTP removal efficiency. PREM6 could complete the estimation without one or both of the two parameters but the results would be refined if they are provided. The following procedures are implemented in PREM6 to prepare the model input data for DtD products:
    a. If the value of WWTP removal efficiency is specified by a user (see Section 8.4 for more information), PREM6 will directly use the provided value for evaluation and thus not need the parameters of SMILES, HLC, or $logK_{OW}$.
    b. Otherwise, if the removal efficiency is to be estimated, PREM6 will check the availability of SMILES, HLC, and $logK_{OW}$ on the interface. If the SMILES is not provided by a user, PREM6 will retrieve it according to the chemical name. If the values for HLC and/or $logK_{OW}$ are not provided, PREM6 will show a message to remind the user (Figure 13).
6) HLC, Heat of Henry (J/mole), and density (g/cm^3) are the required parameters for volatile compounds. Once the pesticide is detected to be volatile (VP ≥ 3.75 torr), PREM6 will ask the user to provide these parameters (Figure 14), which will be used to estimate the air diffusion coefficient. If a user chooses not to provide the required parameters (i.e., select "No" in Figure 14), the pesticide will be modeled as a non-volatile component. HLC and density are usually available in the submitted data volumes while there is no simple approach to estimate Heat of Henry. As recommended by USEPA (Rothman et al., 2015; Young, 2016), it can be estimated via the Estimation Program Interface (EPI) Suite (USEPA, 2012) with some manual processes as summarized in Appendix I.

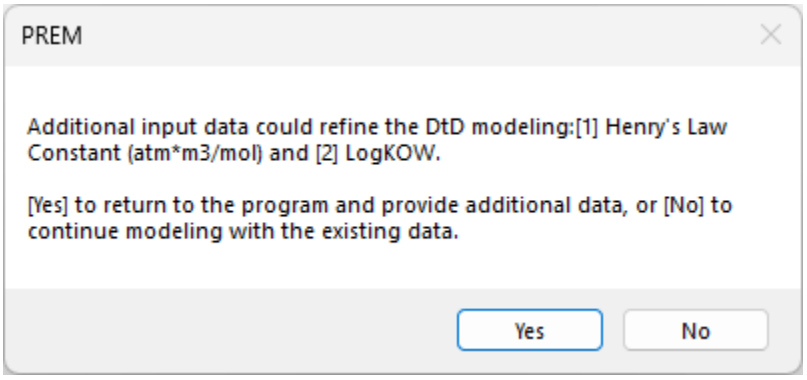


Figure 13. Optional but recommended parameters to refine DtD evaluations

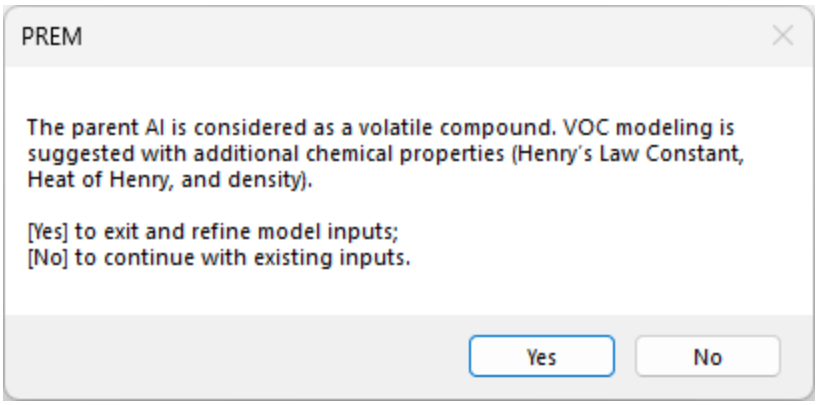


Figure 14. Required parameters for evaluating volatile compounds

7 Degradate evaluation

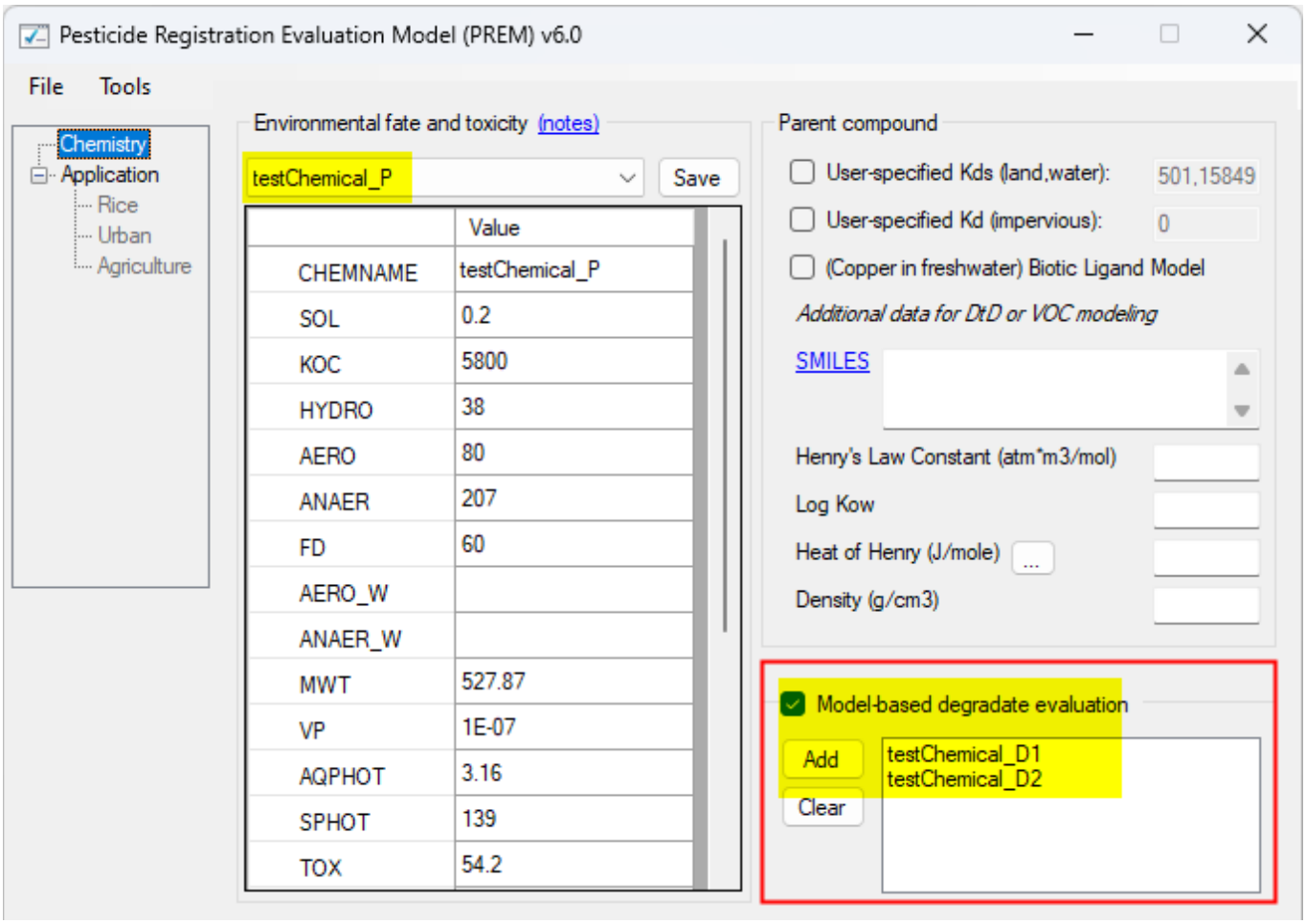


Figure 15. Example of model settings for degradate evaluation (The parent compound is selected in the data viewer/editor, while the degradates for modeling are specified under the option for "model-based degradate evaluation" by using the "Add" button)

The degradate evaluation can be enabled by checking the option for "Model-based degradate evaluation" and specifying the degradates to be modeled (Figure 15). Before the evaluation, the degradates of interest should be added to the database by following the same procedure for adding a parent compound (see Section 8).

A three-step procedure has been developed for evaluating pesticide degradates. The model will handle steps 1 and 3, but step 2 (input data preparation and data analysis for degradates) should be conducted by a model user.

Step 1: Evaluation for the parent compound only, by *unchecking* the option for degradate evaluation. After the evaluation on the parent, the model will also conduct initial screening for its degradates, and provide suggestions for the next step of evaluation:

1) A warning message will show if there are degradates that have high potential to cause aquatic toxicity (Figure 16).
    a. If the modeling results for the parent compound are not to support registration, degradate evaluation is not required. But the initial screening results for the degradates should be included in the evaluation report.
    b. If the modeling results for the parent compound are to support or conditionally support registration, *continue to Step 2* for additional considerations.
2) Otherwise, if there is no warning message for pesticide degradates at the end of the evaluation, degradate evaluation is not required.

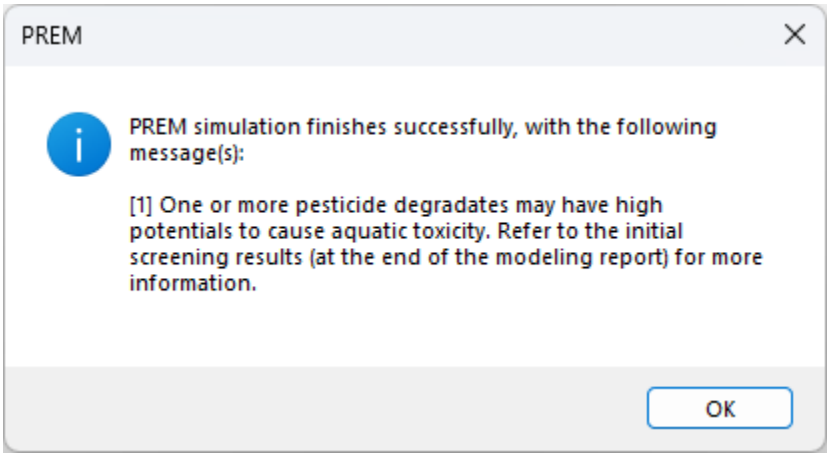


Figure 16. Warning message for potential degradate evaluation

Step 2: Data collection and analysis for degradate toxicity by following the *results of initial screening* for degradates. In the modeling report ("PREM.txt"), the initial screening results include the candidate degradates (by degradation pathways) and associated criteria for potential model-based evaluations (Figure 17). For each of those degradates, toxicity data (water toxicity, and sediment toxicity if its KOC >1000) are needed. If toxicity data are not available from CDPR's ecotoxicology evaluation reports, SWPP will **presume that the data do not support registration** and **request the registrant to submit additional toxicity data**. Details on the data needed for degradate evaluation are provided in Table 2 of the technical report for degradate

evaluation (Luo et al., 2016). Only degradates with toxicity data meeting the criteria reported in the initial screening (e.g., “if they are highly toxic” or “if they are more toxic than the parent compound.”) will *be modeled in Step 3*.

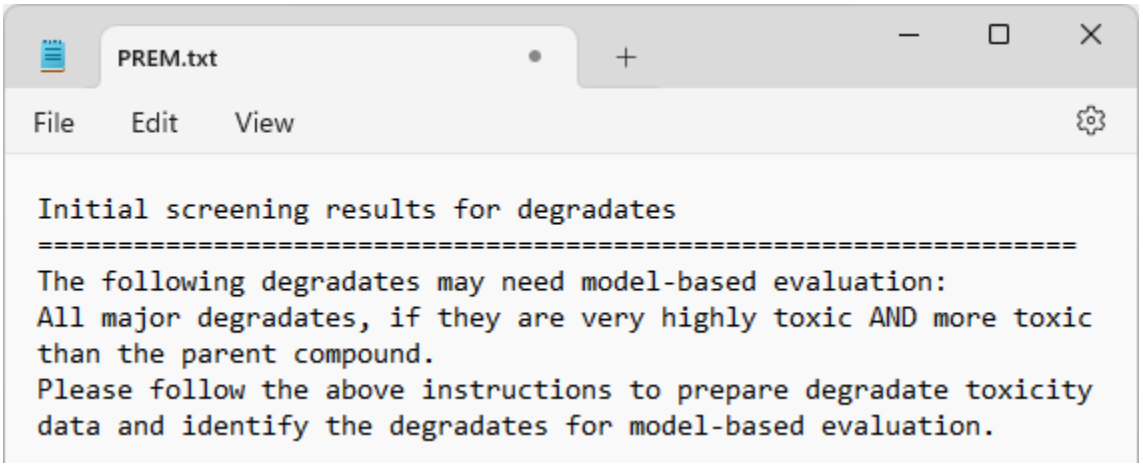


Figure 17. Example of modeling results for parent-only evaluation and initial screening for degradates

Step 3: Model-based evaluation on degradates identified in the previous step.

1) Prepare model input data for the degradates to be modeled by following the guideline in Section 13.
2) Create data entries for the degradates with physicochemical properties and toxicity data (see Section 5.3 “Add a new chemical to the database”).
3) Select the parent compound in the data viewer/editor (Figure 9), and fill all required input data (use pattern, application info, etc.) for the parent compound.
4) Check the option for “Model-based degradate evaluation” and add the degradates to be modeled (Figure 15).
5) Run the model for the combined evaluation of the parent compound and selected degradates.

8 Pesticide use pattern and application data (“Application” tab)

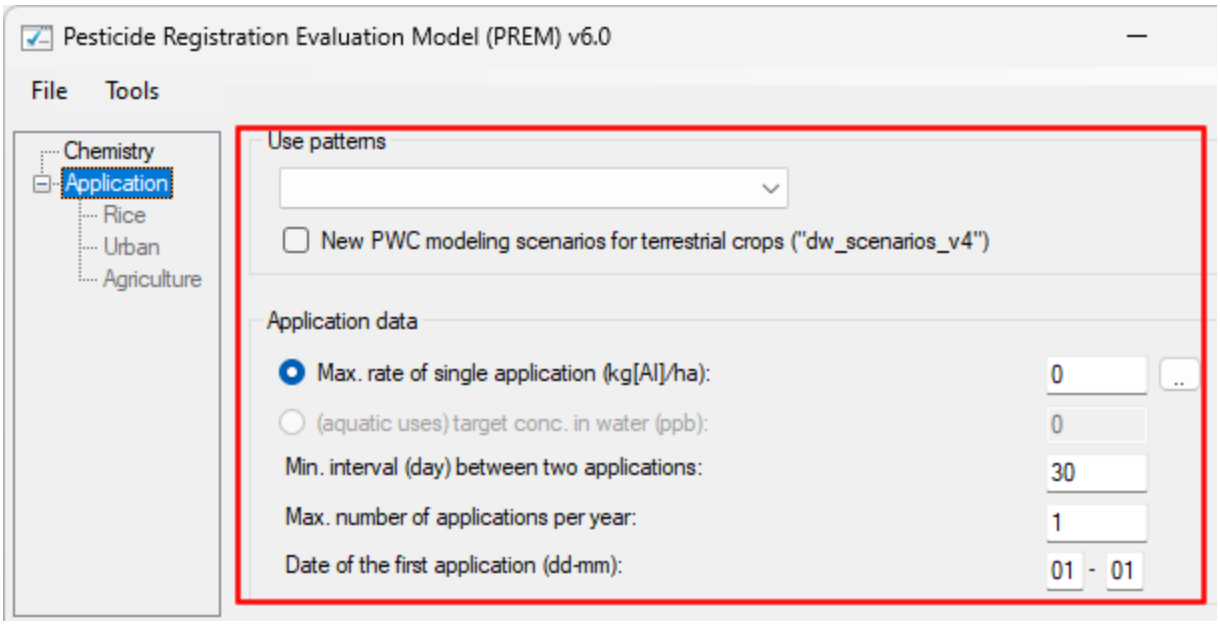


Figure 18. Pesticide use pattern and application data in PREM

8.1 PREM6 standard use patterns

Carefully inspect the application instructions on the product label and summarize the proposed use patterns. If the pesticide product is associated with the listed high-risk use patterns (Figure 19), select the use pattern as a modeling scenario. If more than one listed high-risk use patterns are proposed on the product label, each of them needs to be modeled separately. Otherwise, if none of the use patterns on the label are listed as high-risk patterns, select “Low-risk use pattern” for modeling (the first item in the dropdown menu, Figure 19). For example, if two high-risk use patterns and some low-risk use patterns exist on the label, a user only needs to model those two high-risk use patterns.

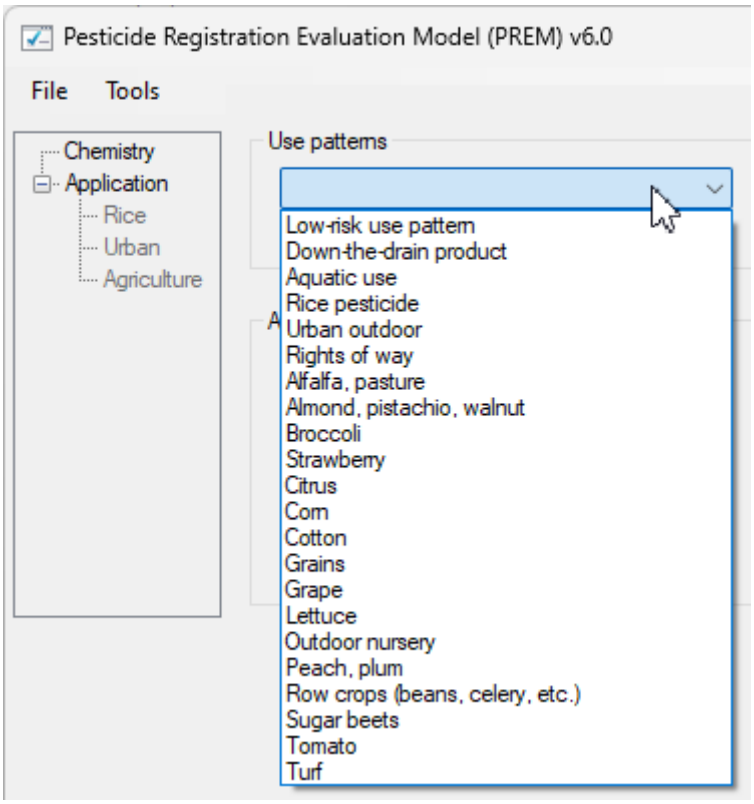


Figure 19. Standard use patterns for modeling in PREM6

When a use pattern is selected from the dropdown menu, PREM6 will provide additional information for users to schedule the applications, usually based on the crop growth calendar incorporated in the corresponding modeling scenarios. In addition, a default date will be set to the first application, which is January 1 for aquatic and urban outdoor uses, or the emergence date of a crop to be modeled. For example, the following message box (Figure 20) will prompt if the use pattern is set as “rice pesticide” and the date of the first application is initiated as May 23, i.e., the date of rice emergence predefined in the modeling scenario.

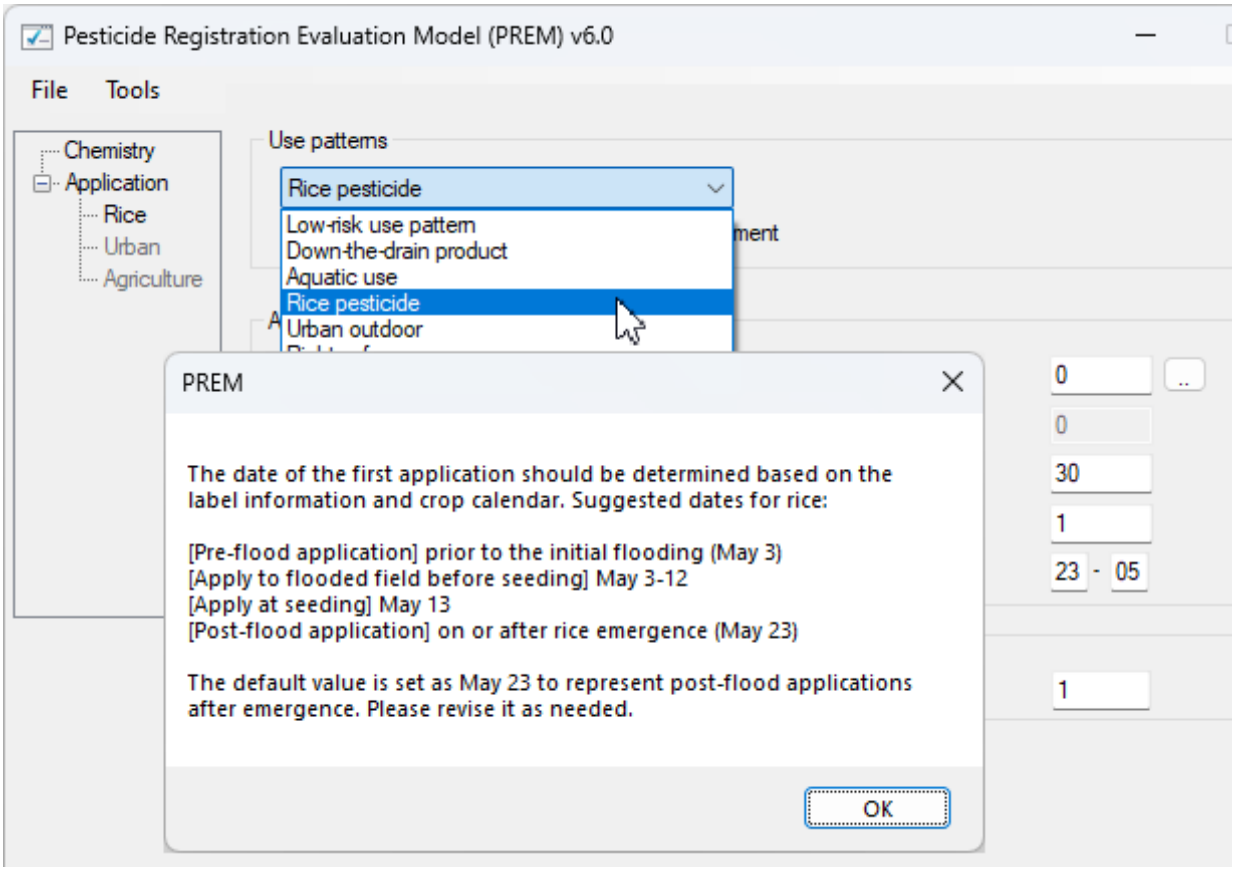
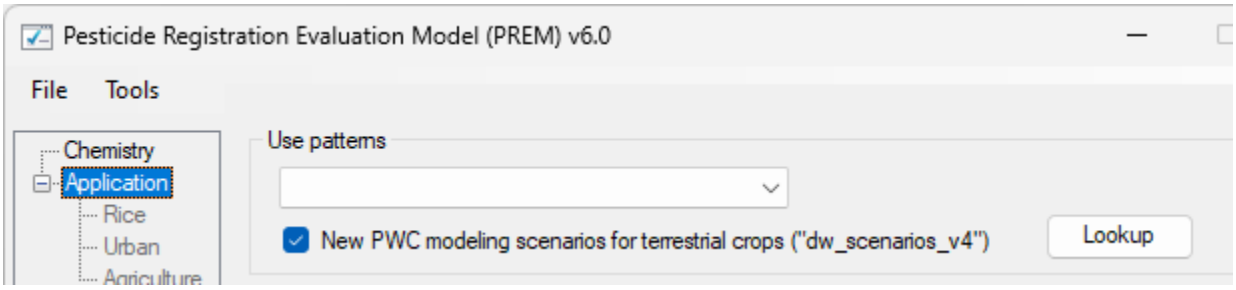


Figure 20. Message for rice pesticides selected as the use pattern for modeling, and the default date of May 23 is assigned to the data of the first application

8.2 New PWC modeling scenarios for terrestrial crops

For terrestrial cultivated crops, in addition to the standard use patterns, PREM6 has the capability to use the new PWC modeling scenarios recently released by USEPA (2023) (Figure 21).

(a)



(b)

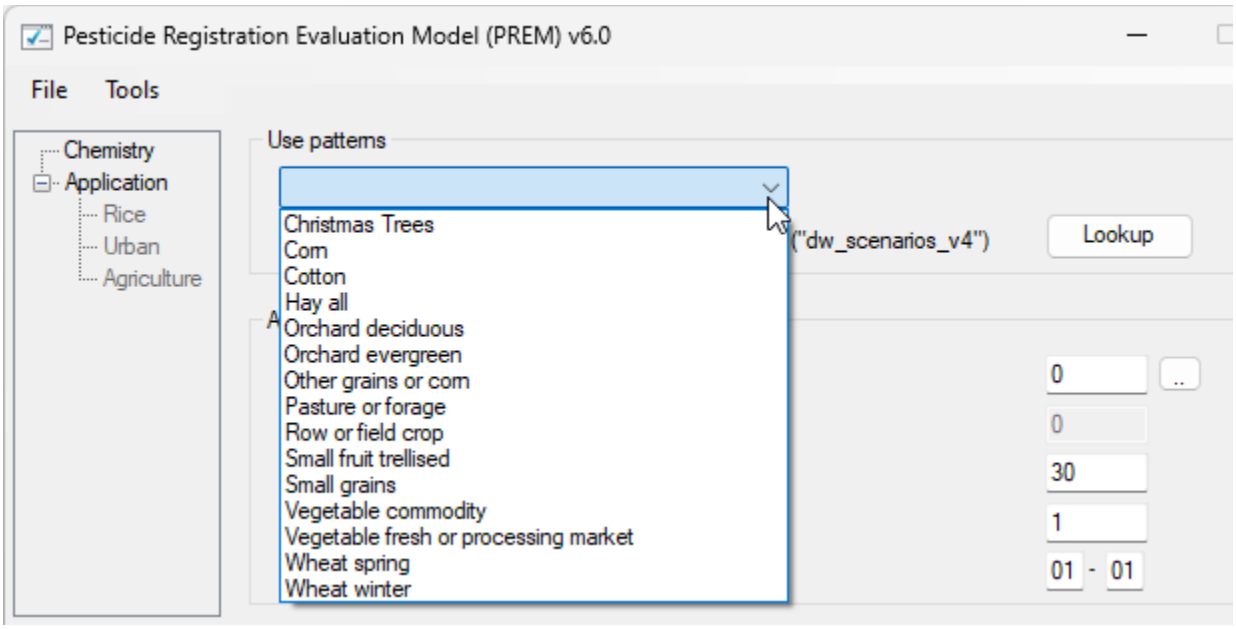


Figure 21. New PWC modeling scenarios

The new modeling scenarios for Pesticide in Water Calculator (PWC) were developed based on the crop classifications in the Cropland Data Layer (CDL) (USEPA, 2020a). PREM6 provides a "lookup" tool to relate a crop to its recommended modeling scenario (Figure 22). A user can retrieve the recommended modeling scenario by browser the list or searching by CDL name or code.

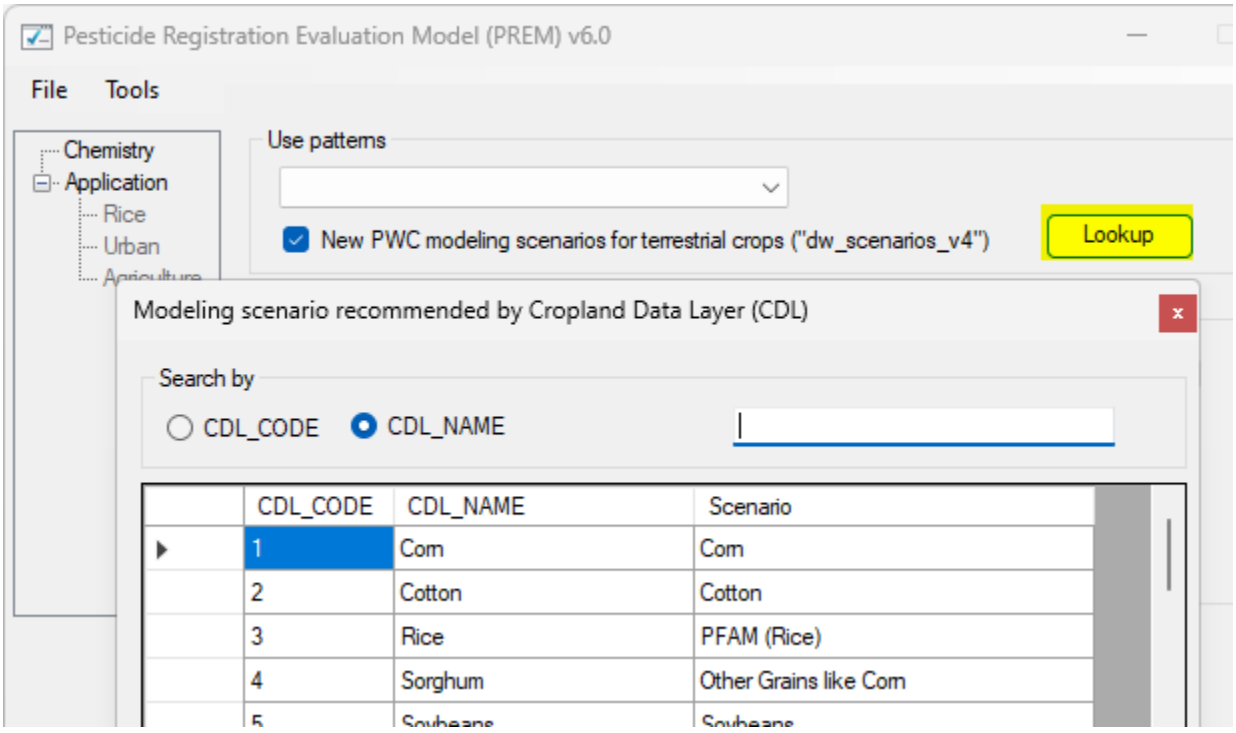


Figure 22. Relating the CDL key to its recommended modeling scenario

The new scenarios do not sufficiently cover all use patterns modeled by PREM6. Therefore, they are only used in PREM6 to refine the modeling results for registration evaluations on pesticide products for use on terrestrial cultivated crops under the following conditions: (1) Modeling results with the standard use patterns do not support registration. In this case, the modeling results based on the new PWC scenarios will be reported. (2) Registration evaluation on a new AI for which none of the proposed use patterns is identified with high-runoff potentials (i.e., not listed in the standard use patterns, Figure 19).

8.3 Application data for low-risk use patterns

Application data are not needed for low-risk use pattern.

8.4 Application data for down-the-drain products

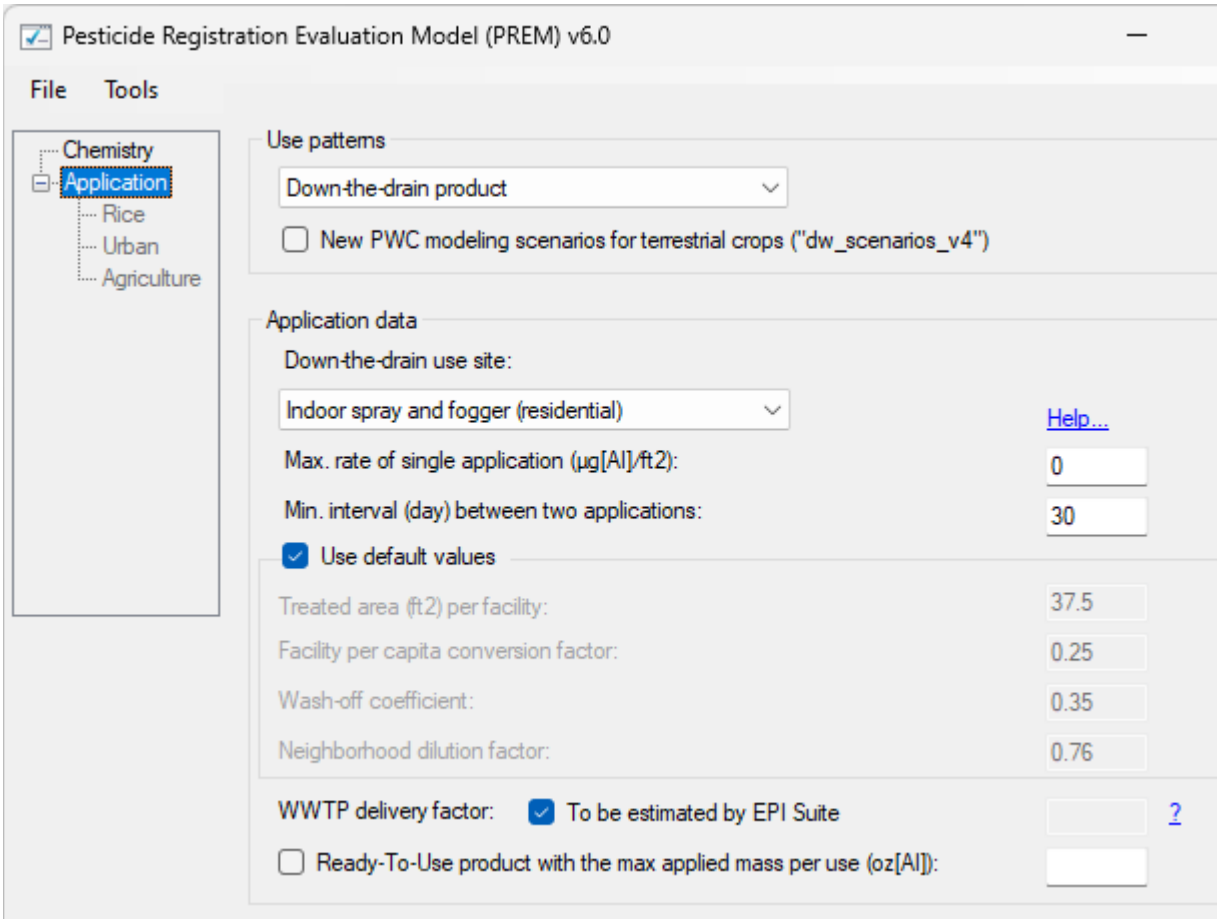


Figure 23. Application data for down-the-drain product, showing the available parameters and options for the use site of "Indoor spray and fogger (residential)" as an example

In addition to the chemistry data (including SMILES, Henry's Law Constant, and $\log K_{OW}$, see sections 5 and 6), the following input data sets are required for PREM6 evaluation of DtD

products: (1) DtD use site (select from a pull-down menu, such as “Floor drains”), (2) the maximum application rate (µg/subject or µg/ft^2) and minimum interval (days), and (3) a set of coefficients.

Use sites

PREM6 models nine use sites for DtD products (Figure 24). Based on the previous registration evaluations by SWPP, these sites are associated with high wash-off potentials to sewer systems and thus required for model-based evaluations. Note that not all indoor uses of pesticides are considered to be high-risk patterns. For example, ear tags, collars, and bait stations/gels, which have relatively low wash-off potentials and low risks to surface water, should be modeled as “low-risk” use patterns (Figure 19).

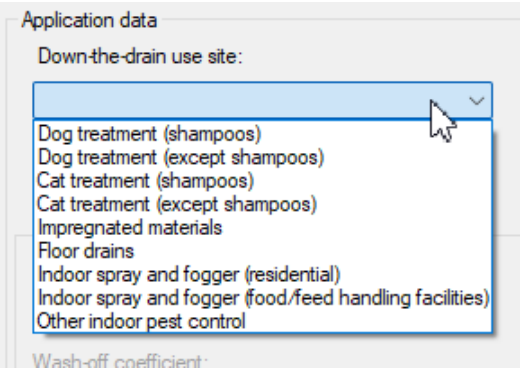


Figure 24. Use sites modeled in PREM6 for down-the-drain (DtD) products

The use sites to be modeled by PREM6 can be categorized in two groups according to the application rate derived from the product label: [1] rate in applied mass per subject (e.g., per dog, per treated article, or per drain), and [2] rate in applied mass per unit area (e.g., µg/ft^2 for indoor spray and fogger). Once a use site is selected, the model interface will be adjusted accordingly, including the descriptions, default values, and related input data and options (Table 4). For example, with “Indoor spray and fogger (residential)” selected as the use site for modeling, the unit of application rate will be changed to “µg[AI]/ft^2” (Figure 23). In addition, the default model input values are provided, if applicable, for treated area, conversion factor, wash-off coefficient, and dilution factor (Figure 23). See the next section for more information on the default values.

Table 4. Use sites and associated model settings for DtD products

PREM6 use sites	Label use patterns	Unit of appl. rate	Default settings?
Dog treatment (shampoos)	Shampoos for dogs and puppies	µg[AI]/dog	Yes
Dog treatment (except shampoos)	Spot-on/powder/spray/lotion for dogs and puppies	µg[AI]/dog	Yes
Cat treatment (shampoos)	Shampoos for cats and kittens	µg[AI]/cat	Yes
Cat treatment (except shampoos)	Spot-on/powder/spray/lotion for cats and kittens	µg[AI]/cat	Yes
Impregnated materials	Pesticide treated fabrics, fibers, clothing, and washable textiles, garments, and gear	µg[AI]/subject	No
Floor drains	Floor drains (to sewer)	µg[AI]/drain	Yes
Indoor spray and fogger (residential)	Indoor applications such as bed bugs, furniture, carpets, floors, and pet bedding	µg[AI]/ft^2	Yes
Indoor spray and fogger (food/feed handling facilities)	Indoor applications at food/feed handling facilities	µg[AI]/ft^2	Yes
Other indoor pest control	At the discretion of Registration Branch or by request of outside stakeholders. Examples include drinking water treatment and animal housing (e.g., professional dog kennels)	µg[AI]/ft^2	No

Note: see Table 5 for the default values of modeling inputs for DtD products predefined in PREM6

Application data and coefficients

PREM6 uses a set of modeling coefficients for DtD evaluation. For most of the use sites, default values for the coefficients have been developed based on the previous registration evaluations by SWPP (Xie and Luo, 2022) and the same processes of parameterization can be used to characterize a new site for modeling. Once a use site is selected, the available default values will be assigned to the associated coefficients. Table 5 summarizes all default values in PREM, and Figure 23 shows an example of the default values for the use site of "Indoor spray and fogger (residential)".

Table 5. Default values of the modeling coefficients predefined in PREM

Down-the-drain use site	Treated area (ft^2)	Subject per capita conversion factor	Washoff coefficient	Neighborhood dilution factor
Dog products (shampoos)	NA	0.22	1	0.07
Dog products (except shampoos)	NA	0.22	0.21	0.07
Cat products (shampoos)	NA	0.25	1	0.05
Cat products (except shampoos)	NA	0.25	0.21	0.05
Impregnated materials	NA	User	User	User
Floor drains	1	0.19	1	0.76
Indoor spray and fogger (residential)	37.5	0.25	0.35	0.76
Indoor spray and fogger (food/feed handling facilities)	269.1	0.02	0.35	0.76
Other indoor pest control	User	User	User	User

Notes: "NA" = the treated area is not appliable to pet products and impregnated materials (Table 4). "User" = no default value, need user's input. See Xie and Luo (2022) for examples of user-specified values.

No default values are provided for the site category of "Other indoor pest control" which involves various use patterns and application methods. For some use patterns in this category, input parameters have been prepared in the previous evaluations and could be considered for future evaluations on the similar products. For example, the following set of parameters have been used for evaluating indoor pest control in professional dog kennels (Budd, 2019; Xie, 2022): treated area (ft^2) = 837, subject per capita conversion factor = 1.07E-5, wash-off coefficient = 1, and neighborhood dilution factor = 0.76

If there are registrant-submitted data available for any of the coefficients specific to the product under evaluation, the submitted data, after the data review by CDPR, should be used to replace the default values. Default values can be changed by unchecking the option to "Use default values" (Figure 23).

If the value for a coefficient is not available after considering all data in the registration data volumes and estimates by PREM6, SWPP will use conservative estimations or request additional data from the registrant.

WWTP delivery factor

The WWTP (wastewater treatment plant) delivery factor is the ratio of pesticide mass between influence and effluence. Mathematically, [delivery] = 1- [removal]. For example, if the WWTP removal efficiency is 0.8 for a pesticide, the corresponding delivery factor is 0.2.

PREM6 provides two options for the delivery factor, manual input or automatic estimation by EPI Suite (the option "To be estimated by EPI Suite", Figure 23). Estimation by the EPI Suite is

generally recommended. The input parameters required and recommended for the estimation include SMILES, Henry's Law Constant, and logK_{OW}. See Section 6 for more information. The EPI Suite actually estimates the removal efficiency, which is further converted to the delivery factor by PREM6 for use in the model. Manual input for user-provided value is more suitable for inorganic pesticides (which cannot be modeled by the EPI Suite) or pesticides with given removal efficiencies. For example, the removal efficiency of 0.72 (thus, the delivery factor = 0.18) has been used in the previous SWPP evaluations for copper pesticides.

Adjustment on residential indoor spray with RTU products

The option of Ready-To-Use (RTU) product adjustment (Figure 23) is provided for the use site of "indoor spray and fogger (residential)". The implied assumption is that, a residential user does not have to treat all potential treatable areas, but only use one container of the RTU product for each application. With the option, PREM6 will adjust the application data according to the coverage area of the user-specified applied mass (oz[AI]). The applied mass is calculated from the total product mass (oz[product] in one container) and AI percentage ([AI]% in the product) shown on the label.

8.5 Application data for aquatic uses

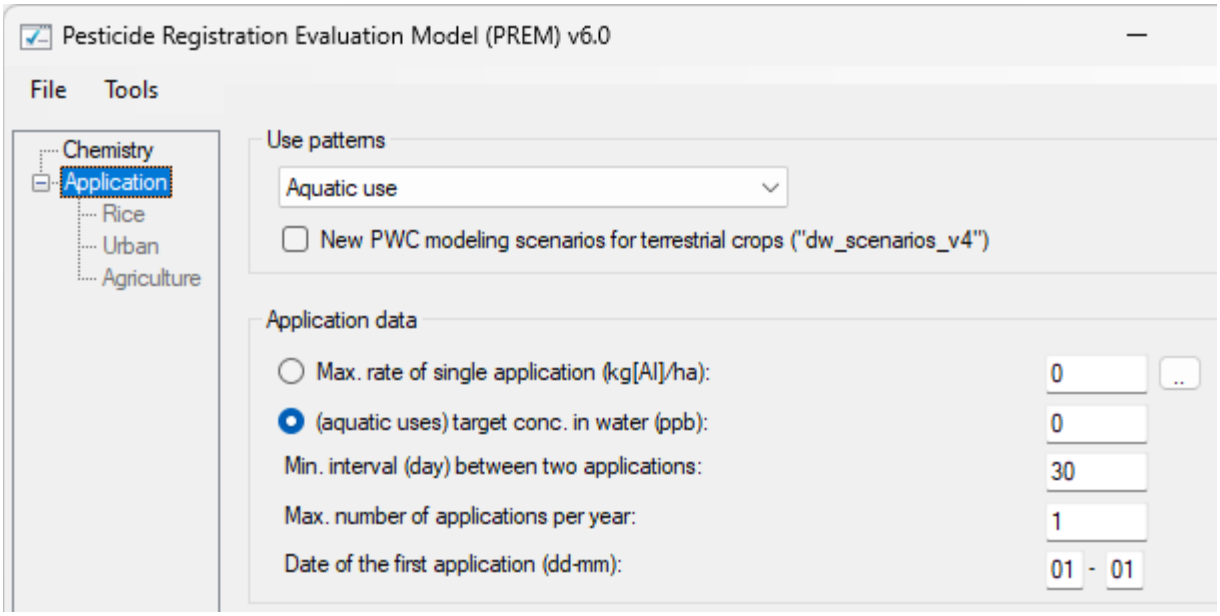


Figure 25. Application data for aquatic uses

Pesticide products for aquatic uses can be evaluated based on either application rate (kg[AI]/ha) or target concentration (ppb) (Figure 25). Other application data required by PREM6 include the minimum application interval (day), the maximum number of applications per year, and the date of the first application. The default date of the first application is set to be January 1 for aquatic uses.

8.6 Application data for rice pesticides

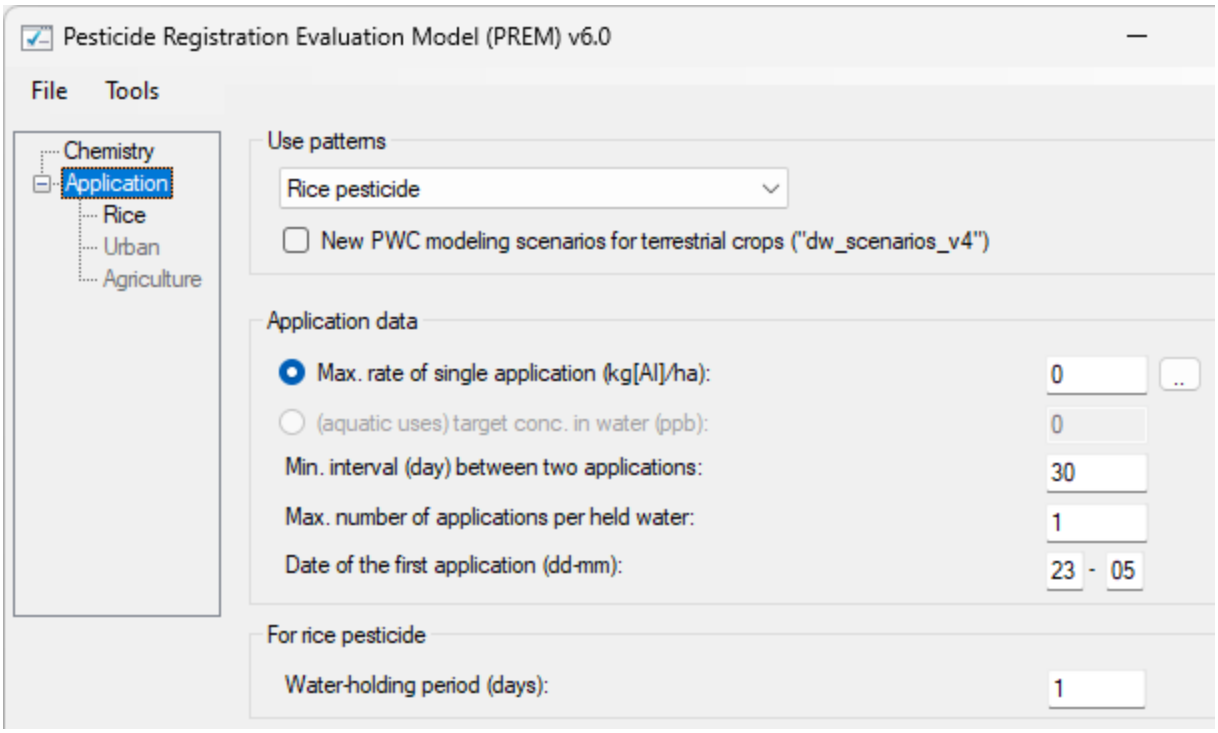


Figure 26. Application data for rice pesticides

For rice pesticide applications, it's required to hold water for a certain number of days (i.e., the water-holding period) after the last application and after the paddy is flooded. In addition to the application rate and schedule, therefore, rice pesticide evaluation also requires a water-holding period (Figure 26). If the period is not specified on the product label, water holding for one day is modeled for conservative estimation.

The date of the first application is used in PREM6 to identify the type of rice pesticide applications: pre-flood or post-flood applications. According to the default modeling scenario for California rice, applications prior to May 3 are modeled as pre-flood applications, and those on or after May 23 are modeled as post-flood applications. The default date is set to be May 23, representing a post-flood application (Figure 27). The date should be changed if the pesticide is proposed for pre-flood applications, e.g., to be used prior to flooding or after a field is drained. For pre-flood application, the date of application is determined based on the minimum dry period required on the label. For example, the statement that "*water must not be reapplied to the field for a minimum of 24 hours following the application*" suggests a 1-day dry period after the pre-flood application, and the date of application could be set to be May 1.

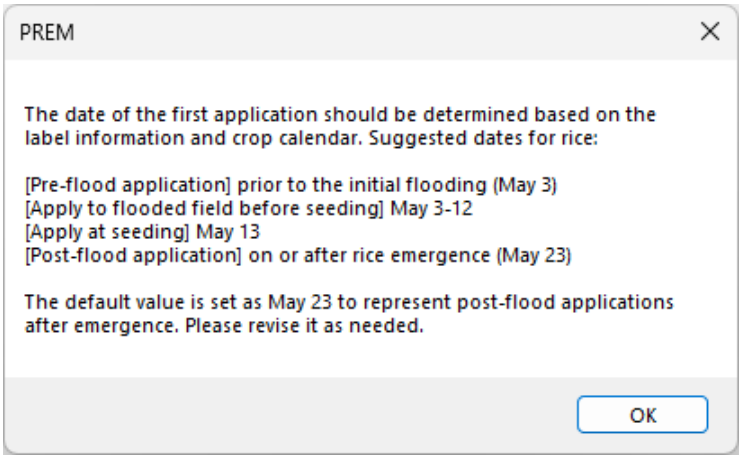


Figure 27. Message for the use pattern of a rice pesticide

8.7 Application data for other use patterns

Other use patterns (urban outdoor, right-of-way, and terrestrial crops including the new PWC scenarios) require the same set of basic application data (Figure 28), including the maximum rate of single application (kg[AI]/ha), the minimum interval (day) between two applications, the maximum number of applications per year or season, and the date of the first applications. Use the "Rate Calculator" in the "Tools" menu to determine the application rate if it is not explicitly provided on the label (Section 4.2).

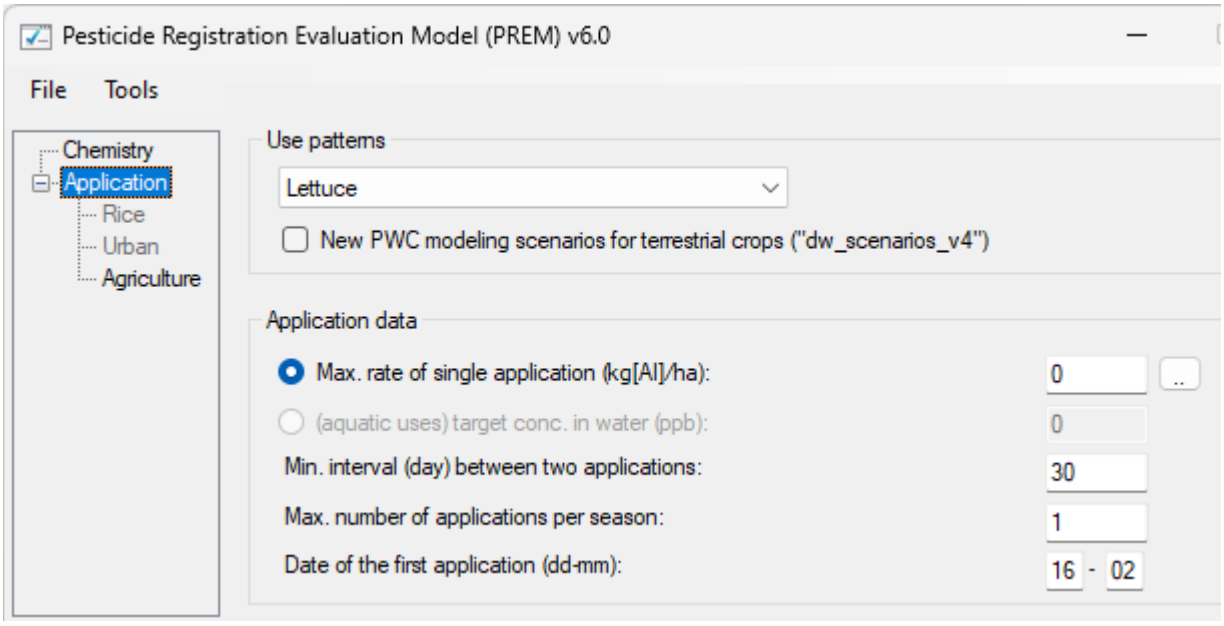


Figure 28. Application data for pesticide uses on urban outdoor, right-of-way, and terrestrial crops

When a user selects a use pattern for modeling, a default date will be set to the first application, which is the emergence date of the crop to be modeled. For example, if the use pattern is set as "Lettuce", the date of the first application is initiated as February 16, i.e., the date of lettuce emergence predefined in the modeling scenario (Figure 28). PREM6 also provides other critical dates (maturity and harvest) in the modeling scenario to help a user to adjust the application timing if the pesticide is proposed to be applied to other stages of crop growth (Figure 29).

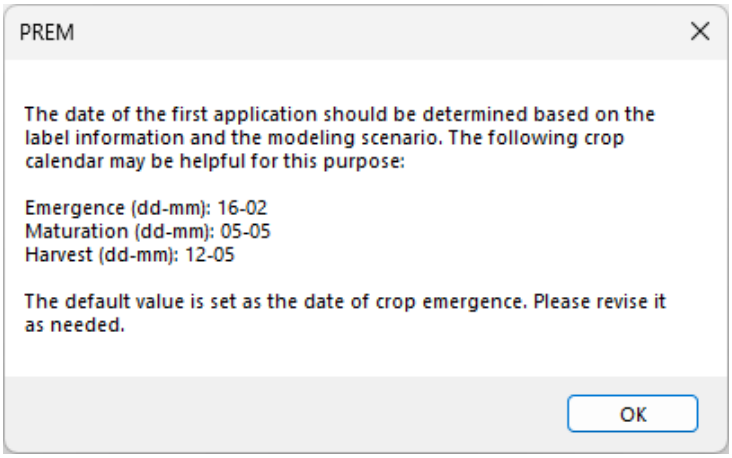


Figure 29. Crop calendar prescribed in the modeling scenario, using "Lettuce" as an example

9 Additional input parameters for rice pesticides ("Rice" tab)

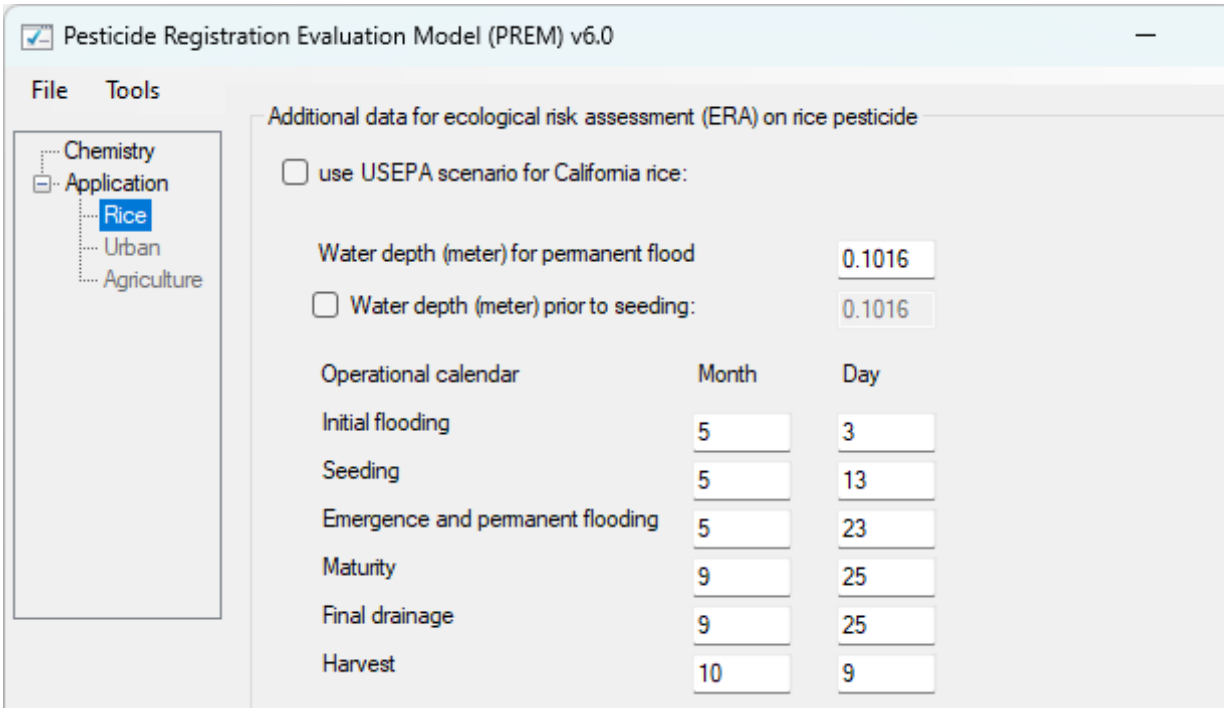


Figure 30. Additional data for pesticide uses in flooded fields

The “Rice” tab becomes available when “Rice pesticide” is selected as the use pattern for modeling (Figure 30). PREM6 incorporates representative parameter values suggested by USEPA for the modeling scenario of California rice production (White et al., 2016), and allows users to revise the values to represent the environmental settings required on the product label.

The predefined water depth in a California rice paddy is 4 in (0.1016 m). For other crops, the water depth may need to be changed. For example, the water depth of 1.5 in (0.0381m) is suggested for watercress (USEPA, 2020b) and 12 in (0.3048 m) for cranberry (USEPA, 2016).

A new option is developed to model a different water depth prior to seeding (Figure 30). This option is used to evaluate a pesticide which is applied to a flooded rice paddy and prefers a shallow water depth.

For most of registration evaluations on rice pesticides, it’s not necessary to modify the rice growth calendar and water management schedules provided as default values in PREM6 (Figure 30). The more important factors influencing rice modeling results are (1) the water depth at the time of application (i.e., pre- vs. post-flood applications indicated by application timing), and (2) the water-holding period and (for pre-flood applications only) the dry period required on the label. See Section 8.6 for more information on water-holding period and pre-flood application.

10 Additional input parameters for urban out door uses ("Urban" tab)

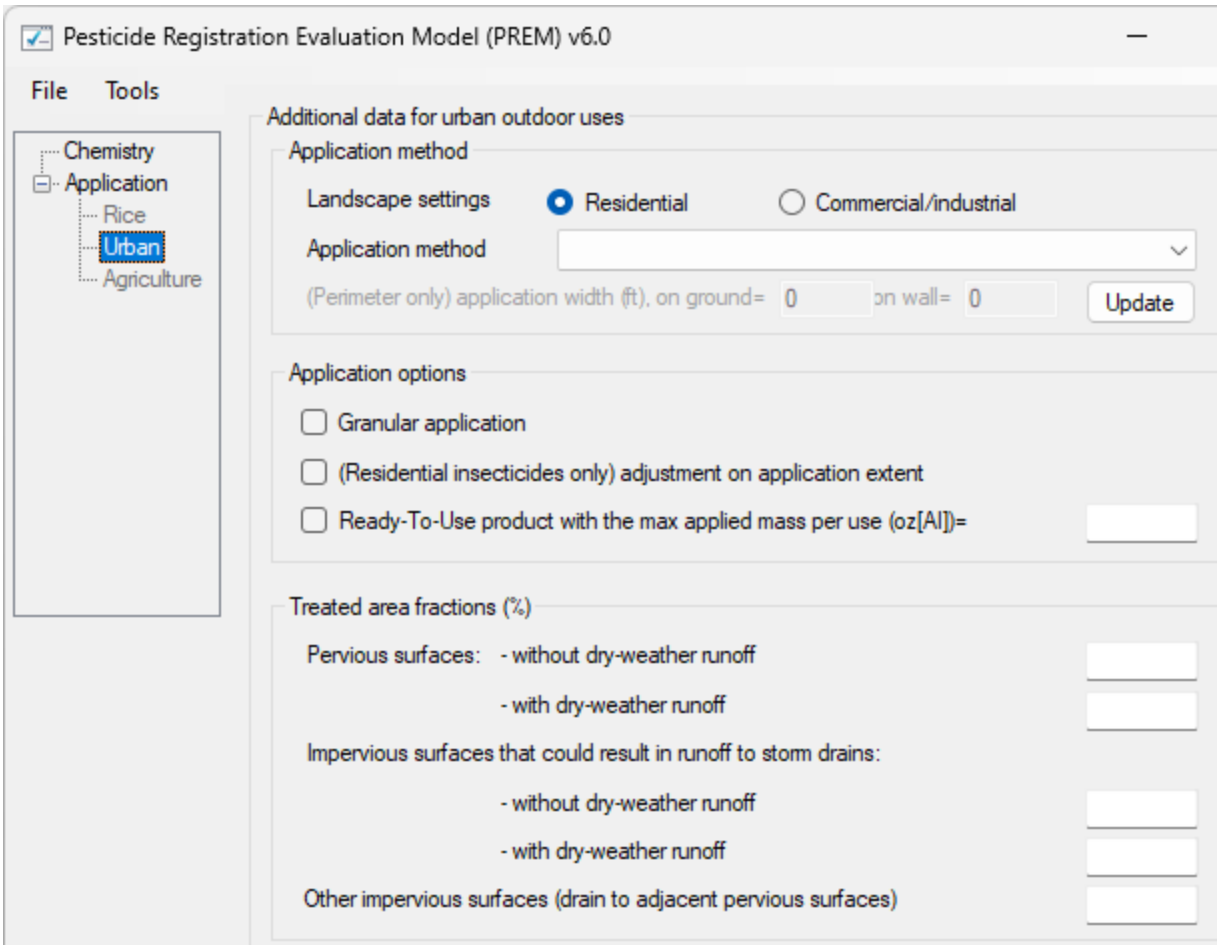


Figure 31. Additional data for pesticide uses in urban outdoor settings

The "Urban" tab becomes available when "Urban outdoor" is selected as the use pattern for modeling (Figure 31). Modeled application methods are associated with intended or unintended (e.g., overspray to adjacent paved areas during lawn treatment) applications to impervious surfaces. Application methods are mathematically represented by a series of treated area fractions (in percentage) (Figure 31).

Six types of general application methods have been predefined in the model (Figure 32). For perimeter treatment, a user should provide application bandwidths for horizontal and vertical surfaces. The model will automatically calculate the treated area fractions of each modeled surface. The model also allows users to manually change the treated fractions in order to represent mitigation measures or other application methods not predefined in the model. Please refer to the document for urban evaluation (Luo, 2014) for details to characterize the urban environment and pesticide applications in California.

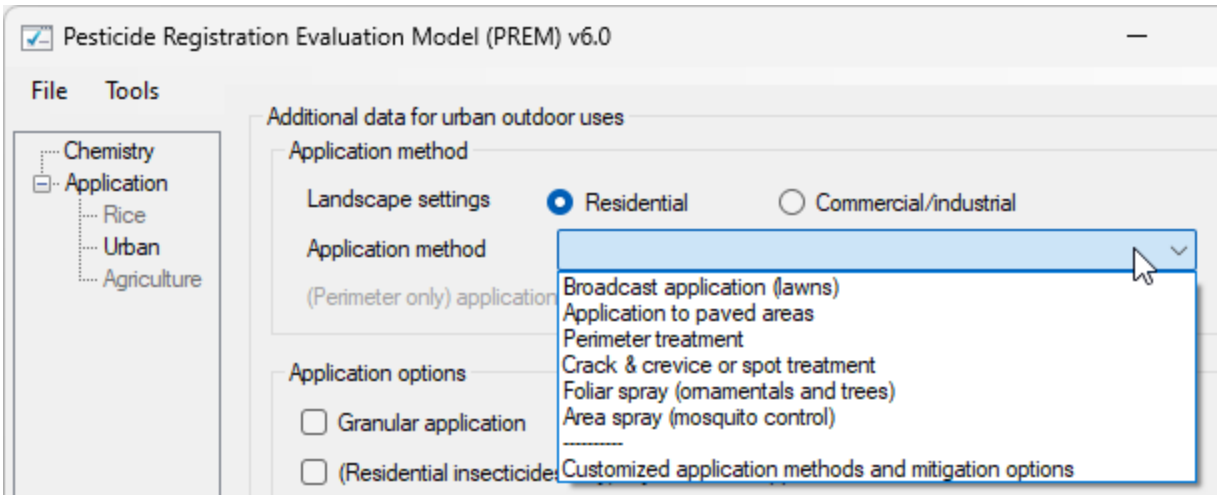
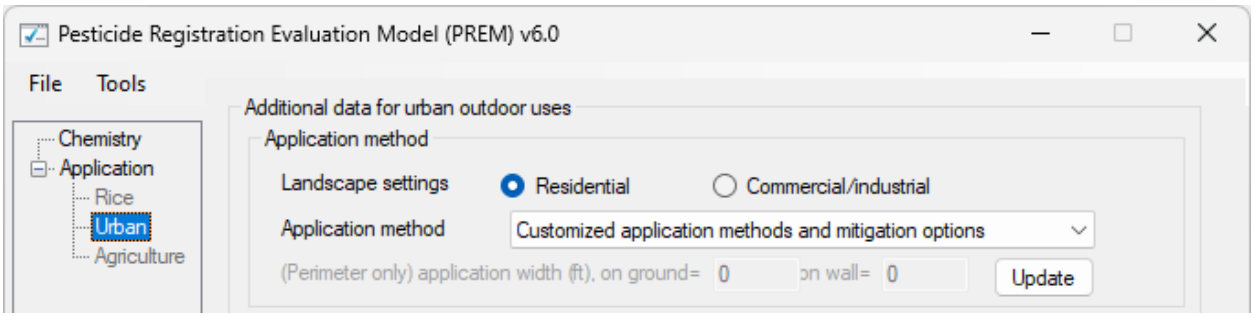


Figure 32. Application methods modeled for urban outdoor uses

In addition to the six predefined application methods, PREM6 provides an advanced option for users to customize application parameters for each landscape component in the urban settings. This option is developed for the mitigation practices required by the product label and/or regulations, which cannot be sufficiently modeled with the general application methods.

The new tool is available by selecting "Customized application methods and mitigation options" and clicking the "Update" button (Figure 33a). A user could edit the application method on each landscape component. For example, Figure 33b demonstrates that a 6-inch perimeter treatment is assigned on the residential driveway. Select "Not treated" or leave the box blank if applications are prohibited on the corresponding surface. Additional mitigation options are provided to restricting applications to vertical surfaces (walls) or pervious surfaces adjacent to paved areas.

(a)



(b)

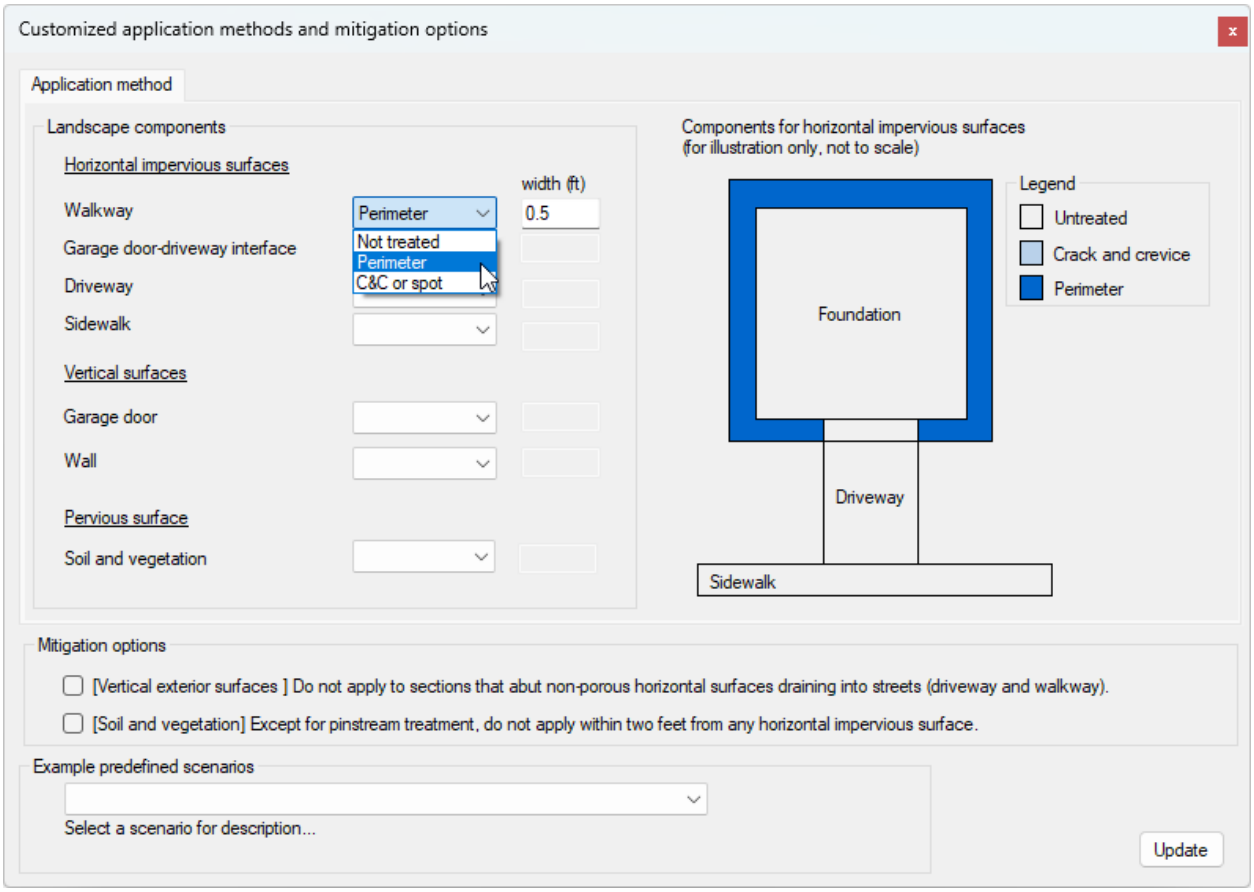


Figure 33. Advanced modeling options for urban outdoor pesticide uses

PREM6 provides three examples for customized application scenarios based on the label changes and regulations on pyrethroids and fipronil products proposed for urban outdoor uses (Table 6). More details on the modeling scenarios have been previously documented in CDPR modeling studies (Budd and Luo, 2016; Luo, 2017b, 2023). Figure 34 shows an example for "(Fipronil) 2018 label change".

Table 6. Examples for customized application methods and mitigation options

Modeling scenario	Description
(Bifenthrin) 2013 label change, bifenthrin MOA, and CDPR Surface Water Regulations	2-ft up but NOT to vertical surfaces connected to driveway/walkway that drain into street, and restricted applications to all horizontal impervious surfaces.
(Other pyrethroids) 2013 label change and CDPR Surface Water Regulations	2-ft up (pin stream to garage door) and restricted applications to all horizontal impervious surfaces.
(Fipronil) 2018 label change	6-in up and 6-in out, NO application to garage door and driveway.

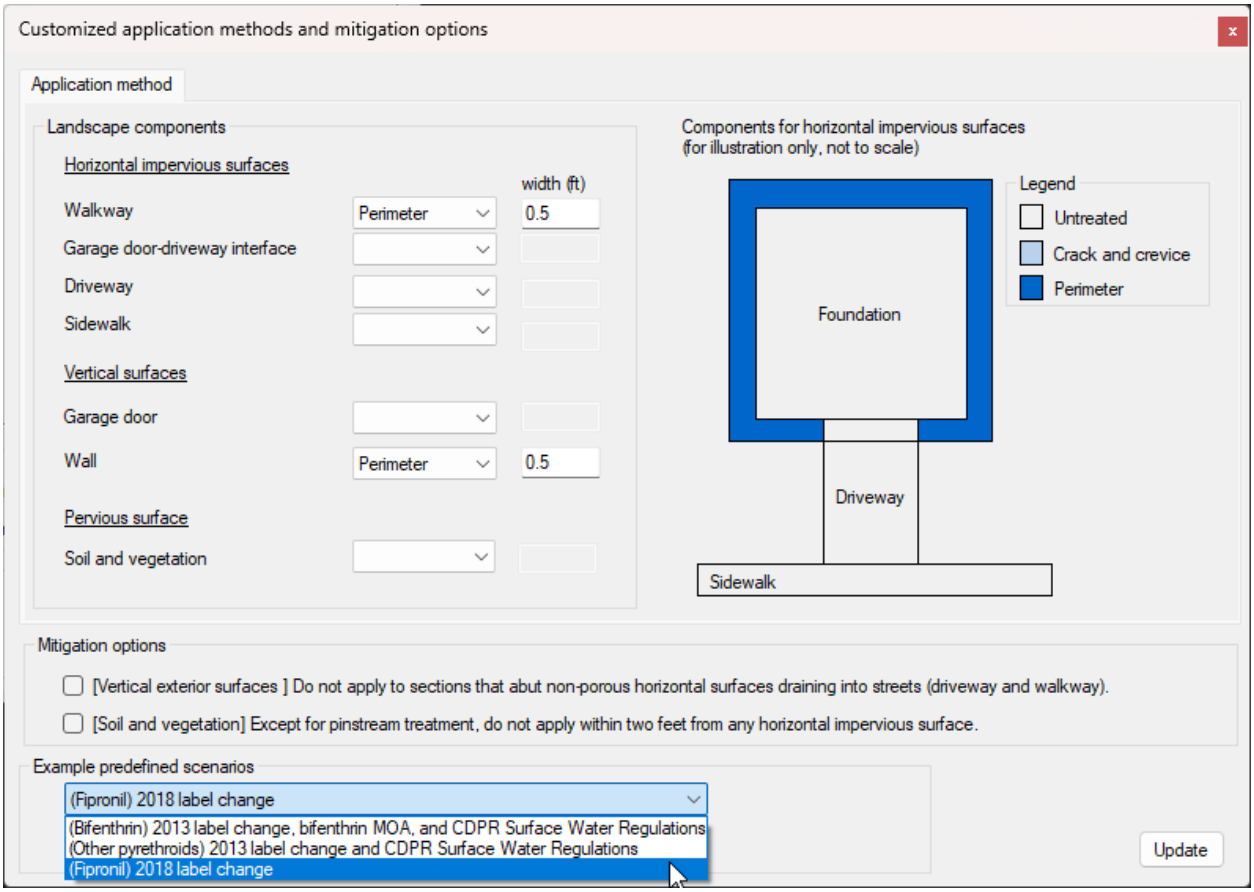


Figure 34. Predefined modeling scenarios, "(Fipronil) 2018 label change" as an example

The general procedures to characterize urban outdoor uses are as follows:

1) Read the product label and summarize the product formulation, use pattern, and application method.
2) Select landscape settings (residential or commercial/industrial).
3) Select one of the predefined application methods (Figure 32), or customize the method with mitigation options (Figure 33). Click "Update" to calculate the treated area fractions.
4) (Perimeter treatment only) specify the widths of application.
5) If the pesticide product is applied as a granular form, the option for "Granular application" should be checked. In this case, the fraction of incidental application to a non-target surface (e.g., overspray to adjacent paved areas during lawn treatment) is set to be zero (Luo, 2014; USEPA, 2018).
6) (Residential uses only) check the option for "Adjustment on application extent" if the pesticide product is evaluated as insecticides. With this option, the label rate is adjusted by the fraction of households treated with residential outdoor pesticide products (75.9%) (Luo, 2017a).
7) (Residential uses only) if the pesticide product is in a ready-to-use formulation and with an assumed maximum applied mass per use (e.g., one container per use), check the option for ready-to-use product and provide the maximum use applied mass per use in oz[AI].

11 Additional input parameters for agricultural applications ("Agriculture" tab)

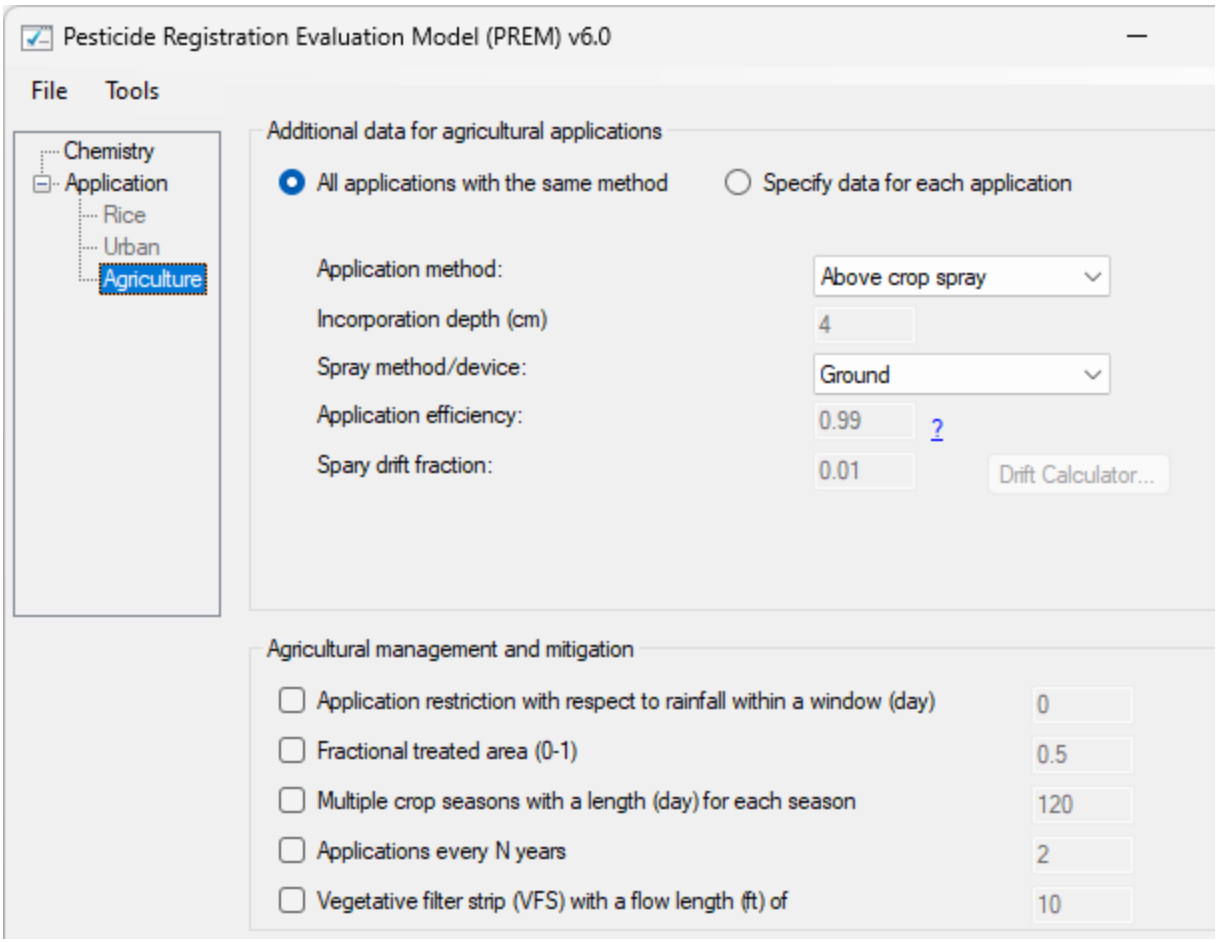


Figure 35. Additional data for agricultural application methods and mitigation practices

Application methods and mitigation practices can be specified in the "Agriculture" tab (Figure 35) for agricultural applications to terrestrial crops and other vegetations (e.g., forestry, outdoor nursery, and rights-of-way). Application methods can be modeled in two ways: [1] assuming all applications with the same method, or [2] specifying method for each application.

11.1 Repeated applications with the same method

With this option, all applications are characterized with the same rate, method, efficiency, and drift fraction, and scheduled according to the application timing, interval, and frequency previously specified in the "Application" tab (Section 7). PREM6 provides five application methods for user to model (Figure 36): "Below crop spray", "Above crop spray" (default), "Soil incorporation (uniform)", "Soil injection", "Soil fumigation", and "In-furrow at seed planting". The last four methods (incorporation, injection, fumigation, and in-furrow) require an application depth (cm).

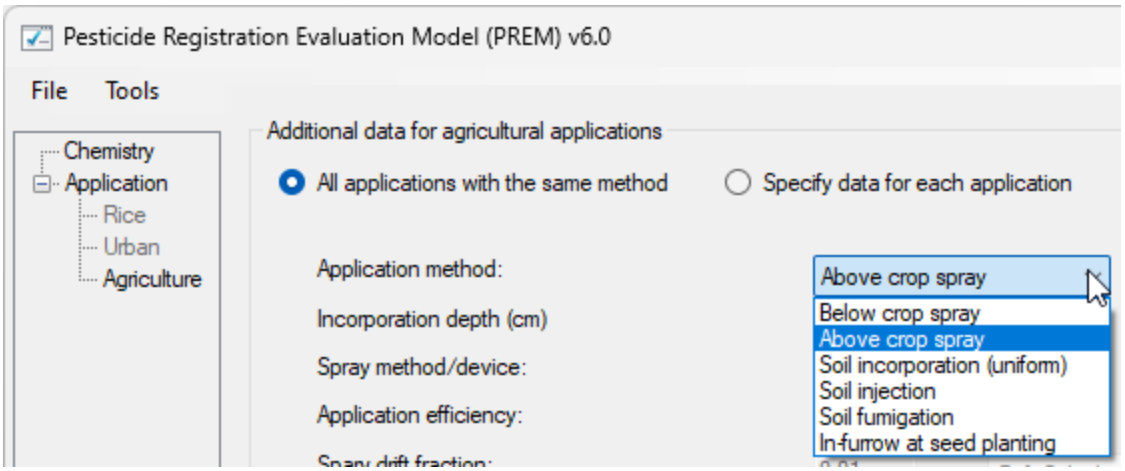


Figure 36. Application methods modeled in PREM6

PREM6 uses USEPA-recommended default values for application efficiency and spray drift fraction (USEPA, 2009) according to user-selected spray method (Figure 37). For example, when a user selects "Air-blast" from the pulldown menu, the default values of 0.99 (application efficiency) and 0.03 (drift fraction) will be automatically filled to the model interface.

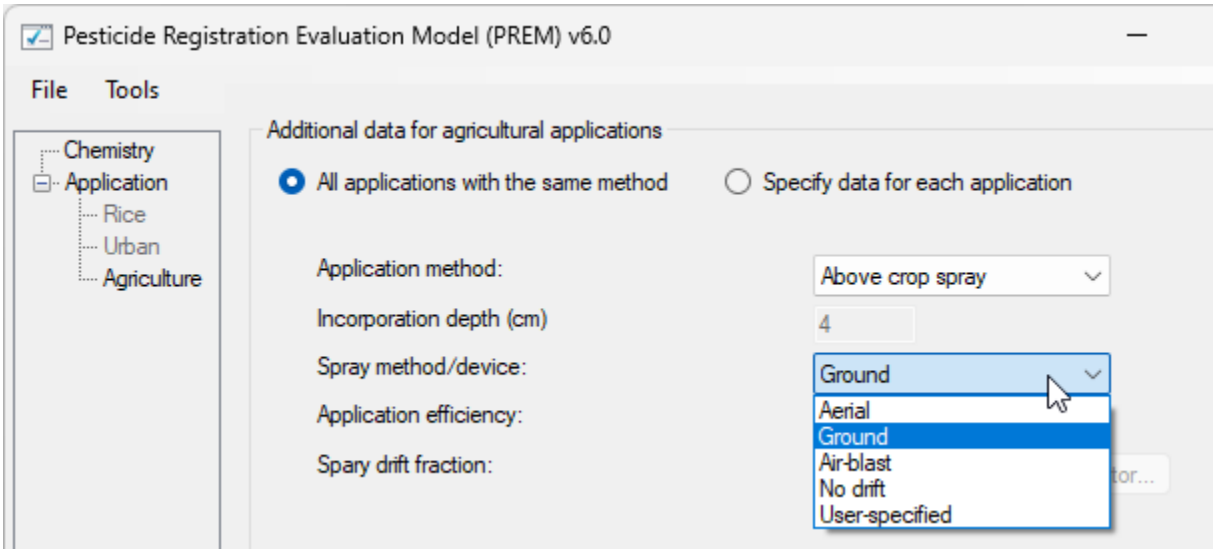


Figure 37. Spray methods modeled in PREM6

The option of "User-specified" could be used to modify the default values to represent the label-required mitigation practices to reduce spray drift. With this option, a user may manually modify the values, or use the "Drift Calculator" (Figure 38) provided in PREM6 which evaluates the mitigation effects of the spray buffer zone distances required on the product label for pesticide applications.

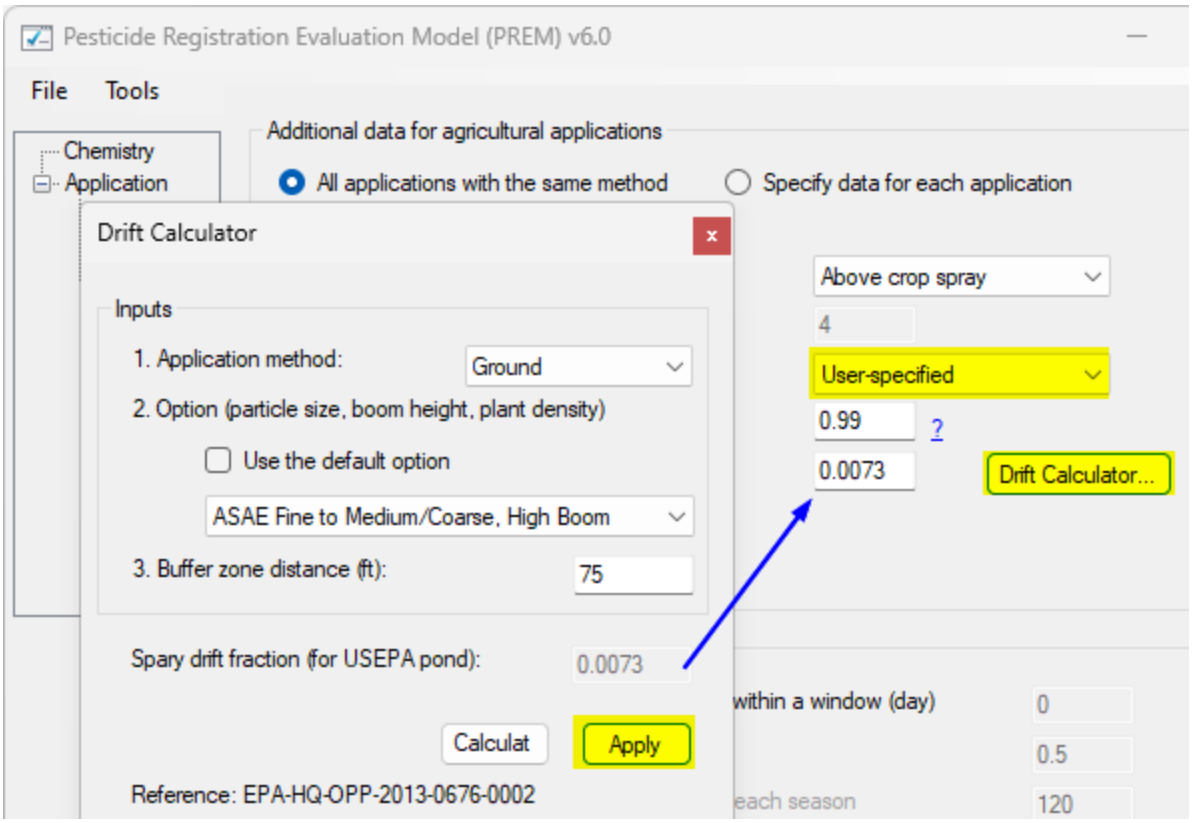


Figure 38. Drift Calculator

11.2 Specify data for each application

An advanced modeling option is provided in PREM6 which allows users to specify parameters for each individual application. With this option, applications may have different rates, methods, efficiencies, and drift fractions, and could be scheduled with different intervals. Figure 39 shows an example for imidacloprid uses on lettuce, modeled by USEPA (2016) as one application as a soil incorporation at a rate of 0.296 kg/ha, followed by foliar applications at a rate of 0.053 kg/ha and an interval of 5 days.

The parameter values specified for each application (Figure 39) will override the general application data provided under the "Application" tab (Figure 28). The only parameter taken from the general application data is the date of the first application. This date is used as a reference date, and all applications are scheduled relative to the reference date. For example, a relative day ("Rday") of 0 is to schedule an application on the reference day, and Rday = 5 for an application in 5 days after the reference day. If the reference is provided as the date of emergence, a negative value of Rday suggests an application prior to emergence. For example, Rday = -10 is used to schedule an application at the time of seeding (USEPA, 2016) (Figure 39).

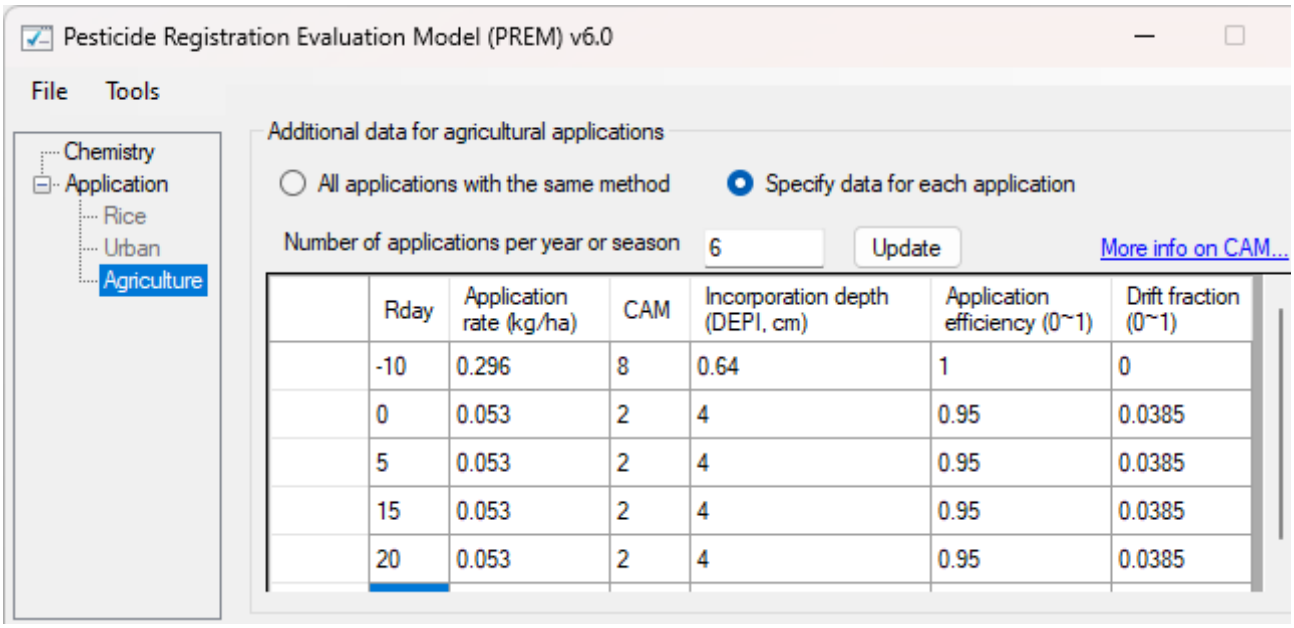


Figure 39. Option to specify application methods for each application event, showing an example with one soil injection and subsequent aerial applications

Descriptions for the input parameters are available when a user moves the mouse over the parameter. Detailed explanations are provided in Table 7.

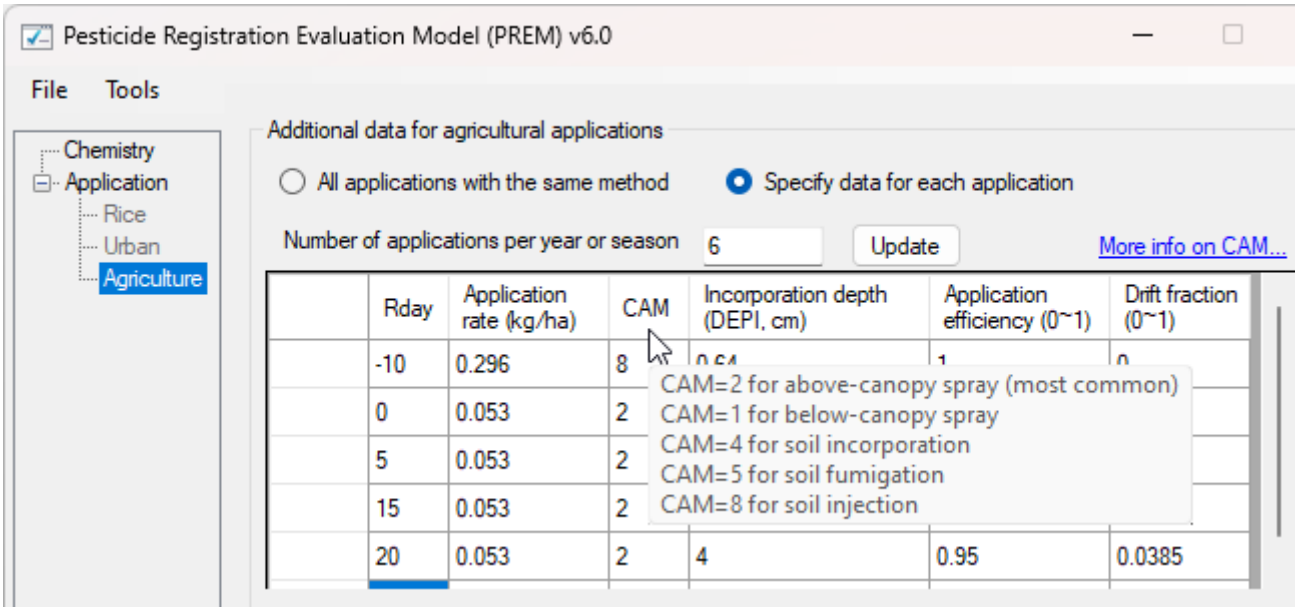


Figure 40. Tip text when a mouse is moving over an input parameter, Chemical Application Method (CAM) as an example

Table 7. Input parameters to specify data for each application

Parameter	Description
Rday	Relative days to the reference date. The default reference data in PREM6 is the date of emergence, as assigned to the "Date of the first application" in the "Application" tab.
Application rate (kg/ha)	Rate for each application
Chemical application method (CAM, 1 to 9)	Application methods predefined in the USEPA modeling (Young, 2020). See Table 8 for details. Commonly used CAMs are below-canopy (CAM=1), above-canopy (2), soil incorporation (4), soil fumigation (5), and soil injection (8) (Figure 40).
Incorporation depth (DEPI, cm)	Set to a fixed value of 4 cm for CAM = 1, 2, and 3; or user-specified value for other CAMs
Application efficiency (0 to1)	Default value of 0.99 for ground or air-blast applications, 0.95 for aerial applications, or estimated by other models
Drift fraction (0 to 1)	Default value of 0.01 for ground applications, 0.03 for air-blast applications, 0.05 for aerial applications, or estimated by other models (e.g., the "Drift Calculator" in PREM6)

Table 8. Definition of Chemical Application Method (CAM) (Young, 2020)

CAM	Description
1	below crop, linearly decreasing incorporation to a soil depth of 4 cm
2	above crop (linear interception), linearly decreasing incorporation to 4 cm
3	above crop (exponential interception), linear decreasing incorporation to 4 cm
4	below crop, uniform incorporation to a user-specified soil depth (DEPI)
5	below crop, linearly increasing incorporation to DEPI
6	below crop, linearly decreasing incorporation to DEPI
7	T-band: below crop, user-defined fraction in the top 2 cm, and maximum depth DEPI
8	below crop, application at DEPI
9	similar to CAM=2, but incorporation to DEPI

Note: also available in PREM6 by clicking the link text "More info on CAM…" (Figure 39)

11.3 Modeling options for agricultural management and mitigation (Figure 41)

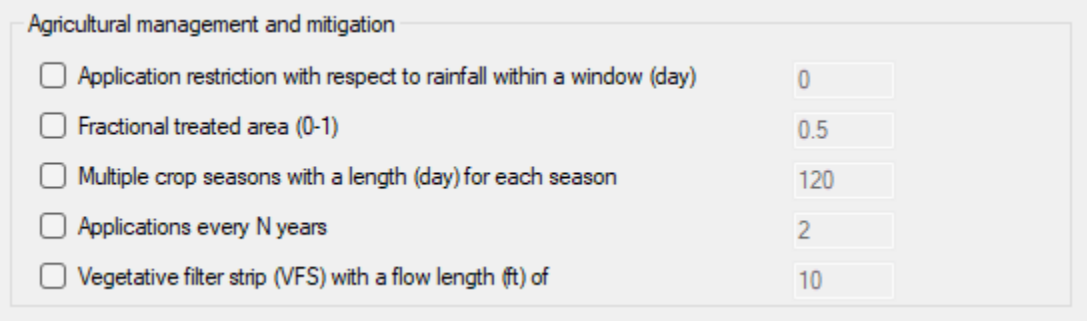


Figure 41. Options for agricultural management and mitigation

Application restriction with respect to rainfall within a window

This option is to represent the restrictions for pesticide applications required on the label. Example label language is "*no application shall occur if … a storm event, forecasted by NOAA or NWS, is to occur within 48 hours following applications; or a storm event is like to produce runoff from the treated area is forecasted by NOAA/NWS to occur within 48 hours following the application*." By checking this option, a user is asked to specify the acceptable window, in days, for an optimum application, e.g., 2 days in the above example.

Fraction treated area

By default, PREM6 assumes that the entire agricultural watershed will be treated by the pesticide under evaluation, i.e., the fraction treated area = 1. This is appropriate for conservative estimation especially for the pesticide products labelled for a wide variety of crops and used in agriculturally dominated watersheds of California. For the pesticide products proposed for special local needs (SLN), PREM6 accepts a user-specified fraction treated area for more realistic modeling according to the proposed use patterns. For example, a fraction of 0.5 was used in the previous evaluations of SLN products for orchards (Luo et al., 2024).

Multiple crop seasons

This option is developed for vegetables for which succession planting is commonly observed in the Central Coast of California. Specifically, this option is applicable to two *standard* use patterns in PREM6 (Figure 19): [1] "Lettuce" representing leafy vegetables, and [2] "Broccoli" representing brassica (cole) leafy vegetables. The corresponding modeling scenarios for the two use patterns were both developed based on the crop production areas in Monterey County (USEPA, 2022). When any of the two use patterns are selected, the option to model "multiple crop seasons" will become available (Figure 41).

With this option selected, PREM6 will model two crop seasons (Luo et al., 2024). The only additional model input is the length modeled for each season in days, i.e., the interval between the first and the second crop seasons. The default value is 120 days. Users are only required to specify pesticide use data for the first season, in the same format as that for single-season modeling. PREM6 will repeat the same set of applications for the second season.

Note that PREM6 does not model multiple crop seasons for the *new PWC scenarios* of "Vegetable commodity" and "Vegetable fresh or processing market" (Figure 21). The new scenarios for vegetables were not developed for the Central Coast of California.

Applications every N years

PREM6 provides an option to skip pesticide applications for some years. The default modeling process assumes that the proposed applications will be repeated every year during the modeling period. The new option allows users to evaluate pesticide applications on a certain number (N) of years as required on the product label. For example, the label language of "applications every

other calendar year" is modeled with N=2. In this case, PREM6 will model applications in the first year, *no application in the second year*, applications in the third year, and so on.

Vegetative filter strip (VFS)

The label-required mitigation by VFS could be evaluated in PREM6. The only input parameter is the flow length (or the VFS width, in feet). Other model parameters and settings incorporated in PREM6 have been described in the technical report (Luo, 2020). Hydrological simulations in the VFS are based on the VFSMOD (Muñoz-Carpena and Parsons, 2020) version 4.5.2. By checking this option, PREM6 will report the updated RQs in the receiving waterbody by introducing a VFS with the user-specified width. More outputs on the VFS effectiveness are provided under the "Tools" menu item to "View VFS modeling results" (Section 4.2), including the incoming amounts of surface runoff, sediment, and pesticide from the treated field and their predicted relative reductions through the VFS (Figure 42).

```
Outputs: VFS modeling results
================================================================
                 hydrology
                 ---------------
          1755 | # of runoff events
         40.22 | event-mean incoming flow (m3)
         15.34 | event-mean incoming sediment (m3)
          99.3 | flow reduction (%)
          99.8 | sediment reduction (%)
                 chemical #0
                 ---------------
         85.52 | event-mean incoming pesticide, dissolved (mg)
         21.52 | event-mean incoming pesticide, adsorbed (mg)
          99.6 | pesticide reduction (%)
       6.80E-5 | mass balance (%)
```

Figure 42. Example output file for additional modeling results of VFS modeling

12 Modeling results and evaluation report template

Each model run will generate a report ("PREM.txt") which summarizes modeling inputs and outputs. This file will be displayed in Notepad (or any default text file editor in your computer) once a model run is completed, and can be found in the same folder of the model executable file ("PREM.exe"). The modeling report should be attached as an appendix to the evaluation report.

PREM6 provides an option to "Report EECs" under the Tools menu (Figure 5). Therefore, there are two types of modeling outputs: (1) Standard modeling results by default with the option to "Report EECs" unselected. PREM6 will report modeling results as RQs and registration recommendations, and (2) EEC-only results by selecting the option to "Report EECs". PREM6 will only report EECs calculated with the user-specified averaging periods (Figure 6).

Previous evaluation reports are posted in the internal website of CDPR's Environmental Monitoring Branch. An evaluation report is typically organized into six sections: recommendation summary, background, evaluation, conclusion, references, and appendix. Some considerations for each section of the report include:

12.1 Recommendation summary

Check one or more boxes for registration recommendations (Figure 43).

[x] Data/Information Support Registration
[ ] Data/Information Support Conditional Registration
[ ] Data/Information Do Not Support Registration
[ ] No Registration Action Required
[x] AI Flagged for Future Surface Water Review

Figure 43. Options for registration recommendations in the evaluation report, showing an example with recommendations to support registration and flag the active ingredient

12.2 Background

Provide basic information for the product, AI, label, use patterns, and target pests. You should provide other noteworthy information such as reasons for why the product is being routed to SWPP (e.g., new AI, direct application to water, previously flagged by SWPP, or request from water agencies), and note previous evaluations if applicable.

12.3 Evaluation

Explain your analysis of how the product(s) could affect surface water quality in this section. Assess whether the product you are evaluating can be appropriately simulated by PREM6. If so, follow subsequent guidance below. If not, you can engage in an open discussion of anticipated impacts to California aquatic environments using other models or a best professional judgment approach.

1) Explain that the SWPP evaluation will be relied upon using data from chemistry and ecotoxicology evaluation reports that have been approved by the Pesticide Registration Branch. Provide references for these data sources, and other documents that you deemed important for your evaluation.
2) For each chemical to be modeled (active ingredients and degradates), provide a table summarizing the input values used for physicochemical and toxicological properties with appropriate references and any notes regarding data selection. If the value for a model input parameter is derived by a reviewer, the detail processes should be documented in the evaluation report. For example, a reviewer may have to calculate the "median" aquatic dissipation half-lives from multiple values approved in the chemistry review report. All data used for the modeling should be specified. See Table 9 for a template.
3) For a chemical which has been modeled in previous evaluation studies: provide description and justification if there are different input values used in this study for

physicochemical and toxicological properties, e.g., newly available or updated test results.

4) Justify your selection of the model use pattern(s) and explain your interpretation or derivation of the label application rate that is used as input to the model. You should also highlight any relevant application specific information that may impact the model results (e.g., maximum applications per year, minimum application intervals).
5) If there are multiple model runs (e.g., for different products, active ingredients, use patterns, and application rates and intervals), you should summarize their results in a table. The key columns to show are the products, modeled use patterns, application rates and intervals, risk quotient(s), and model-based recommendations.
6) When applicable, consider highlighting and discussing important information not sufficiently addressed by the model simulations. Consider these factors together with the modeling results to arrive at the final registration recommendation.

Table 9. Template table for the model inputs of physicochemical and toxicological properties

Property (unit)	Input value	Reference	Note
The input parameter and unit, e.g., "Solubility (ppm)". See Table 3 for a full list of parameters.	A single value as model input	Provide references here	Explain how the input value is determined from the references, e.g., "Median of results from four accepted studies."

12.4 Conclusion

Present your final registration recommendation and briefly summarize how you arrived at your conclusion. Be as clear and succinct as possible.

1) For support, state that the data support the registration of the product.
2) For conditional registration, the registrant is requested to submit water and sediment analytical methods for the chemicals of concern (parent AI and/or degradates). In this case, provide the specifications for method development (Appendix II), and specify a deadline for document submission. You may also ask for other types of data from the registrant to address minor issues that you would like to see resolved (e.g., toxicity data, half-life data).
3) For registration denial, the reviewer needs to clearly delineate the likely factors for the denial. Look for opportunities to provide helpful guidance to the registrants here as they will want to resolve issues quickly. Registration denial is associated with the following conditions:
    a. Data are sufficient for registration evaluation, but result in high-risk quotients in surface water. In this case, the reviewer may provide suggestions on potential label changes that will prevent or mitigate potential risks to surface water
    b. Data are not sufficient to complete registration evaluation for surface water protection. The reviewer will specify the requests for additional data (such as degradate toxicity data, toxicity data for marine/estuarine species) to continue and refine the evaluation.

12.5 References

Provide references for all your citations and list them alphabetically. A reference style that is consistent with those used for peer-review scientific journals is preferred. References for registrant-submitted documents should have sufficient identifiers for an independent party to successfully recover the document and verify the citations. Identifiers include titles, authors, dates, CDPR document numbers, and CDPR tracking I.D. number.

12.6 Appendix

Attach the model outputs ("PREM.txt") as an appendix. Use a monospace font (e.g., Consolas) to format the text of model outputs. If there are multiple model runs and output files, organize them with a table of contents.

13 Guideline for physicochemical and toxicological data preparation

13.1 Data sources

Input parameters for the model are listed in Table 3, which are generally categorized as physicochemical properties (for the parent compound and degradates), aquatic toxicity data (for the parent compound and degradates), and molar formation fractions (for degradates only). For newly submitted AIs, representative values of the input parameters should be prepared only based on the **evaluation reports in the areas of Chemistry and Ecotoxicology**, in which registrant-submitted data are reviewed by CDPR's Pesticide Registration Branch. There may be **multiple versions** available for the reports, and each adds or replaces values to the previous one. In this case, the latest version should be used in the data preparation.

Registration packages with previously registered AIs may rely on data submitted from previous data submissions. For input parameters not available or not approved in CDPR's previous evaluations, data from reputable sources in the open literature could be used. Data sources commonly used by SWPP include the Pesticide Properties Database (PPDB) by International Union of Pure and Applied Chemistry (IUPAC) and modeling studies by USEPA. References must be provided for any data values used in the data preparation.

13.2 Physicochemical properties

Physicochemical properties for the parent compound and degradates are taken from the chemistry evaluation report. First, take a look at the table at the end of the report, which summarized most of the required input parameters (KOC, SOL, AERO, ANAER, and HYDRO) for the comparison with groundwater leaching criteria (Figure 44).

	Property	SNV	Experimental Values	Criteria Exceeded?
			Mobility	
			Soils	
	K_{OC}	< 1900 mL/g	*Maximum:* 96.0 mL/g	Yes
			Minimum: 11.1 mL/g	
			Median: 53.6 mL/g	
			Mean: 52.3 mL/g	
			Std Dev: 31.7 mL/g	
or	Water solubility	> 3 ppm	26.5 mg/L @ 20°C	Yes
			and	
			Persistence	
	Hydrolytic half-life	> 14 days	72.5 ± 0.52 days[1]	Yes[1]
or	Aerobic soil metabolism half-life	> 610 days	< 1 day	No
or	Anaerobic soil (or aquatic) metabolism half-life	> 9 days	< 2 days	No

Figure 44. Example of data summary table in the chemistry review reports

If **a single representative value** is provided in the summary table (e.g., SOL=26.5 ppm, Figure 44), it should be used for the corresponding parameter. For a parameter reported as **a range of values** (e.g., KOC=11.1 to 96.0, or AERO <1 day, Figure 44) or **not summarized** in the table, individual values of the parameter should be retrieved from the main text of the chemistry report. In this case, the following considerations should be incorporated in the data preparation:

1) Only use the test results from registrant-submitted studies and considered to be **acceptable** by the chemistry evaluation.
2) Generally, the representative value of an input parameter is the **median value** of the accepted individual test results.
3) If there were tests performed under **California field conditions**, use the test results from those studies. For half-lives, in addition, the median of *all* accepted values should be also calculated. Use the global median if it is significantly higher than the California value.
4) For a "**stable**" degradation process, a half-life significantly larger than the test duration should be used. Or model users can leave the corresponding cell blank in the data viewer/editor (Figure 45), and the model will consider those as missing data and assign a default half-life of 99,995 days (see Section 13.4 for "Missing data handling").
5) For degradation studies, if both half-life ($t_{1/2}$ or $T_{1/2}$) and degradation half-time (DT50) are provided, use **half-life ($t_{1/2}$ or $T_{1/2}$)** in calculating the median value.
6) If test studies were conducted under various pH values, use the results under **neutral pH** conditions (pH=7 or around 7).
7) For **photolysis** half-life (SPHOT), if results are provided for both direct (buffered water) and indirect (natural water) tests, use the results from indirect photolysis test.

8) For **aerobic aquatic metabolism half-life** (AERO_W), if results are provided for "water" and "total system" tests, use the results in water.

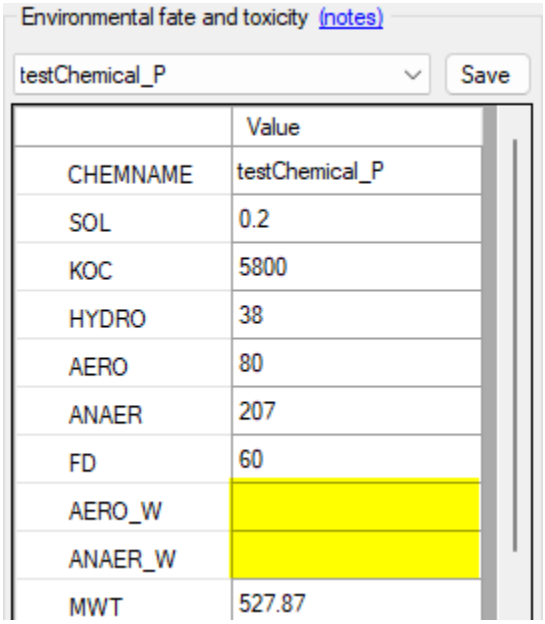


Figure 45. Blank cells in the data viewer/editor for half-lives, representing stable degradation process

The same procedures can be used for the data preparation for **degradates**. See Section 7 for the determination of degradates requiring model-based evaluations. The formation fractions (DKs) can be estimated from active radioactivity (AR, reported in percentage). Usually very limited data are available for degradates, therefore, in addition to the laboratory test results, physicochemical properties from estimation programs (such as USEPA EPI suite) could be considered for model inputs of degradates.

13.3 Aquatic toxicity data

Toxicity values are summarized at the end of the ecotoxicology evaluation report (Figure 46). The following procedures and worksheets have been developed to assist the data preparation for aquatic toxicity (TOX and TOXSED as input parameters):

Test Animal	Type of Study	Acute Toxicity Value**	Relative Toxicity
Rat	Acute oral	> 300 mg/kg (male) > 425 mg/kg (female	Toxicity Category II
Daphnia magna	Chronic toxicity (21-day)	1.4 µg/l NOEC	N/A
Eastern oyster	Water exposure (96 hrs)	5.4 µg/l EC_{50} < 3.1 µg/L NOEC	Extremely toxic
Brown shrimp	Water exposure (96 hrs)	15 µg/L LC_{50}	Extremely toxic
Larval midge	Chronic toxicity (28-day)	0.00265 mg/L NOEC	N/A
Rainbow trout	Water exposure (96 hrs)	3.8 µg/l LC_{50} 2.9 µg/l NOEC	Extremely toxic
Sheepshead minnow	Water exposure (96 hrs)	43 µg/L LC_{50} 30 µg/L NOEC	Extremely toxic
Rainbow trout	Chronic toxicity (**63-day**)	0.96 µg/l NOEC	N/A
Bluegill sunfish	Water exposure (96 hrs)	34.1 µg/l LC_{50} 20.4 µg/l NOEC	Extremely toxic

Figure 46. Example of toxicity data summarized in the ecotoxicology evaluation report

1) Only use the test results that are considered to be **acceptable** by the ecotoxicology evaluation.
2) Toxicity data may be reported for both technical-grade active ingredient (AI) and the formulated product, usually summarized in separate tables in the evaluation report. The **technical-grade AI product toxicity** should be used for registration evaluation.
3) Water toxicity is required for all chemicals, while sediment toxicity is only required for chemicals with KOC >1000. In the case of KOC ≤1000, skip all the processes and descriptions below for sediment toxicity.
4) Use **LC_{50} and EC_{50}** values from **acute** toxicity test (as indicated in the "Type of study," Figure 46, this is usually 48-hour or 96-hour for water tests, but there is no standard test duration for sediment tests) for freshwater and marine/estuarine species of fishes and invertebrates.
5) For sediment toxicity, if no LC_{50} or EC_{50} is available, use other reported data (e.g., LOEC or NOEC) for preliminary evaluation. See the section 13.4 "Missing data handling" for more information.
6) If a toxicity value is reported as "larger than (>)" or "less than (<)" a certain value, the provided value will be used.
7) If a toxicity value of the pesticide, reported in the format of water or pore-water concentration, is larger than its water solubility, the value of solubility should be used. For example, in a previous registration evaluation by SWPP, the active ingredient has the lowest acute toxicity of 87 mg/L in the water, larger than its water solubility of 62.6 mg/L. Therefore, the value of solubility (converted to the unit of µg/L, i.e., 62,600 µg/L) was used for modeling.
8) For water toxicity, the retrieved values should be converted into the unit of **µg/L**. For sediment toxicity, the retrieved values should converted into the model-required unit according to the mass basis of the reported data, i.e., **µg/kg[dry weight]** for sediment mass based concentration (TOXSED_UNIT=1, Table 3), **µg/L** for pore-water

concentration (TOXSED_UNIT=2), or **µg/g[OC]** for organic carbon based concentration (TOXSED_UNIT=3).

9) Fill the following worksheet with retrieved toxicity values (Figure 47). For sediment toxicity, if the retrieved values are reported on a different mass basis, they should be further converted into a pore-water concentration (µg/L) for calculating the lowest value:
   a. from µg/kg[dry weight] to pore water µg/L: (value in µg/kg[dry weight])/KOC/FROC2, where FROC2 (dimensionless) is the organic carbon fraction of the benthic sediment used in the toxicity test. If FROC2 is not reported, use the default value (0.04) in the modeling scenario of the USEPA pond.
   b. from µg/g[OC] to pore water µg/L: (value in µg/g[OC])/KOC*1000

10) Use the lowest toxicity values **for freshwater species as the initial trial** of input parameters TOX and TOXSED, and run the model. The model will determine the exposure potential of the product to marine/estuarine species (Xie and Luo, 2016), and make suggestions for the use of freshwater or marine/estuarine toxicity values:
   a. The product may have **low** exposure potential to marine/estuarine species (Figure 48). In this case, **keep using the lowest toxicity values for freshwater species** for TOX and TOXSED in the evaluation.
   b. The product may have **high** exposure potential to marine/estuarine species according to the use patterns (Figure 49). In this case, if the product label restricts its use in estuarine areas, keep using the lowest toxicity values for freshwater species for TOX and TOXSED in the evaluation. Without such restrictions, toxicity data for marine/estuarine species are required, and **the lowest toxicity values for all species** should be set for TOX and TOXSED in the evaluation. If toxicity data for marine/estuarine species are not available, SWPP will presume that data do not support registration and request the registrant to submit additional data.
   c. The product may have high exposure potential to marine/estuarine species according to the physicochemical properties of its AI (Figure 50). In this case, toxicity data for marine/estuarine species are required, and **the lowest toxicity values for all species** should be set for TOX and TOXSED in the evaluation. If toxicity data for marine/estuarine species are not available, SWPP will presume that data do not support registration and request the registrant to submit additional data.

Water toxicity, freshwater	Sediment toxicity, freshwater
Individual values, with potential test species ▪ Bluegill (*Lepomis macrochirus*) ▪ Common carp (*Cyprinus carpio*) ▪ *Daphnia pulex* ▪ Fathead minnow (*Pimephales promelas*) ▪ Rainbow trout (*Oncorhynchus mykiss*) ▪ Water flea (*Daphnia magna*) ▪ Others **The lowest value** ("NA" if no data in this category) =	**Individual values**, with potential test species ▪ *Hyalella azteca* ▪ Midge larvae (*Chironomus dilutus*, formerly named as *Chironomus tentans*) ▪ Others **The lowest value** ("NA" if no data in this category) =
Water toxicity, marine/estuarine	Sediment toxicity, marine/estuarine
Individual values, with potential test species ▪ Eastern oyster ▪ Saltwater mysid (*Americamysis bahia*) ▪ Sheepshead minnow ▪ Others **The lowest value** ("NA" if no data in this category) =	**Individual values**, with potential test species ▪ *Eohaustorius estuarius* ▪ *Leptocheirus plumulosus* ▪ *Rhepoxynius abronius* ▪ Others **The lowest value** ("NA" if no data in this category) =
The lowest value of water toxicity (all species) =	**The lowest value** of sediment toxicity (all species) =

Figure 47. Worksheet to determine the input values for toxicity data in water and sediment

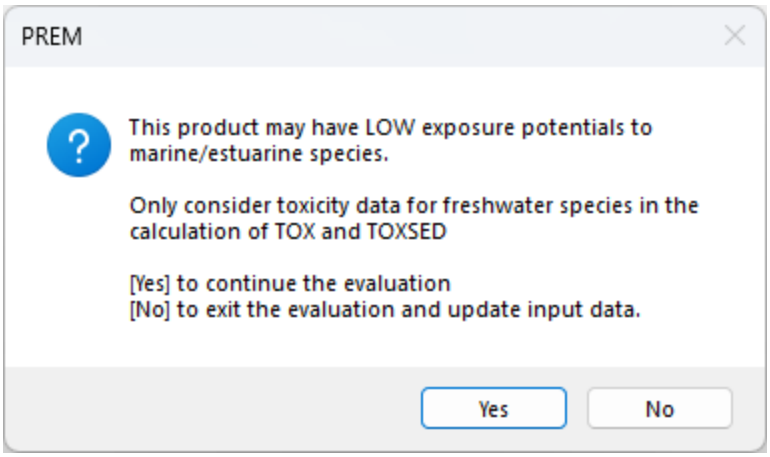


Figure 48. Warning message for a product with low exposure potential to marine/estuarine species

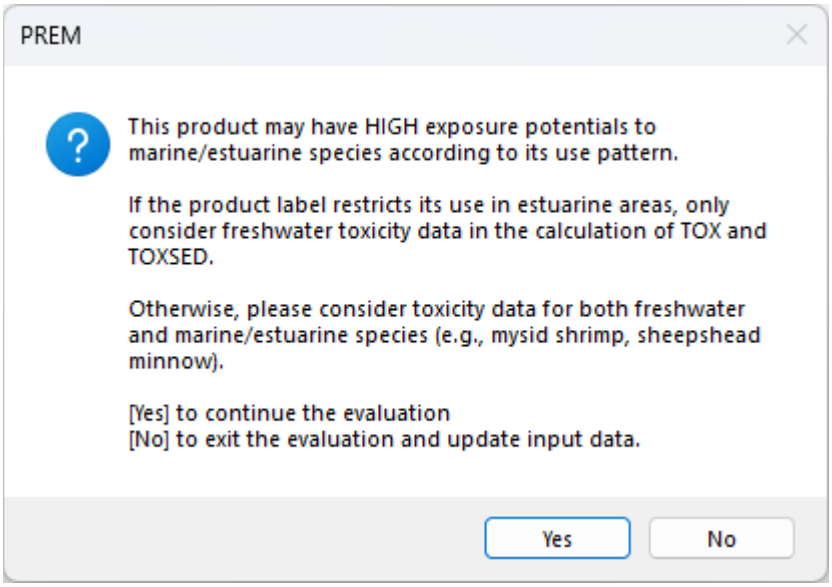


Figure 49. Warning message for a product with high exposure potential to marine/estuarine species according to the use patterns

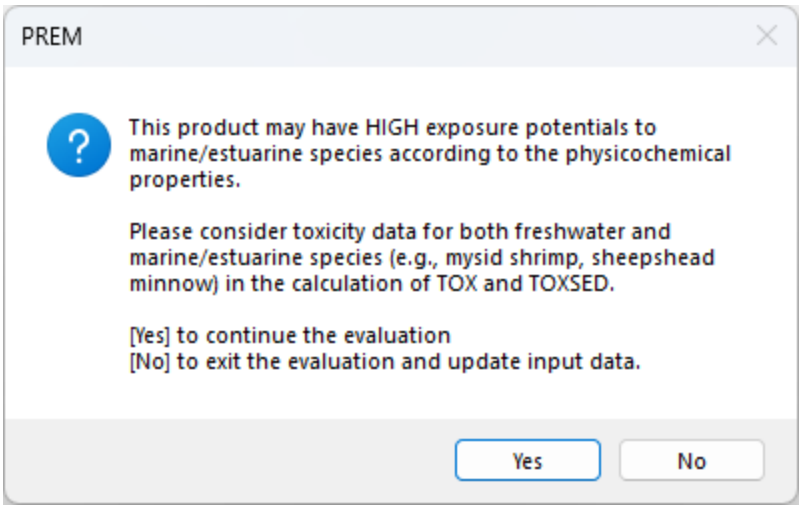


Figure 50. Warning message for a product with high exposure potential to marine/estuarine species according to the physicochemical properties

13.4 Missing data handling

If there are still missing data (blank cells in the data editor) by following all procedures in the guideline, the model will first determine if the parameters with missing data are essential to the evaluation. If so, the model will give warning message and ask for user's input. In summary, SOL, KOC, MWT, and TOX are required for the parent compound, and KOC, MWT, TOX, and at least one of the DKs are required for degradates. Figure 51 shows an example message if the water solubility (SOL) value is missing.

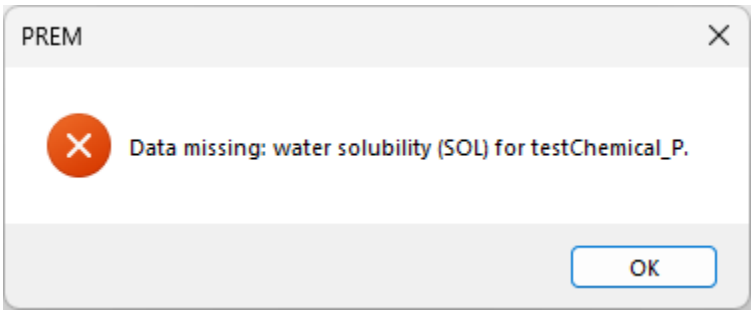


Figure 51. Warning message for missing data of water solubility

For other parameters with missing data, PREM6 uses the following procedures to estimate the input values:

1) Parameters for half-lives (HYDRO, AERO, ANAER, FD, AERO_W, ANAER_W, AQPHOT, and SPHOT) will be set to 99,995 days, which is an arbitrary large value representing a "stable" or "persistent" degradation process.
2) Vapor pressure (VP) will be set as 1e-15 torr, based on the 90th percentile of vapor pressure data in the Pesticide Property Database (IUPAC, 2023).

3) Sediment toxicity (TOXSED), if KOC >1000, will be estimated with the water toxicity (TOX) value as the pore-water concentration. In this case, the model will confirm with users (Figure 52), and give a warning message at the end of the evaluation (Figure 53).

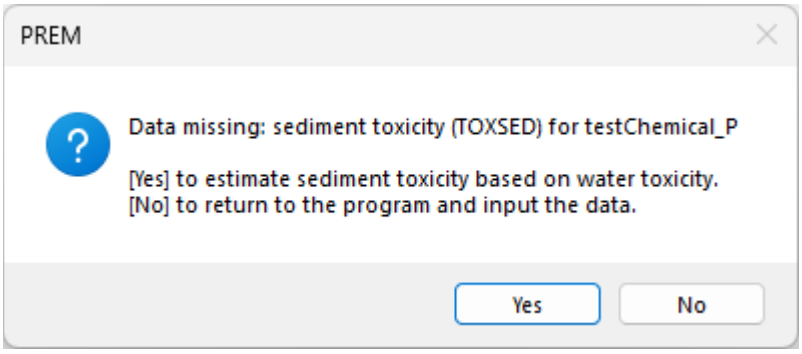


Figure 52. Warning message: sediment toxicity is missing

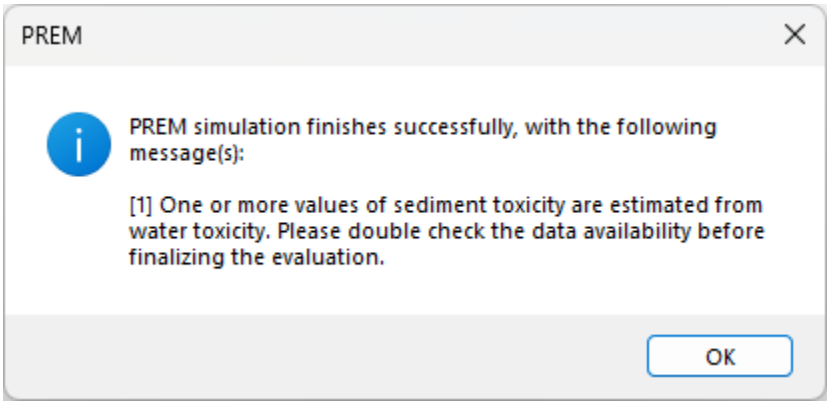


Figure 53. Warning message: estimated sediment toxicity was used in the evaluation

Acknowledgement

The authors would like to acknowledge Robert Budd, Nels Ruud, Michael Ensminger, Minh Pham, Jennifer Teerlink, Nan Singhasemanon, and Kean S. Goh for critical reviews on the current and previous versions of the User's Manual.

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Appendix I. Estimating Heat of Henry by the Estimation Program Interface (EPI) Suite

Heat of Henry (or enthalpy of vaporization, ENPY) is the energy required for the phase change for volatilization of a solute from solution (J/mol). ENPY is used in pesticide modeling to adjust Henry's Law constants at various temperatures,

$$HLC(T) = HLC_{ref} \exp[-\frac{ENPY}{R}(\frac{1}{T} - \frac{1}{T_{ref}})]$$

where HLC(T) is the Henry's Law constant at the temperature T (K), and HLC_{ref} is the Henry's Law constant at the temperature T_{ref} (K), and R is the universal gas constant (8.314 J/K/mol).

The USEPA guidance for volatilization algorithm suggests the EPI Suite for estimating ENPY (Rothman et al., 2015). Specifically, ENPY is determined based on the temperature variation of HLC. The following procedures can be used to estimate the Heat of Henry for a volatile compound with EPI Suite 4.11 (USEPA, 2012):

1) Open the EPI Suite
2) Open the HENRYWIN program from the navigation bar on the left of the main interface (Figure 54)
3) Check the option to "show temperature variation with results" in the HENRYWIN (Figure 54)
4) Set the chemical by name or by SMILES notation. Use the [NameLookup] button to confirm the chemical if it is in the built-in database
5) Click the [Calculate] button on the HENRYWIN program. The model outputs are shown on a new window. Scroll to the section of "Henry LC Temperature Variation" (Figure 55).

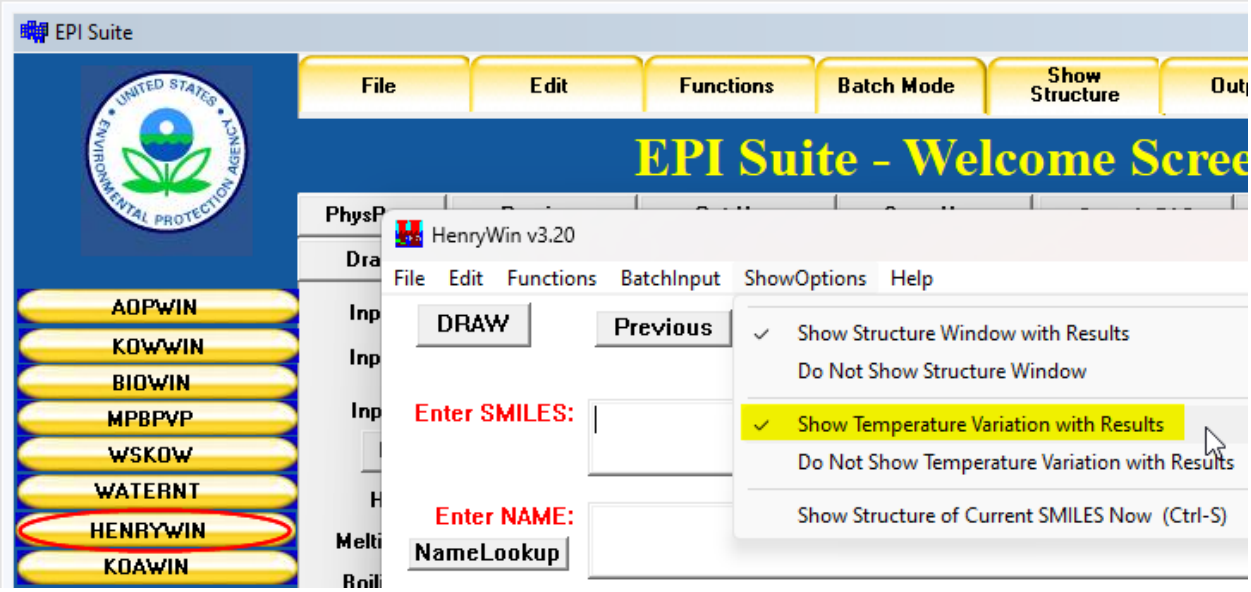

Figure 54. HENRYWIN program in EPI Suite and the option for ENPY calculation

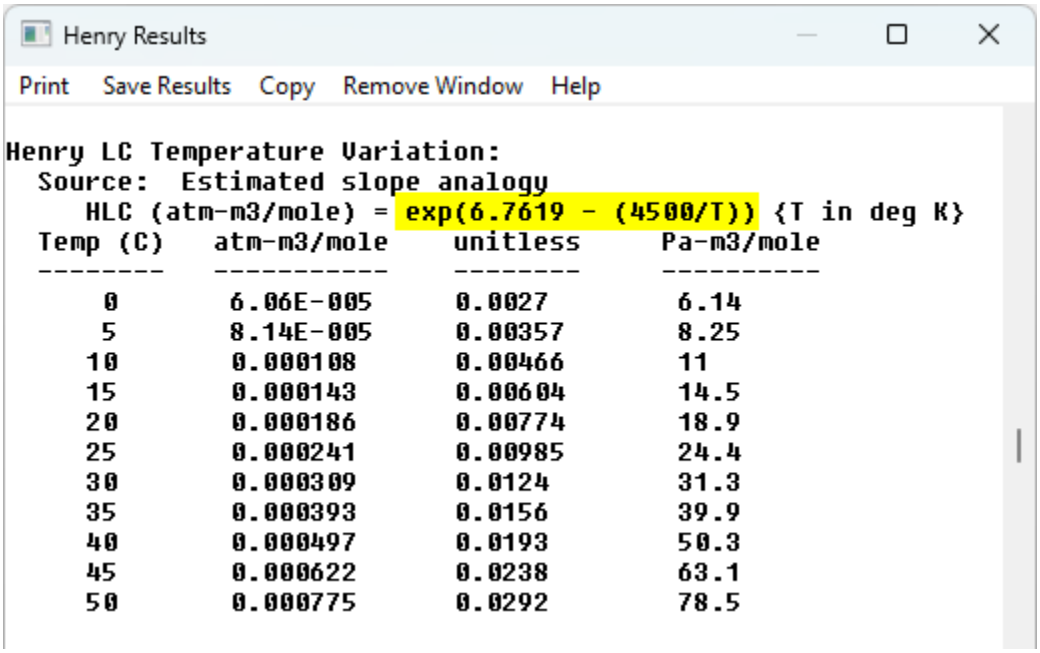

Figure 55. Example HENRYWIN results. The estimated regression relationship between Henry's Law Constant and temperature is highlighted.

The HENRYWIN program generates the temperature variation of HLC in the format of a regression equation HLC= exp(A-B/T) where T is temperature (K) and A and B are calibrated regression coefficients (Figure 55). ENPY is then calculated as 8.314×B, where 8.314 is the gas constant in the unit of J/K/mol.

Appendix II. SWPP's analytical method requirements

CDPR Surface Water Protection Program's Analytical Method Requirements

(Revised December 2016)

(For complete description of requirements and terminology reference, see CDPR Standard Operating Procedure #QAQC012.00)

1) Methods should be routinely executable by commercial laboratories.
2) Analytical method(s) submissions shall include the following: 1) a list of the materials, reagents, equipment and instruments used, 2) description of the preparation, extraction and analytical procedures, 3) description of the data analysis, and 4) calculations and units.
3) Calibration procedures must be provided. The calibration standard curve should include a minimum of 4 concentration points. The two fortification levels used in the study (i.e., LOQ and 10xLOQ) should be within the calibration range.
4) Method detection limits (MDL) are typically determined as described in CDPR Standard Operating Procedure #QAQC012.00, Appendix 1: 40 CFR Ch.1, part 136 appendix B, "Definition and Procedure for the Determination of the Method Detection Limit – Revision 1.11." Information on the limit of detection (LOD) may be substituted for MDL information. Replicates used for MDL determination must have analyte recoveries between 70–120% of spiked concentration with a relative standard deviation (RSD) <20%.
5) Reporting limits (RL) should be set at 3–5 times the MDL. Submitted methods may substitute the limit of quantification (LOQ) for RL. RLs for natural surface water should be no greater than 10% of the lowest acute water toxicity value (LC_{50} or EC_{50}) for a water column dwelling species (e.g., fish, invertebrates). For registrant-submitted methods, the lowest toxicity value will be determined from the set of toxicity studies submitted to DPR to support pesticide registration. Sediment RLs should be no greater than 10% of the lowest acute or chronic sediment toxicity value (LC_{50} or EC_{50}) for a sediment-dwelling organism. If no acute sediment toxicity studies are submitted, RLs for sediment should be no greater than 1 μg/kg.
6) The method should utilize mass spectrometry or tandem mass spectrometry paired with either gas chromatography (GC) or liquid chromatography (LC). Other methods (e.g., high performance liquid chromatography (HPLC) with fluorescence detection or GC with thermionic specific detection) may be used with justification. Justification must explain why mass spectrometry was not the chosen instrument for analysis. Instrument operating conditions, analyte retention times and quantification and confirmation ions must be specified.
7) Method validation requires a minimum of five analyses at two matrix spike concentrations (typically LOQ and 10XLOQ).
8) Analytical method documentation shall include reporting on all QA/QC (including) blank concentrations, method recovery data, LOD/MDL, and RL/LOQ.

9) Overall mean method recoveries are acceptable from 70% < *recovery* < 120% with a relative standard deviation (RSD) of <20%.
10) A 28-day (minimum duration) storage stability study in both surface water and sediment matrices. The objective of the storage stability test is to determine how long environmental samples could be stored and still remain viable. Surface water matrices should be stored in a refrigerator at 2–7 ºC and sediment samples stored in a freezer below 0 ºC for the duration of the test. The test should include at least four sampling intervals and two replicate samples at each interval to validate the residue's rate of decomposition in representative matrices. Clean water and sediment matrices should be spiked with the analyte of interest at an environmentally-relevant concentration (i.e., 10X LOQ). Analysis should be conducted with fully-validated analytical methods and acceptable recovery range (70–120%) and RSD (<20%).
11) Independent laboratories hired to develop analytical methods for registrants must follow the above requirement and provide the required data, including storage stability data.
12) Independent laboratories hired to validate registrant provided analytical methods must provide validation of the analytical methods including all of the above requirements with the exception of storage stability data.