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**SWPP Pesticide Registration Evaluation Model (PREM) User Manual
(Version 5.0)**

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1 Overview

The Surface Water Protection Program (SWPP) 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 scenarios that the model is capable of simulating. Details for the original and improved model development have been documented in the technical reports (Luo and Deng, 2012a, b; Luo, 2014; Luo et al., 2016; Xie and Luo, 2016; Luo, 2017). A computer program has been developed to implement the model with a graphical user interface. The purpose of this document is to provide instructions to use the program. PREM 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, and urban outdoor uses, but not capable of evaluating indoor uses, marine antifouling paint products, and other unique pesticide use patterns. Recent refinements to the model include evaluation of primary degradates of pesticide active ingredients (AIs), and discharge into estuarine/marine environments.

2 Installation

PREM has been developed based on the common computer settings in DPR. The system requirements include:

- 1) 64-bit Windows, and
- 2) Microsoft Access Driver ver. 16

The data driver comes with a full installation of Microsoft Access 2016 (as a part of Microsoft Office Professional Plus 2016), or can be downloaded from “Microsoft Access Database Engine

2016 Redistributable” (<https://www.microsoft.com/en-us/download/details.aspx?id=54920>). After installation, the driver will be listed in the ODBC Data Source (Figure 1).

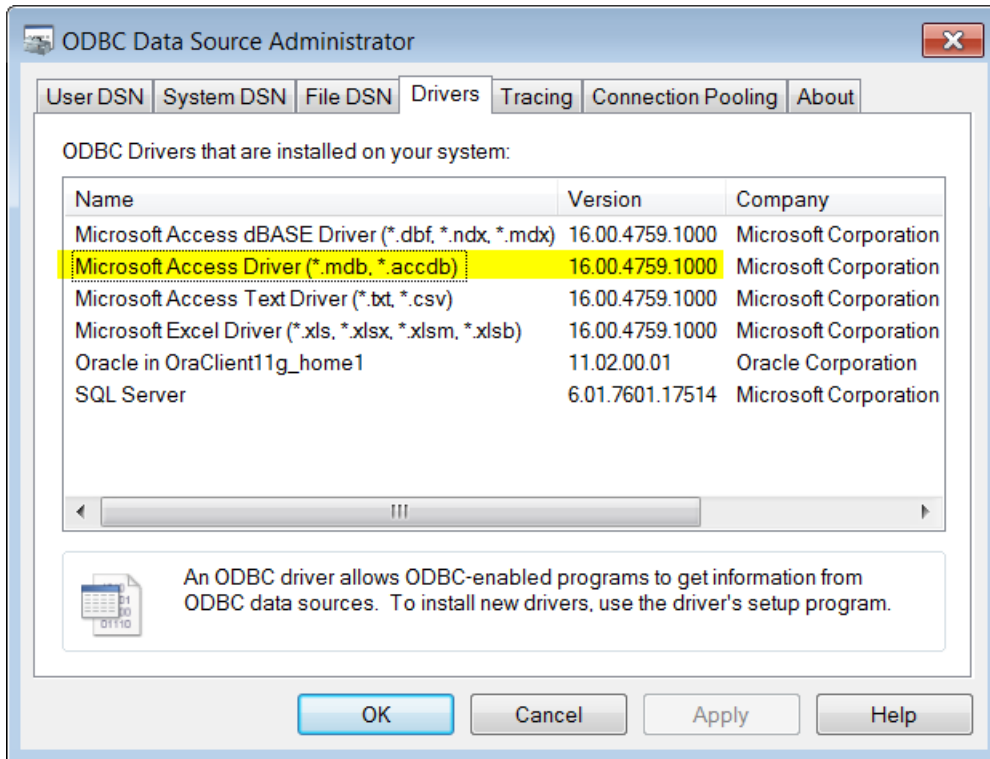


Figure 1. Screenshot showing the required data driver successfully installed

The installation package of PREM can be downloaded from DPR webpage of “Surface Water Models” (http://cdpr.ca.gov/docs/emon/surfwttr/sw_models.htm) as a .ZIP compressed file. Please unzip the file and extract its contents into a local hard disk of your computer. Figure 2 shows an example of the model package in D:\PREM5\. The package includes the executable file (PREM.exe), database (PREM.dat), and supporting files (in the sub-folder of “PL6”). Double click “PREM.exe” to start the model.

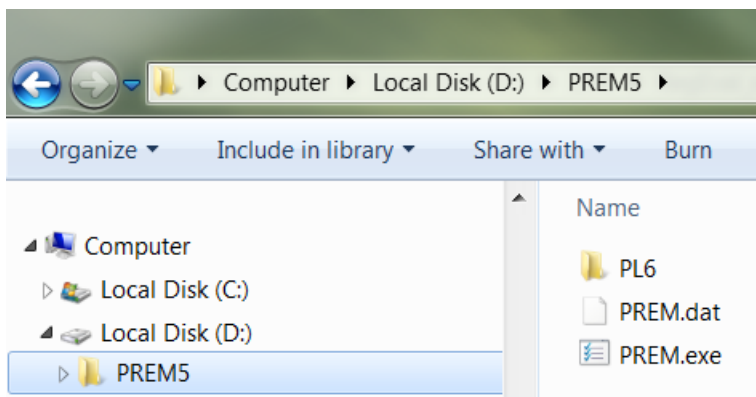


Figure 2. PREM package in a local computer

3 The model GUI (Graphical User Interface)

3.1 Physicochemical properties and toxicity data

3.1.1 Model input parameters

The viewer/editor for pesticide physicochemical properties and toxicity data (Figure 3) is developed for two purposes: [1] to prepare model input data for the chemicals under evaluation, including the AI and its degradates; and [2] to set the parent compound for evaluation (the chemical showing in the pull-down menu before a model run is considered as the parent compound).

	CHEMNAME	SOL	KOC	HYDRO	AERO	ANAER	FD	AERO_W	ANAER_W	MWT	VP	AQPHOT	SPH
▶	testChemical_P	0.2	5800	38	80	207				527.87	1E-07	3.16	139

Figure 3. Editor for physicochemical properties and toxicity data of pesticides

Table 1 lists input parameters, descriptions, and units required by PREM for physicochemical properties and toxicity data. The same information is also available by clicking the text “notes” on the program (Figure 4). Users are asked to prepare representative values for all parameters based on the data submitted by registrants and reviewed by DPR’s Pesticide Registration Branch. Detailed instructions are provided in the Section 5 “Guideline for data preparation” of the manual. Care must be taken when selecting input values including the units.

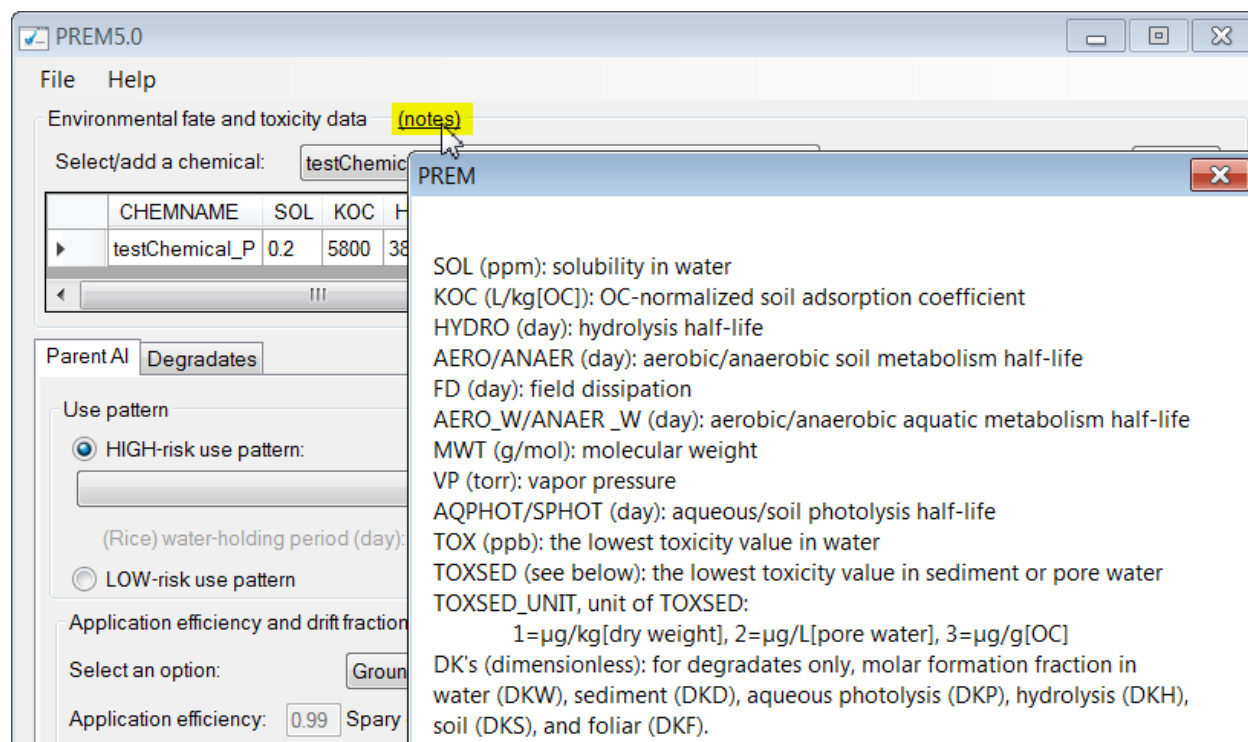


Figure 4. Popup window showing the detailed information for model-required input parameters

Table 1. Model input parameters for physicochemical properties and toxicity of pesticide

Input parameter	Description	Unit
CHEMNAME	chemical name	-
SOL	<i>(only needed for parent compound)</i> 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	<i>(only needed for urban outdoor uses)</i> soil photolysis half-life	day
TOX	the lowest 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= $\mu\text{g}/\text{kg}$ [dry mass of sediment]; 2= $\mu\text{g}/\text{L}$ [pore water]; and 3= $\mu\text{g}/\text{g}$ [OC]	-
DK's	<i>(only needed for degradates)</i> 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)	-

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

Use the pull-down menu to list all the chemicals with data available in the model database (Figure 5). Data can be retrieved by selecting the chemical name in the list. It is critical that the users verify the data values and make changes as needed before the model simulation. After all changes have been made, confirm the changes by clicking “Save” (Figure 5). The program will also warn users if unsaved changes are detected.

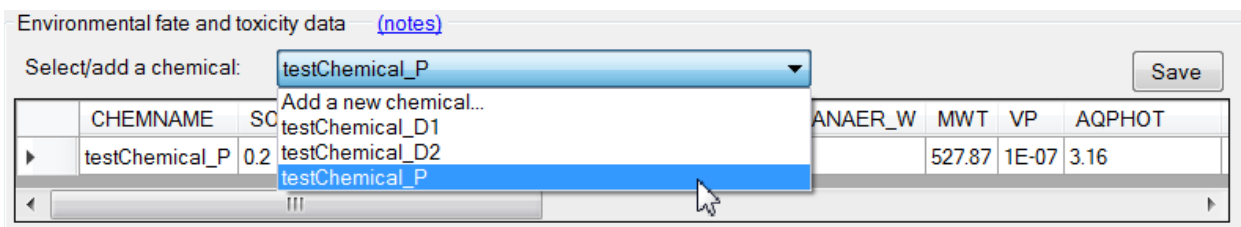


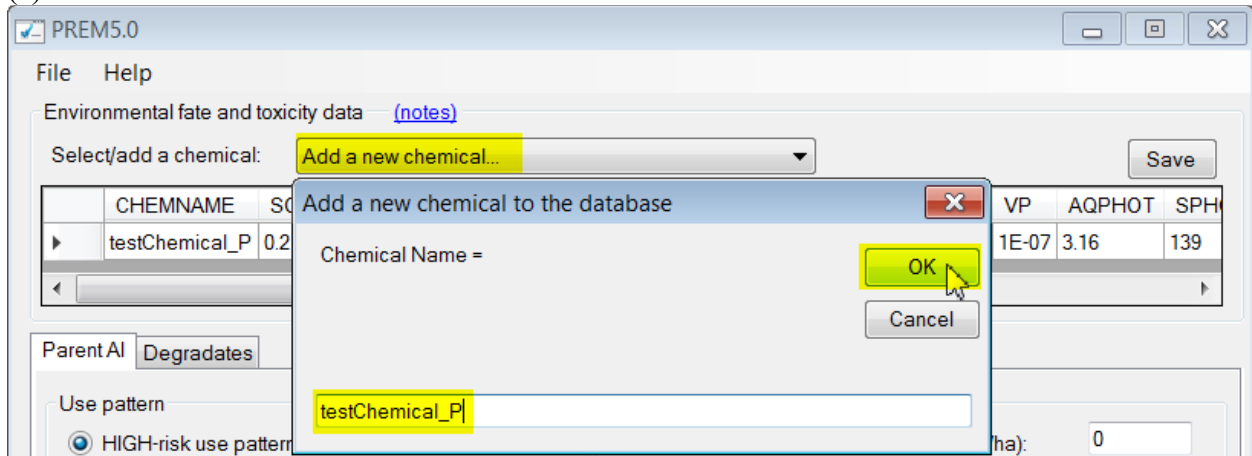
Figure 5. Select an existing chemical for data review and editing

3.1.3 Add a new chemical to the database

If the chemical (AI or degradates) to be evaluated is not in the built-in database, users can create a new data entry for the chemical (Figure 6a). 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.

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. After all the changes have been done, confirm the changes by clicking the “Save” button (Figure 6b). The program will warn users if unsaved changes are detected. Scientific notation is allowed in the data viewer/editor, and encouraged for smaller values, e.g., “1e-4” or “1E-4” is used for “0.0001”.

(a)



(b)

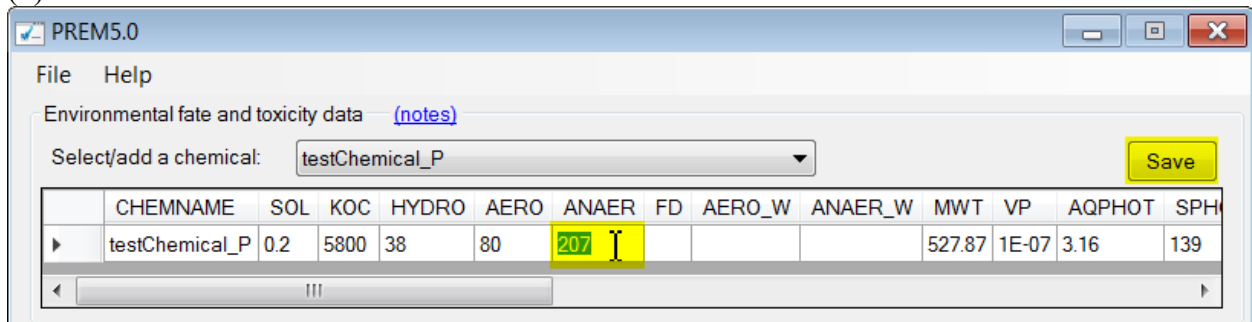


Figure 6. Create a data entry for a new chemical in the database

3.2 Pesticide applications

3.2.1 Pesticide use patterns and associated modeling scenario

Carefully inspect the application instructions on the product label. If the pesticide product is associated with the listed high-risk use patterns (Figure 7), select the use pattern as a modeling scenario. If more than one listed high-risk use patterns are listed on the product label, each of them needs to be modeled separately. Water-holding time is needed for rice pesticides.

Otherwise, if none of the use patterns in the label are listed as high-risk patterns, check the option for “Use pattern with LOW runoff potential to surface water”.

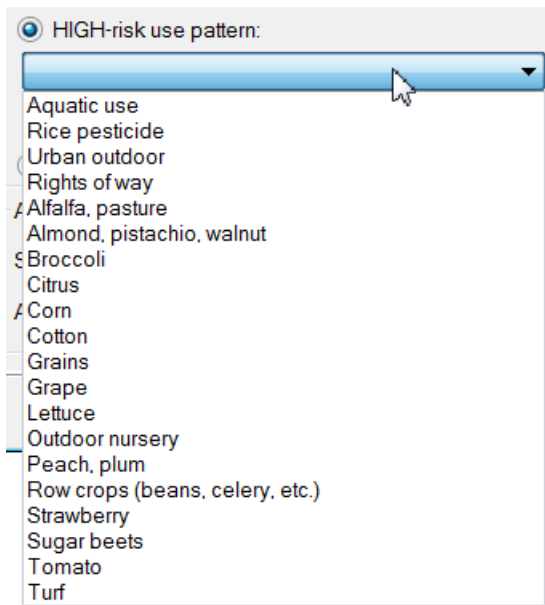


Figure 7. High-risk use patterns to be evaluated in the model

Two special cases of pesticide use pattern:

- Seed treatment: model-based evaluation is not recommended at this time since the required physicochemical properties and application information may not be available for a product labeled for seed treatment.
- Vector control: use patterns for vector control is determined based on the landscape characteristics of the treated area. For example, the modeling scenario of “alfalfa, pasture” has been used to evaluate an adult mosquito insecticide in agricultural areas). Vector control can be modeled in PREM by specifying the application efficiency (deposition to the target surface) and drift fraction. See the next section for more information.

3.2.2 Application efficiency and drift fraction

Both application efficiency and drift fraction are defined based on the areal deposited mass of pesticide relative to the application rate. For example, 10 kg of pesticide are applied to the 10-ha agricultural field, suggesting an application rate of 1 kg/ha. If 9.9 kg are deposited on the field (10 ha) and 0.03 kg on the receiving water body (1 ha),

- Application efficiency = $[9.9 \text{ kg}] \div [10 \text{ ha}] \div [\text{Application rate of } 1 \text{ kg/ha}] = 0.99$
- Drift fraction = $[0.03 \text{ kg}] \div [1 \text{ ha}] \div [\text{Application rate of } 1 \text{ kg/ha}] = 0.03$

Five options are provided in PREM for specifying application efficiency and drift fraction (Figure 8): [1] Aerial application, [2] Ground application, [3] Air-blast application, [4] No drift, and [5] User-defined values. The first three methods are consistent to the USEPA modeling settings (USEPA, 2009), with suggested values for application efficiency and spray drift fraction in Table 2. The option of “No drift” is used for urban outdoor applications, representing condition with the highest application efficiency (1.00) and lowest spray drift fraction (0.00).

With the option for “User-defined” values, the model allows manual revisions on the default values of application efficiency and spray drift fraction. Refined estimates from external models, such as AgDRIFT or AgDISP, can be used in the model. For example, AgDISP model has been used to estimate application efficiency of an adult mosquito insecticide in agricultural areas.

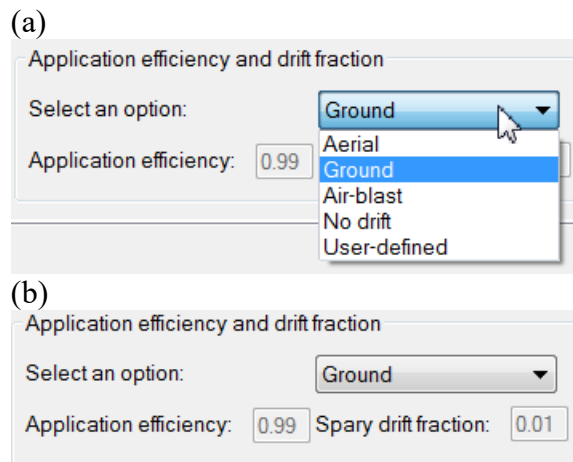


Figure 8. Application efficiency and drift fraction: (a) available options and (b) example of model inputs

Table 2. USEPA suggested application efficiency and spray drift fractions by application methods (USEPA, 2009; Young, 2014)

	Aerial	Ground	Air-blast
Application efficiency	0.95	0.99	0.99
Spray drift fraction	0.05	0.01	0.03

3.2.3 Application rate and associated data

Characterization of a single application (with application rate and application date)

For each single application event, the application rate is defined as the applied pesticide mass divided by the target surface area of treatment, with unit of kg[AI]/ha. A rate calculator is provided to assist with the determination of application rate when information from the product label is in alternative units (Figure 9).

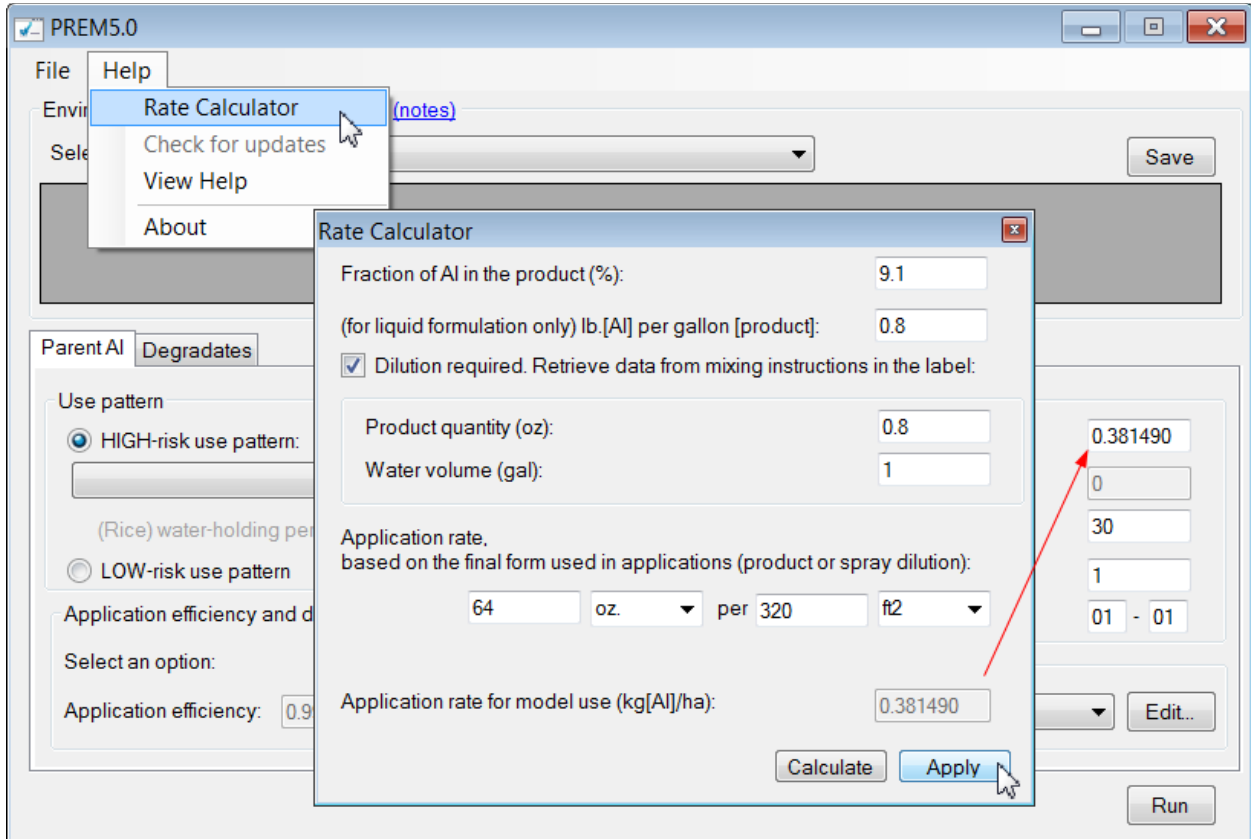


Figure 9. Application rate calculator

For aquatic uses, pesticide application can be characterized by either application rate (kg/ha) or target concentration (ppb) (Figure 10).

The screenshot shows a software interface for configuring application rates for aquatic uses. It is organized into four main sections:

- Use pattern:** Includes radio buttons for "HIGH-risk use pattern" (selected) and "LOW-risk use pattern". Below is a dropdown menu set to "Aquatic use" and a text input field for "(Rice) water-holding period (day)" with the value "0".
- Application rate and date(s):** Includes radio buttons for "Max. rate of single application (kg[Ai]/ha)" and "(aquatic uses) target conc. in water (ppb)" (selected). Below are input fields for "Min. interval (day) between two applications" (30), "Max. number of applications per year" (1), and "Date of the first application (dd-mm)" (01 - 01).
- Application efficiency and drift fraction:** Includes a dropdown for "Select an option" set to "No drift". Below are input fields for "Application efficiency" (1.00) and "Spray drift fraction" (0.00).
- Receiving-water scenario:** Includes a dropdown menu set to "USEPA pond" and an "Edit..." button.

Figure 10. Options for the application rate for aquatic uses

The date for the first application is dependent on the proposed use patterns, application methods, and target pests, and should be derived from the product label. For pesticide uses on terrestrial crops, crop profiles provided by the Western Integrated Pest Management Center (<http://westernipm.org/index.cfm/searchable-data-sources/pmsps-and-crop-profiles/>) should be helpful for the determination of application dates. For rice pesticides, pre- or post-flood applications can be scheduled, respectively, before and after the first flooding event (e.g., May 25th by default). If no relevant information is provided, the model will use the first day of the month of crop maturation for terrestrial crops, based on the USEPA Tier-2 modeling scenarios (USEPA, 2016), June 1st for rice pesticides, and January 1st for other use patterns (e.g., aquatic, urban, and rights-of-way applications).

Characterization of multiple applications (application interval and number of applications)

Multiple applications are defined by the minimum application interval and the maximum number of applications per year. The maximum number of applications should be determined based on the maximum allowable use amount per year, which includes potential uses over multiple crop seasons.

Rice cultivation often requires water holding times prior to release. As a result, multiple applications of rice pesticides are defined in a different way than other use patterns. The number of applications is counted for each water holding period (as shown in the model interface as "Max. number of applications per held water"). The model will confirm this with a user if multiple applications of rice pesticides are to be modeled (Figure 11).

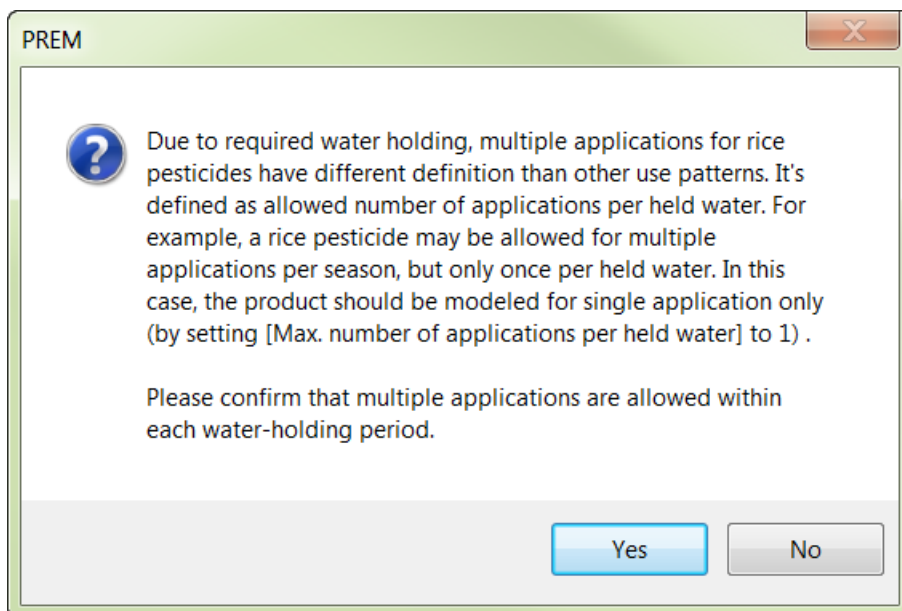


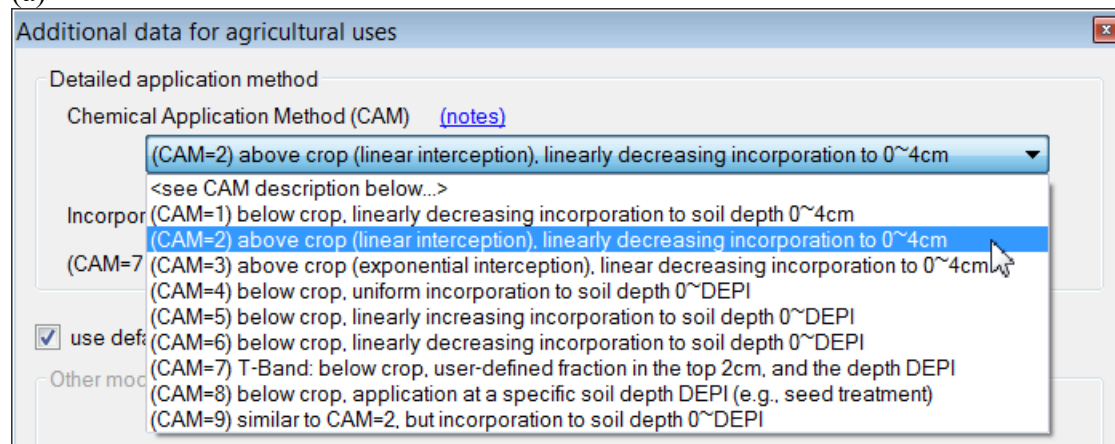
Figure 11. Warning message for multiple applications of rice pesticides

Some products may allow for multiple use patterns with varying application rates and frequencies. In this case, the potential combinations of use patterns, rates, and frequencies should be evaluated individually. The results are tabulated to determine the greatest risk quotient.

3.2.4 Additional data for agricultural uses

For terrestrial agricultural uses, the model will ask for additional data mainly for ground application method and characteristics of the canopy-soil system to be evaluated (Figure 12). Pesticide application method is defined in the model by crop interception (above vs. below canopy) and soil incorporation (depth and distribution) (Young, 2016). CAM=1 (for below-crop application including soil incorporation) or CAM=2 (above-crop application) with USEPA default values are recommended for registration evaluation, unless there are specific requirements in the product label for application method.

(a)



(b)

The screenshot shows a software window titled "Additional data for agricultural uses". It contains the following elements:

- Detailed application method:**
 - Chemical Application Method (CAM) [\(notes\)](#): A dropdown menu with the selected option "(CAM=2) above crop (linear interception), linearly decreasing incorporation to 0~4cm".
 - Incorporation depth (cm) DEPI: A text input field containing the value "4".
 - (CAM=7 only) fraction incorporated into the top 2cm: A text input field containing the value "0.5".
- use default values as suggested by USEPA
- Other model inputs (use USEPA default values unless field data are available):**
 - Foliar extraction (1/cm) FEXTRC: 0.5
 - Volatilization rate from foliage (1/day) PLVKRT: 0
 - Decay rate on foliage (1/day) PLDKRT: 0
 - Plant uptake factor (decimal) UPTKF: 0
 - Post-harvest foliar pesticide disposition IPSCND (1=surface applied, 2= removed, 3=left alone): 1

Figure 12. Additional data required for terrestrial agricultural uses: (a) options for chemical application method and (b) example model inputs

3.2.5 Additional data for rice pesticides and applications to other flooded fields

For rice pesticides or pesticide applications to other flooded fields, the model will ask for additional data detailing water management and crop growth. The model incorporates representative parameter values suggested by USEPA for the modeling scenario of California rice production (Figure 13), and allow users to revise the values to represent the environmental settings required in the product label.

Additional parameters for evaluation in flooded fields

use California rice scenario

Operational calendar

Water management	Month	Day	Target water depth (m)
Initial flooding	5	3	0.1016
Final drainage	9	25	0

Crop data	Month	Day	Max. areal coverage
Seedling	5	23	
Maturity	9	25	1
Harvest	10	9	

Built-in assumptions

heat of enthalpy (J/mol)=59,000 leakage (m/d)=0
reference temperature (C)=20 slow release (1/day)=0
weather data=Sacramento (WBAN# 23232)

Other physical parameters follow the parameterization in "USEPA pond".
Please refer to the "receiving-water scenario" for more information.

Submit

Figure 13. Additional data for pesticide uses in flooded fields

3.2.6 Additional data for urban outdoor uses

For urban outdoor uses, the model will ask for additional data on the land use (residential or commercial/industrial) and application method (Figure 14). Modeled application methods are associated with intended or unintended (e.g., overspray to adjacent paved areas during lawn treatment). Four types of application methods are predefined in the model, including applications to lawns, paved areas, foundation perimeter, and cracks and crevices. For perimeter treatment, users should provide application bandwidth for horizontal and vertical surfaces. The model will automatically calculate the total fractions and treated fractions (in percentage) 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.

(a)

Additional data for urban outdoor uses

Label information for urban uses

Landscape settings Residential Commercial/industrial

Application method

- Broadcast application (lawn)
- Application on paved areas (driveway and walkway)
- Perimeter treatment (including wall treatment)
- Crack & crevice treatment

0

(b)

Additional data for urban outdoor uses

Label information for urban uses

Landscape settings Residential Commercial/industrial

Application method

Perimeter treatment (including wall treatment)

For perimeter application only

Width of application (ft), on ground= 1 wall= 1

Granular application

Adjustment on application extent, for residential insecticides only

Update

Treated area fractions

Pervious surfaces:

- without dry-weather runoff 0 %
- with dry-weather runoff 0 %

Impervious surfaces that could result in runoff to storm drains:

- without dry-weather runoff 1.756 %
- with dry-weather runoff 0.482 %

Other impervious surfaces (drain to adjacent pervious surfaces) 3.642 %

Submit

Figure 14. Additional data for urban outdoor uses: (a) options for application methods for urban outdoor pest control, and (b) example input data

The general procedures to characterize urban outdoor uses are:

- (1) Read the product label and summarize the product formulation, use pattern, and application method.
- (2) Select landscape settings (residential or commercial/industrial).
- (3) If the proposed application method can be represented by the predefined ones, continue with step (4); otherwise, go to step (8).
- (4) Select application method, and specify widths of application (for perimeter treatment only).
- (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) If the pesticide product is evaluated as insecticides for residential uses, the option for “Adjustment on application extent” should be checked. With this option, the label rate is adjusted by the fraction of households treated with residential outdoor pesticide products (75.9%) (Luo, 2017).
- (7) Confirm the inputs by clicking “update” button.
- (8) Manually revise the treated area fractions as needed. This is mainly used to characterize an application method that is not predefined in the model.
- (9) “Submit” the input data to the model.

3.3 Receiving water body

The USEPA standard farm pond is used as the default modeling scenarios for receiving water body in PREM. SWPP evaluated various scenarios and concluded that the pond scenario is appropriate for the screening-level regulatory exposure assessment in the agricultural (Xie et al., 2018) and urban (Luo, 2014) settings of California. The associated parameters can be displayed by selecting the scenario then clicking the “Edit...” button (Figure 15). The model also allows users to create their own modeling scenarios by altering numerical values for the receiving-water parameters.

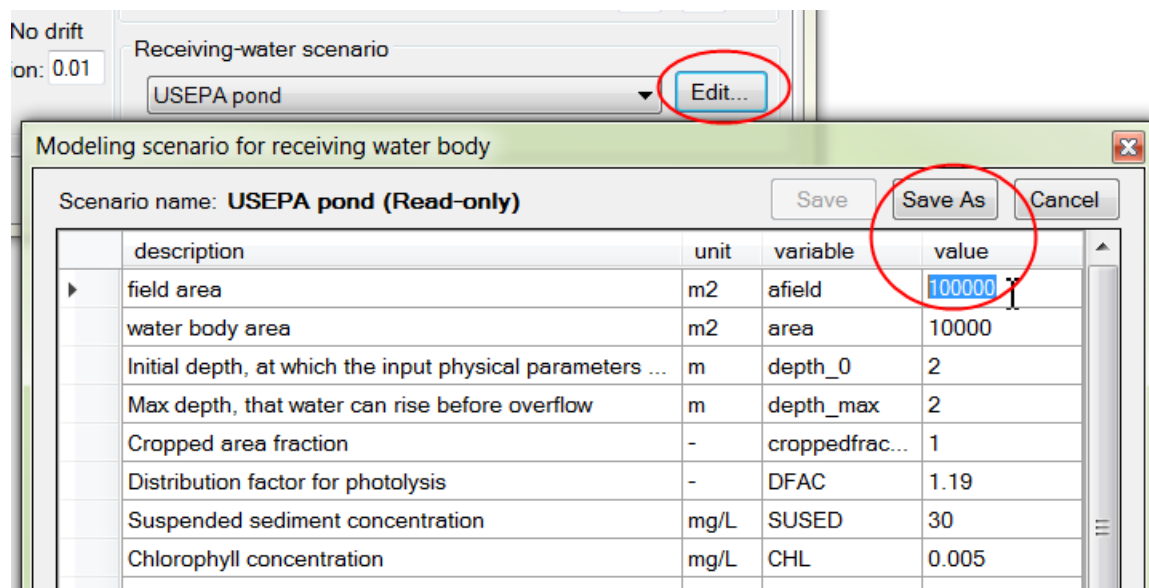


Figure 15. Editors for receiving-water modeling scenario

A receiving water body does not apply to rice pesticides. According to the guidance for modeling pesticide concentrations in rice growing areas (Biscoe et al., 2016): for ecological risk assessment, exposures to aquatic invertebrates and vertebrates are assessed in the rice paddy.

3.4 Degradate evaluation

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 done by model users.

- **Step 1** (by the model): **Evaluation for the parent compound only, by *unchecking* the option for degradate evaluation** (Figure 16). After the evaluation on the parent, the model will also conduct initial screening for pesticide degradates, and provide suggestions for the next step of evaluation:
 - A warning message will show if there are degradates that have high potential to cause aquatic toxicity (Figure 17a).
 - 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.
 - If the modeling results for the parent compound are to support or conditionally support registration, *continue to Step 2* for additional considerations.
 - If there is no warning message for pesticide degradates at the end of the evaluation, degradate evaluation is not required.

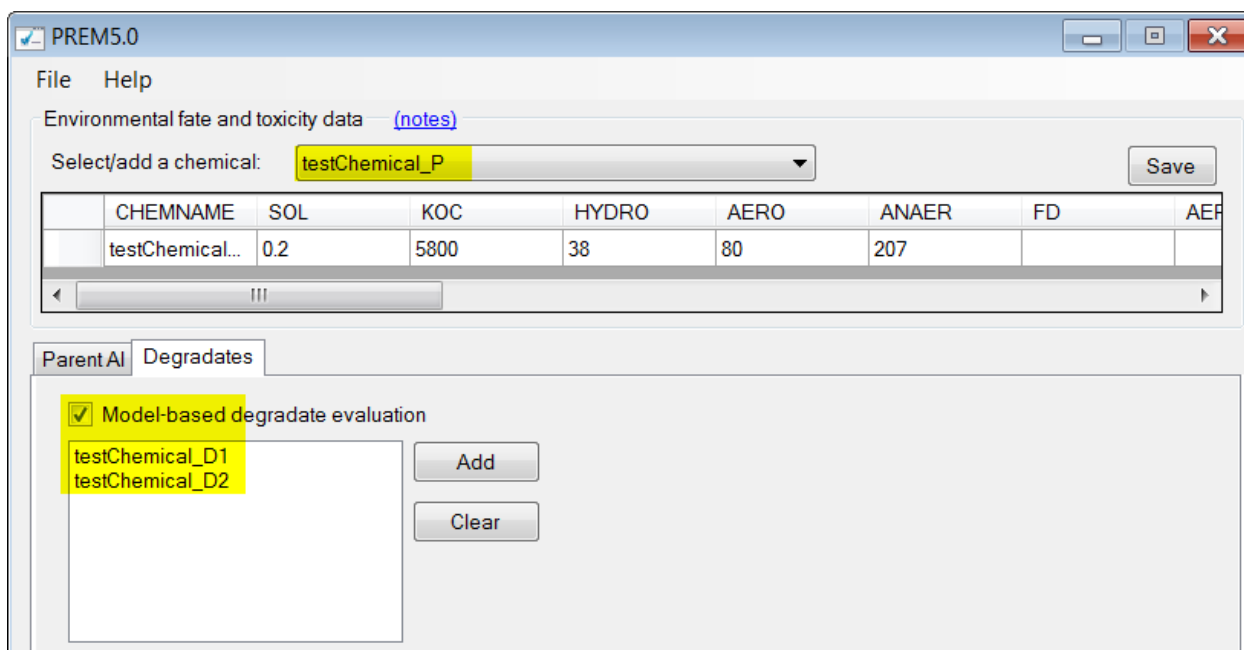


Figure 16. Example of model settings for degradate evaluation. The parent compound is selected in the data viewer/editor, while the degradates for modeling are specified in the “Degradates” panel.

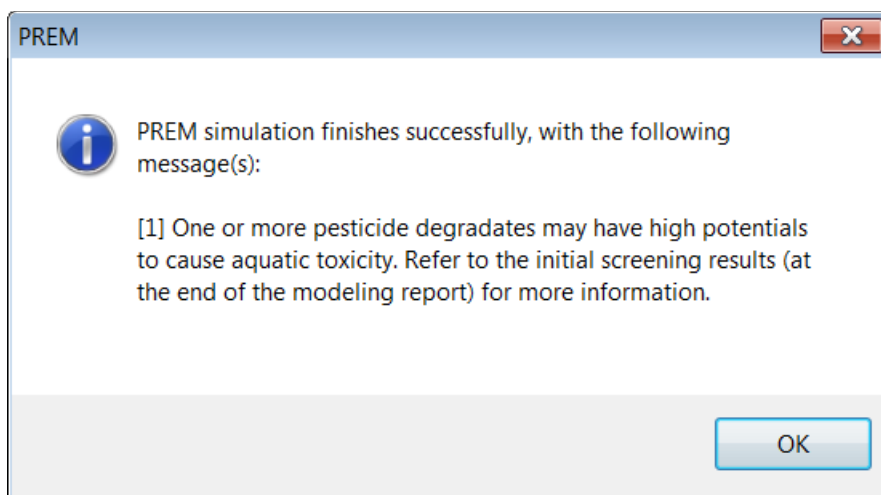


Figure 17. Warning message for potential degradate evaluation

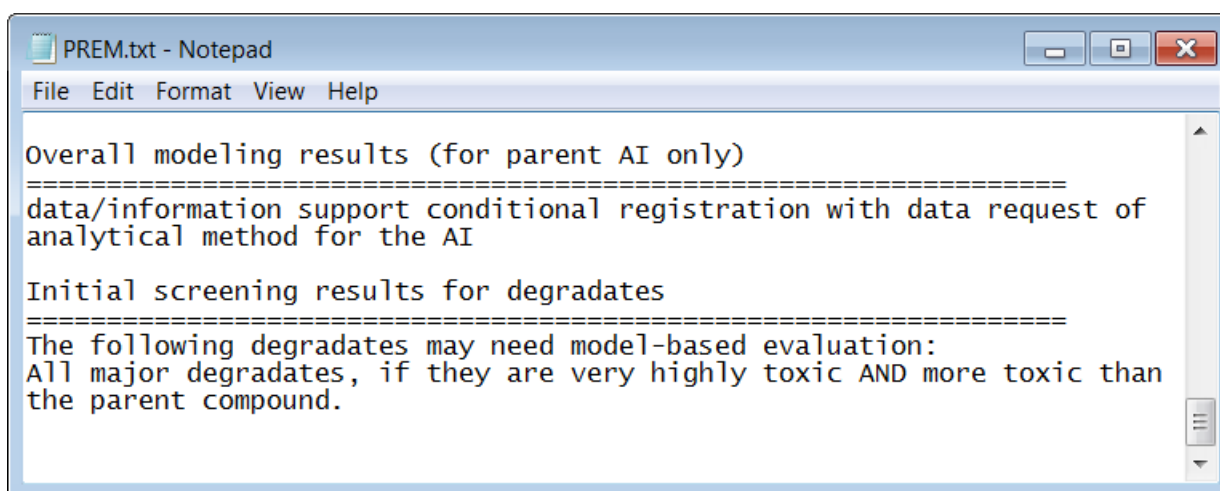


Figure 18. Example of modeling results for parent-only evaluation and initial screening for degradates

- Step 2 (by users): **Data collection and analysis for degradate toxicity by following the results of initial screening for degradate.** In the modeling report, the initial screening results include the candidate degradates (by degradation pathways) and associated criteria for potential model-based evaluations (Figure 18). 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 DPR’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 the 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*. The results of initial screening may also be a request to flag the parent compound for future evaluations if its use pattern changes (Figure 18).

- **Step 3 (by the model): Model-based evaluation on degradates identified in the previous step.**
 - Prepare model input data for the degradates to be modeled by following the guideline in Section “Guideline for data preparation;”
 - Create data entries for the degradates with physicochemical properties and toxicity data (see Section “Add a new chemical to the database”);
 - Select the parent compound in the data viewer/editor (Figure 16), and fill all required input data (use pattern, application info, etc.) for the parent compound;
 - In the panel of “Degradate,” list the degradates to be modeled, and *check* the option for “model-based evaluation” (Figure 16); and
 - Run the model for the combined evaluation of the parent compound and selected degradates.

4 Modeling results and evaluation report template

For each modeling scenario, two text files will be generated:

- (1) Modeling report (“PREM.txt”) with model inputs, outputs, and model-based recommendations. 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.
- (2) Daily time series of risk quotients (“RQ.txt”) in water column and in pore water of the modeled receiving water body. Save this file for your own reference.

An evaluation report is typically organized into five sections: recommendation summary, background, evaluation, conclusion, and references.

5 Guideline for data preparation

5.1 Data Sources

Potential input parameters for the model are listed in Table 1, 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 DPR’s Pesticide Registration Branch (PRB).

Registration packages with previously registered AIs may rely on data submitted from previous data submission. For input parameters not available or not approved in DPR’s previous evaluations, data from open literature could be used. Please provide references for the sources you used to retrieve the data.

5.2 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, FD, and HYDRO) for the comparison with groundwater leaching criteria (Figure 22). If **a single representative value** is provided in the table (e.g., SOL=0.1 ppm, Figure 22), it should be used for the corresponding parameter. For a parameter reported as **a range of values** in the table (e.g., KOC=54–487, Figure 22), or **not summarized** in the table (e.g., AERO_W), individual values of the parameter should be retrieved from the main text of the chemistry report. In this case, the following procedures are proposed for input data preparation:

Property	Potential to Leach if:	Experimental Values	Exceed Criteria?
<i>U.S. EPA</i>			
Water Solubility	> 30 ppm	0.1 ppm	No
Adsorption Coefficient (K _d)	< 5 mL/g	54-487	No
Hydrolytic Half-Life	> 175 days	20-34 days	No
Photolytic Half-Life (days) ¹	> 7 days	28 days	Yes
Aerobic Soil Metabolism	> 21 days	122 days	Yes
Anaerobic Soil Metabolism	> 21 days	No data	
Field Dissipation Half-Life	> 21 days	26-83 days	Yes
<i>CA EPA</i>			
K _{oc}	< 1900 mL/g	15800-42100	No
or Water Solubility	> 3 ppm	0.1 ppm	No
Hydrolytic Half-Life	> 14 days	20-34 days	Yes
or Aerobic Soil Metabolism	> 610 days	122 days	No
or Anaerobic Soil Metabolism	> 9 days	No data	

¹Photolysis in water

Figure 19. Example of data summary table in the chemistry review reports

- (1) Only use the test results from registrant-submitted studies, which are considered to be **acceptable** by the chemistry evaluation.
- (2) If there were tests performed under **California field conditions**, use the test results from those studies.
- (3) Generally, the representative value of an input parameter is the **median value** of the individual test results. Taking Figure 23 as an example, the field dissipation half-life is set as 44 days, as the median of all reported and accepted values.

Study No./Location/Soil Type	Length of Sample Collection (days)	Depth of Movement (cm)	T _{1/2} (Days)	Final Residue (ppm)	Volume/ Study Record No.
DowElanco GHE-P-3610 (1994)/Germany (Herford-Eickum)/Loamy silt. Bareground plot ¹	216	5	55 (R ² = 0.86)	0.013	0070/253037
DowElanco GHE-P-3610 (1994)/Germany (Adelshausen)/Loamy sand. Bareground plot ¹	215	5	41 (R ² = 0.84)	0.006	
DowElanco GHE-P-4517 (1996)/Italy (Grugno)/Loam. Bareground plot ²	369	10	44 (R ² = 0.99)	<0.005	0071/253038
DowElanco GHE-P-4517 (1996)/Italy (Fognamo)/Clay loam. Bareground plot ²	368	20	75 (R ² = 0.62)	0.006	
DowElanco GHE-P-3222 (1993)/Germany (Lauter)/Loamy silt. Bareground plot ³	363	5	26 (R ² = 0.95)	<0.005	0072/253039
DowElanco GHE-P-3222 (1993)/Germany (Landsberg)/Silty clay loam. Bareground plot ³	365	5	83 (R ² = 0.93)	0.007	
DowElanco GHE-P-3222 (1993)/Germany (Grebien)/Silt loam. Bareground plot ³	360	5	66 (R ² = 0.84)	<0.005	
DowElanco ABC 0417 (1988)/[¹⁴ C]-XDE-436 /Indiana, Loam. Soil enclosed in a metal ring ⁴	112	22.9	38 (R ² = 0.99)	Not recorded	0069/253036
DowElanco ABC 0417 (1989)/[¹⁴ C]-XDE-436 /Indiana, Loam. Soil enclosed in a metal ring ⁴	168	30.5	34 (R ² = 0.96)	Not recorded	

Figure 20. Test results summarized in a chemistry evaluation report, field dissipation studies as an example.

- (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, and the model will consider those as missing data and assign a default half-life of 99,995 days (see Section “Missing data handling”).

Environmental fate and toxicity data [\(notes\)](#)

Select/add a chemical:

	CHEMNAME	SOL	KOC	HYDRO	AERO	ANAER	FD	AERO_W	ANAER_W	MWT	VP	AQPHOT
▶	testChemical_P	0.2	5800	38	80	207				527.87	1E-07	3.16

Figure 21. Blank cells in the data viewer/editor for input parameters of half-lives, representing stable degradation process

- (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, the results under **neutral pH** conditions (pH=7 or around 7) should be used for registration evaluation.

The same procedures can be used for the data preparation for **degradates**. 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 if they have been submitted by the registrant and reviewed by PRB.

5.3 Aquatic toxicity data

Toxicity values are usually summarized at the end of the ecotoxicology evaluation report (Figure 25). 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
<i>Daphnia magna</i>	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 22. 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 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 **LC50 and EC50** values from **acute** toxicity test (as indicated in the “Type of study,” Figure 25, 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 LC50 or EC50 is available, use other reported data (e.g., chronic LOEC or NOEC) for sediment-dwelling organisms. If no data are provided in the ecotoxicology evaluation report, please refer to the section “Missing data handling.”
- (6) 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.
- (7) If a toxicity value is reported as "larger than (>)" or "less than (<)" a certain value, the provided value will be used.
- (8) For water toxicity, retrieved values should be converted into the unit of **µg/L**. For sediment toxicity, retrieved values should be converted into the model-required unit according to the mass basis of the reported data, i.e., **µg/L** for pore-water concentration,

µg/kg[dry weight] for sediment mass based concentration, or **µg/g[OC]** for organic carbon based concentration.

(9) Fill the following worksheet with retrieved toxicity values. 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:

(9.1) 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.

(9.2) from µg/g[OC] to pore water µg/L: (value in µg/g[OC])/KOC*1000

<p><u>Water toxicity, freshwater</u></p> <p>Individual values, with potential test species</p> <ul style="list-style-type: none"> ▪ Bluegill (<i>Lepomis macrochirus</i>) ▪ Common carp (<i>Cyprinus carpio</i>) ▪ <i>Daphnia pulex</i> ▪ Fathead minnow (<i>Pimephales promelas</i>) ▪ Rainbow trout (<i>Oncorhynchus mykiss</i>) ▪ Water flea (<i>Daphnia magna</i>) ▪ Others <p>The lowest value (“NA” if no data in this category) =</p>	<p><u>Sediment toxicity, freshwater</u></p> <p>Individual values, with potential test species</p> <ul style="list-style-type: none"> ▪ <i>Hyalella azteca</i> ▪ Midge larvae (<i>Chironomus dilutus</i>, formerly named as <i>Chironomus tentans</i>) ▪ Others <p>The lowest value (“NA” if no data in this category) =</p>
<p><u>Water toxicity, marine/estuarine</u></p> <p>Individual values, with potential test species</p> <ul style="list-style-type: none"> ▪ Eastern oyster ▪ Saltwater mysid (<i>Americamysis bahia</i>) ▪ Sheepshead minnow ▪ Others <p>The lowest value (“NA” if no data in this category)=</p>	<p><u>Sediment toxicity, marine/estuarine</u></p> <p>Individual values, with potential test species</p> <ul style="list-style-type: none"> ▪ <i>Eohaustorius estuarius</i> ▪ <i>Leptocheirus plumulosus</i> ▪ <i>Rhepoxynius abronius</i> ▪ Others <p>The lowest value (“NA” if no data in this category) =</p>
<p>The lowest value of water toxicity (all species) =</p>	<p>The lowest value of sediment toxicity (all species) =</p>

(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:

(10.1) The product may have **low** exposure potential to marine/estuarine species (Figure 26). In this case, **keep using the lowest toxicity values for freshwater species** for TOX and TOXSED in the evaluation.

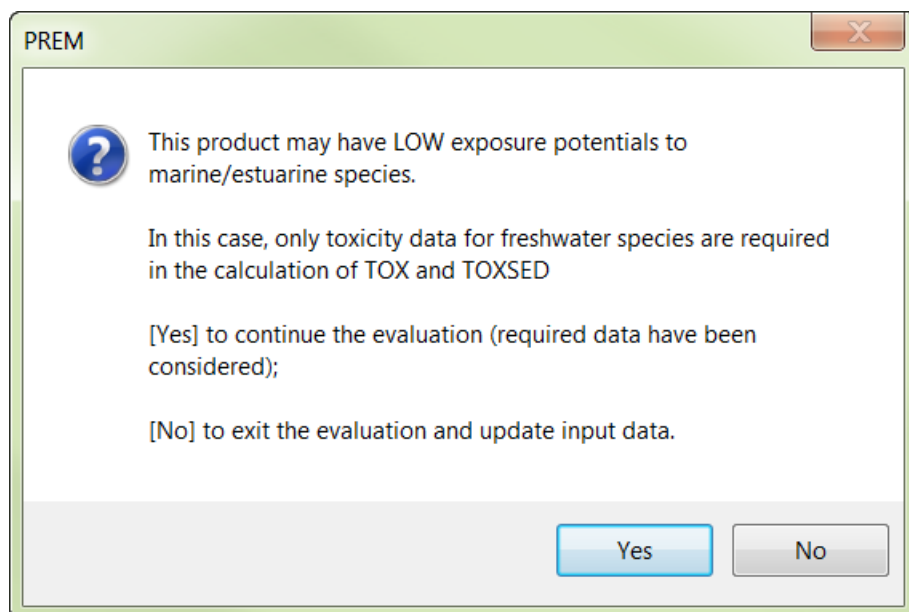


Figure 23. Warning message for a product with low exposure potential to marine/estuarine species

(10.2) The product may have **high** exposure potential to marine/estuarine species according to the use patterns (Figure 27). 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.

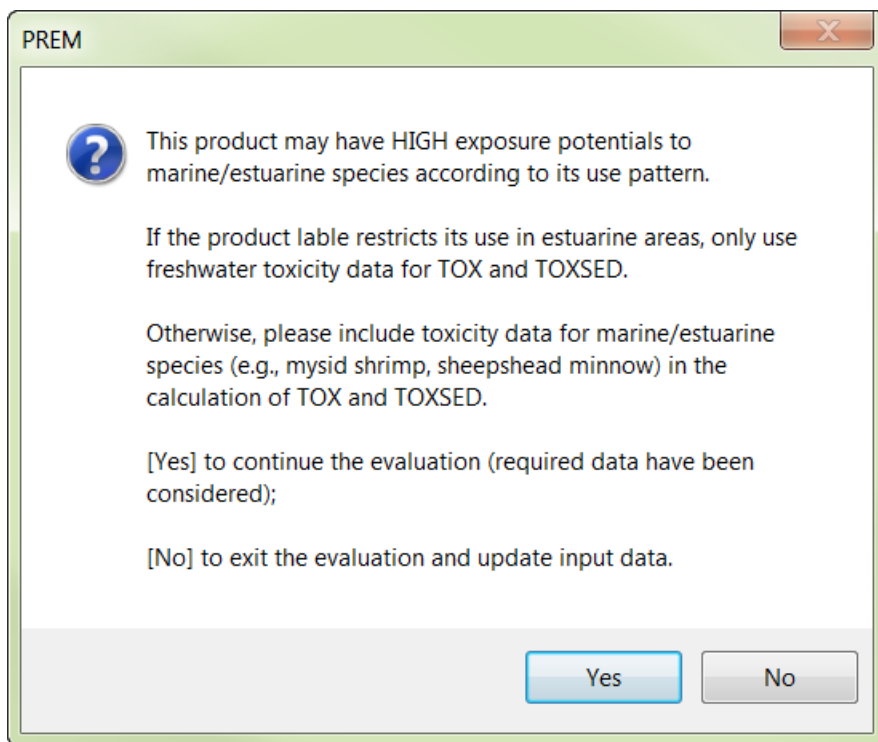


Figure 24. Warning message for a product with high exposure potential to marine/estuarine species according to the use patterns

(10.3) The product may have high exposure potential to marine/estuarine species according to the physicochemical properties of its AI (Figure 28). Similar to (9.2), 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.

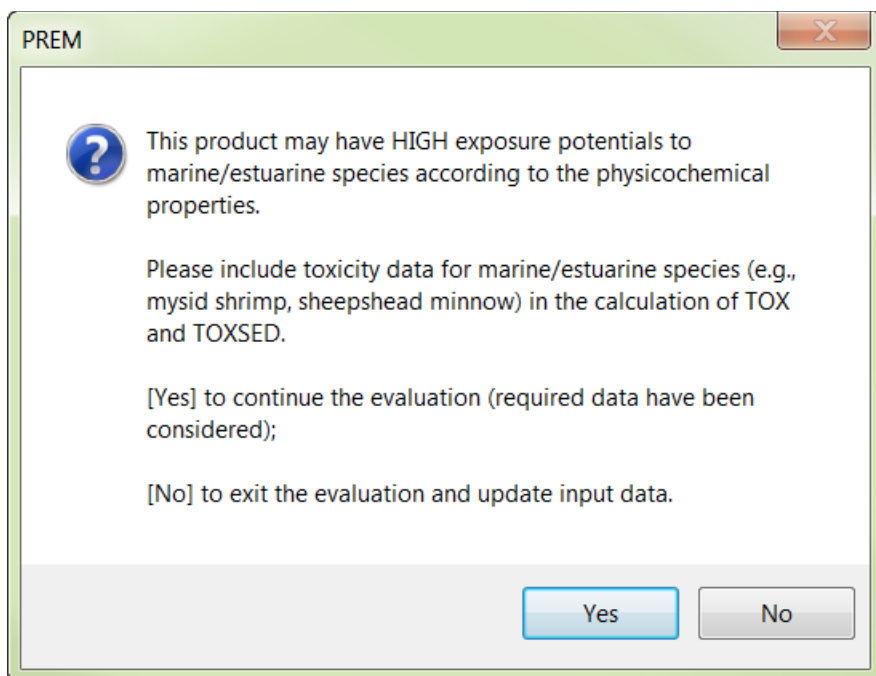


Figure 25. Warning message for a product with high exposure potential to marine/estuarine species according to the physicochemical properties

5.4 Molar formation fractions (for degradate only)

Molar formation fractions are only required for degradates, when some of them are required for model-based evaluations (see section “Degradate evaluation”). If the fractions are not provided by the registrants, SWPP will either calculate the fraction values (with data from dissipation studies) or conservatively estimate the values (without sufficient data for calculation).

5.5 Missing data handling

If there are still missing data (presented as blank cells in the data editor) by following all procedures in the guideline, the model will:

- (1) 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 DK’s are required for degradates. Figure 29 shows an example message if the water solubility (SOL) value is missing for a parent compound.

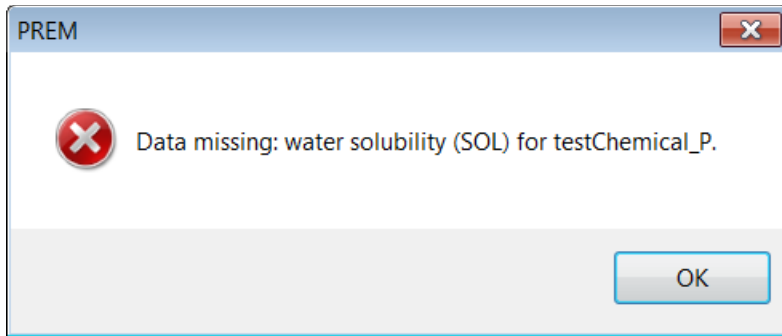


Figure 26. Error message for missing data of water solubility

(2) Replace missing data with default values or estimates:

(2.1) 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. For soil photolysis (SPHOT) which is only used for urban evaluation, the model will confirm with users before using the default value (Figure 30)

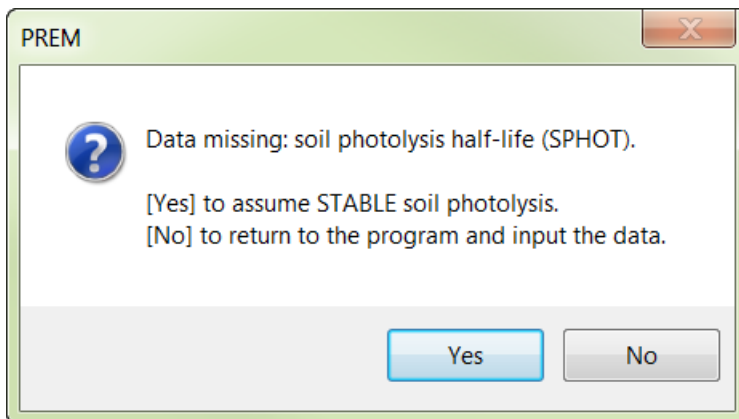


Figure 27. Warning message for missing data of soil photolysis

(2.2) Vapor pressure (VP) will be set as 1e-15 torr, based on the 90th percentile of vapor pressure data in the Pesticide Property Database (FOOTPRINT, 2017).
(2.3) 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 31), and give a warning message at the end of the evaluation (Figure 32).

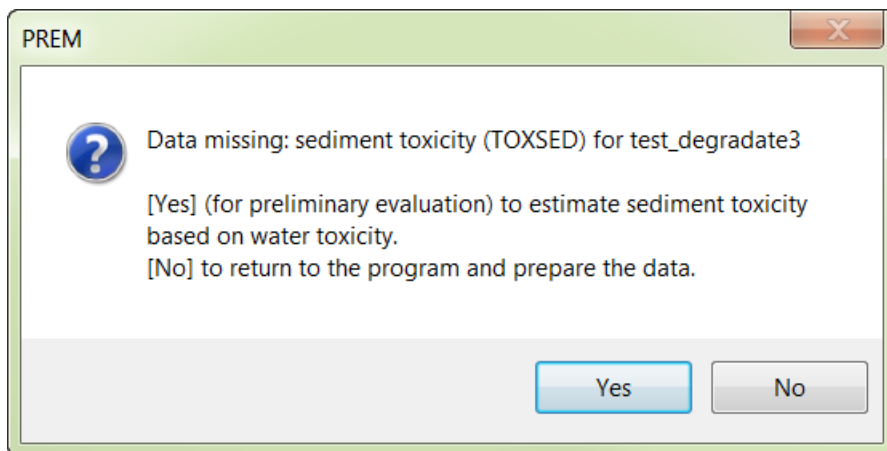


Figure 28. Warning message: sediment toxicity is missing

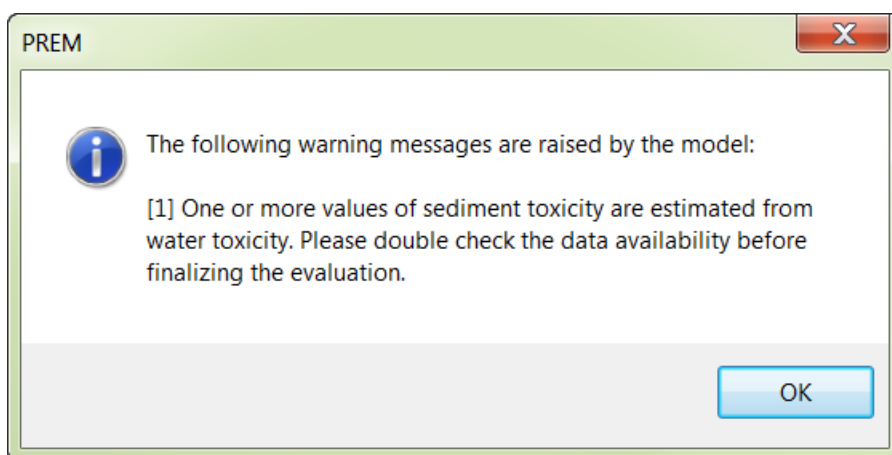


Figure 29. Warning message: estimated sediment toxicity was used in the evaluation

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