

## SWPP Registration Evaluation Model User Manual (Version 3.1)

Revision Date: October 2, 2014

### Contact Information:

Yuzhou Luo, Ph.D.  
Research Scientist III  
[yuzhou.luo@cdpr.ca.gov](mailto:yuzhou.luo@cdpr.ca.gov)

Nan Singhasemanon  
Senior Environmental Scientist  
[nan.singhasemanon@cdpr.ca.gov](mailto:nan.singhasemanon@cdpr.ca.gov)






Surface Water Protection Program, Environmental Monitoring Branch  
California Department of Pesticide Regulation, Sacramento, CA 95812

## OVERVIEW

The Surface Water Protection Program (SWPP) is developing a more consistent and transparent method for evaluating registration packages. Details of the model development and validation have been documented in the technical reports (Luo et al., 2012a, b; Luo, 2014). A computer program is developed to implement the model with a graphical user interface. The purpose of this document is to provide instructions to use the program.

General use patterns of a pesticide should be determined from the proposed product labels before the model-based evaluation. Table 1 listed the included use patterns and modeling capabilities in the current version of the model. Unlisted use patterns, such as antimicrobial products for indoor use and antifouling paint products, cannot be evaluated with the model.

Table 1. Overview in terms of modeling scenarios for registration evaluation (version 3.1)

General use pattern	Initial screening	RQ <sup>1</sup> without dilution by receiving water	RQ with dilution in the USEPA standard farm pond (EXAMS)
Aquatic uses	 USEPA scenarios are not available, SWPP <sup>3</sup> evaluation based on initial screening only	See Note <sup>2</sup>	
Rice pesticides	 USEPA scenario is available, and modified in SWPP model by considering water-holding time	Not considered in SWPP evaluation	
Agricultural uses (non-rice)	 USEPA scenarios are available, and used in SWPP model	 Will consider when SWPP model recommends to deny registration	
Urban uses	 SWPP urban scenario is developed for California urban conditions		

Notes: <sup>1</sup>RQ = risk quotient

<sup>2</sup> If target concentrations of aquatic application are presented or can be derived by a reviewer from the product label, the values should be used for RQ calculation. No modeling is needed in this case.

<sup>3</sup> SWPP = Surface Water Protection Program

## MODEL AND DOCUMENTATION

- Computer implementation: available in DPR internal share drive, [\\dprhq01\SurfaceWater\Registration Evaluation\\[version number\]](\\dprhq01\SurfaceWater\Registration Evaluation\[version number])
- Technical reports (<http://cdpr.ca.gov/docs/emon/surfwtr/review.htm>)
  - Luo, Y. and X. Deng (2012). Methodology for evaluating pesticides for surface water protection, I: initial screening
  - Luo, Y. and X. Deng (2012). Methodology for evaluating pesticides for surface water protection, II: refined modeling
  - Luo, Y. (2014). Methodology for evaluating pesticides for surface water protection, III: Module for urban evaluation
- Supporting documents, data, and model applications
  - Luo, Y., F. Spurlock, et al. (2011). "Use-exposure relationships of pesticides for aquatic risk assessment." PLoS ONE 6(4): e18234.
  - Luo, Y. (2012). Standard Operating Procedure, Methodology for evaluating pesticides for surface water protection (<http://cdpr.ca.gov/docs/emon/pubs/sopadmin.htm>)
  - Luo, Y. (2013). Guideline of data preparation in the registration evaluation for surface water protection (<http://em/localdocs/pubs/reviews/em1301.pdf>, DPR internal webpage). **Note: the guideline has been updated in this document (please see Appendix 1).**
  - Previous model-based evaluations: Environmental Monitoring Registration Evaluation Reports ([http://em/localdocs/pubs/rr\\_revs/rr-rev.htm](http://em/localdocs/pubs/rr_revs/rr-rev.htm), DPR internal webpage)
  - Source codes, previous versions, and other related materials (<\\dprhq01\SurfaceWater\Registration Evaluation\SupportingMaterials>, DPR internal share drive)

## INSTALLATION AND UPDATING

The model is available in DPR internal share drive, [\\dprhq01\SurfaceWater\Registration Evaluation\\[version number\]](\\dprhq01\SurfaceWater\Registration Evaluation\[version number]). Please copy the entire folder, including the executable file (RegEval.exe), supporting database (RegEval.dat), and model input files (the sub-folder of "PL5") into a local hard disk of your computer. Figure 1 shows an example of the model package in D:\RegEval\. Double click "RegEval.exe" to start the model.

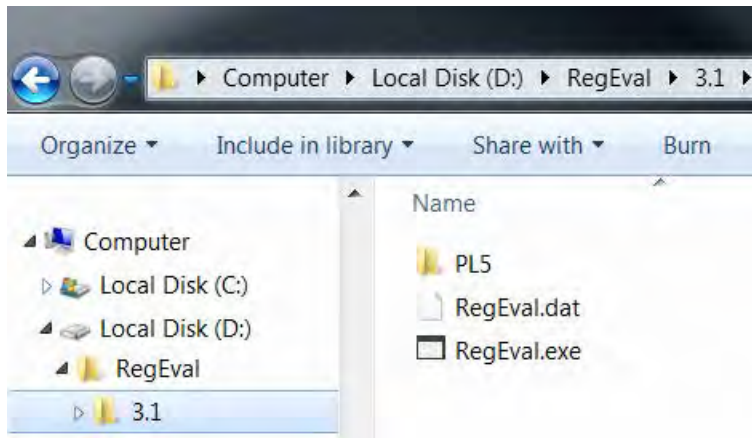


Figure 1. Registration evaluation model in a local computer

The model will automatically check the availability of new versions. A user will be notified if a newer version has been uploaded in the share drive (Figure 2). In this case, please copy new model/data and replace the old ones in your computer.

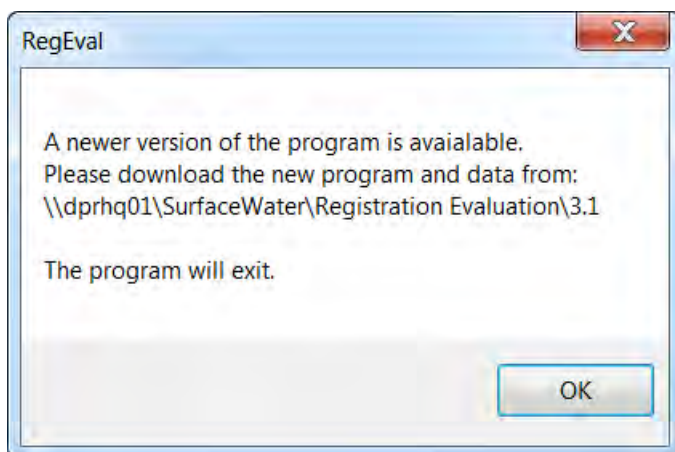


Figure 2. Message for model updating

## OVERVIEW OF THE MODEL GUI (GRAPHICAL USER INTERFACE)

The main GUI includes three panels (environmental fate and toxicity data, modeling scenarios, and application rate) and a “Run” button.

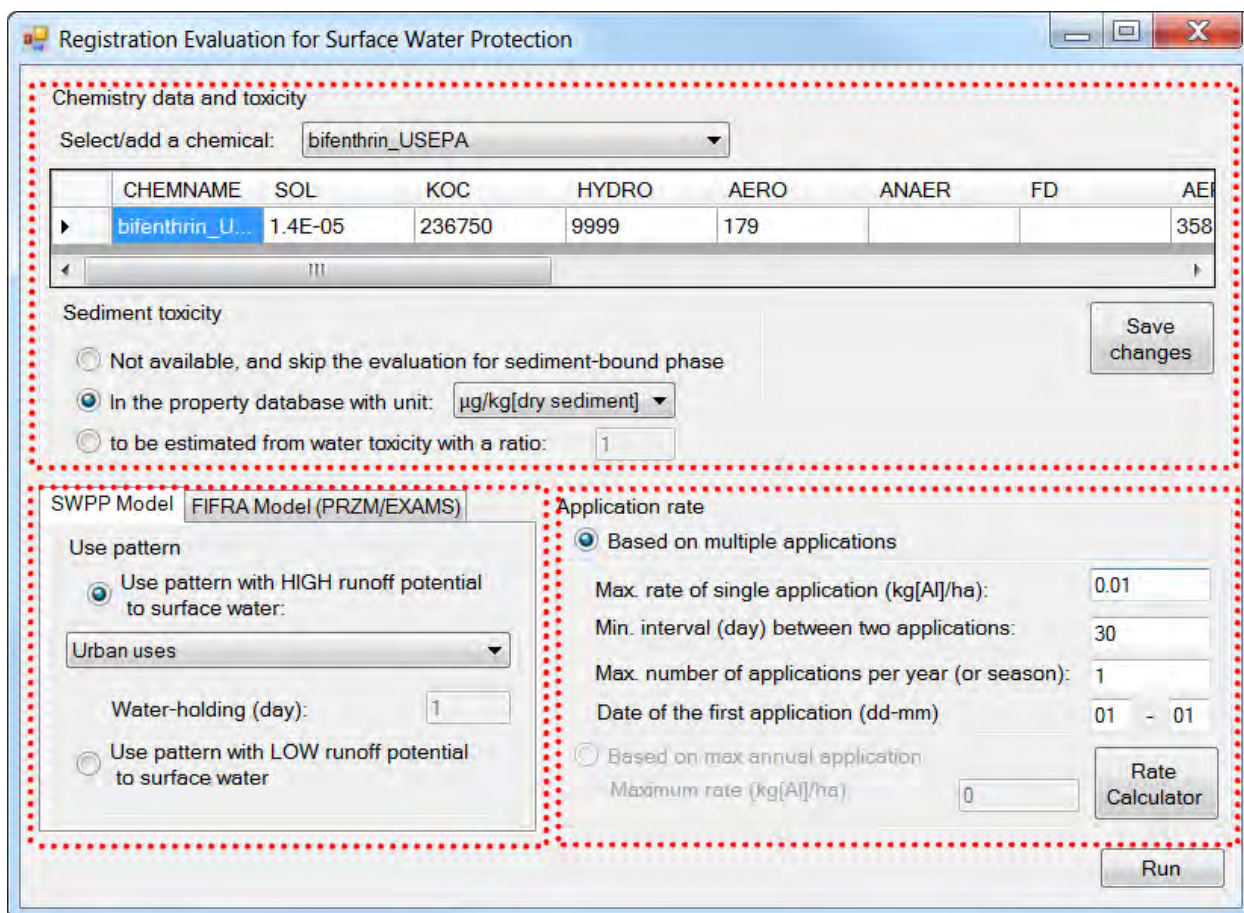


Figure 3. The main GUI of the registration evaluation model

## ENVIRONMENTAL FATE AND TOXICITY DATA


Physicochemical properties and acute aquatic toxicity data of the pesticide should be specified in this panel. Typical operations for this purpose are [1] to prepare input data, [2] to view/edit data for an existing AI in the database, and [3] to create dataset for a new active ingredient (AI).

[1] Prepare input data

**For SWPP modeling approaches including urban uses, please refer to Appendix 1 for data preparation.** For PRZM/EXAMS modeling approaches, please refer to the USEPA guidance for selecting input parameters (USEPA, 2013a).

Sediment toxicity is not required for all pesticides. The program will determine the evaluation process according to the USEPA data requirement (USEPA, 2007a) and availability of user-defined input data (Table 2).

Table 2. Data check for sediment toxicity and subsequent evaluation processes

Sediment toxicity available?	KOC>1000?	Evaluation for pesticide in sediment-bound phase
Yes	Any	Specify the unit, and conduct the evaluation based on the input value
No	No	Don't conduct the evaluation
No	Yes	Estimate sediment toxicity, and conduct the evaluation based on the estimated value.  This is also a warning message according to USEPA data requirements for pesticide registration. In this case, please check the fish & wildlife review report, discuss with Pesticide Registrant Branch, and try to fill sediment toxicity. This option (evaluation based on estimated sediment toxicity) was designed for model validation with previous reviews, but not recommended for new AI's.

[2] View and edit data for an existing AI

Use the pull-down menu to display all chemicals with data available in the built-in database (Figure 4). Data can be retrieved by selecting the chemical name in the list. **It is critical that the user verifies the existing data and make changes as needed** before using the data retrieved from the database. After all changes have been done, please confirm the changes by click the button of “save changes” (Figure 4). Before model simulation, the program will warn the user if unsaved changes are detected.

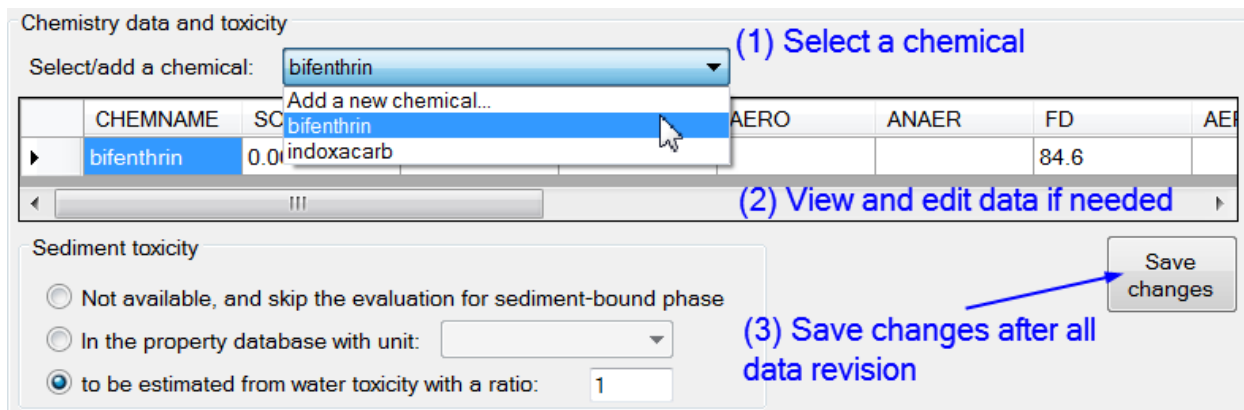


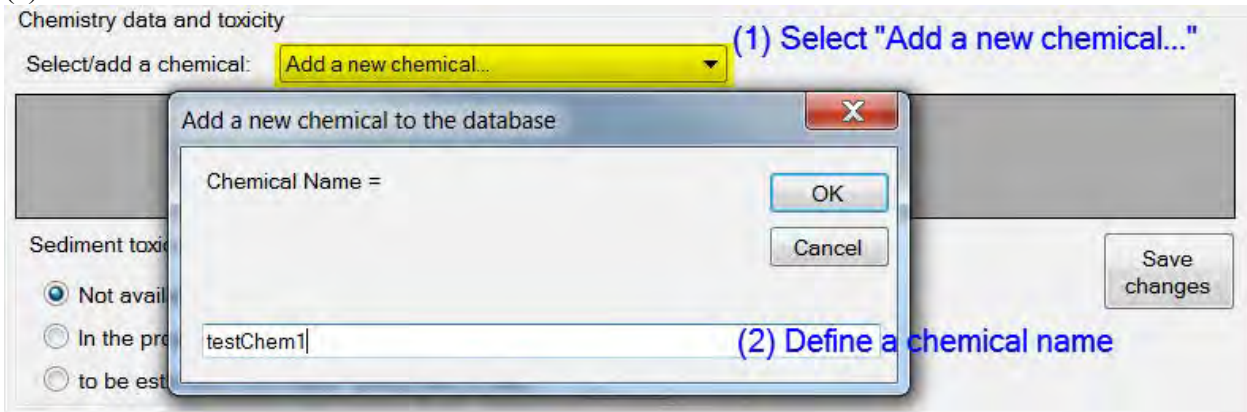
Figure 4. Data review and revision

[3] Add a new chemical to the database

If the chemical to be evaluated is not in the built-in database, one can create a new data record for the chemical (Figure 5). Chemical name should be unique in the database. If you want to test various parameter values for the same AI, consider using different names and adding the user initials, such as “diazinon1\_yl”, “diazinon2\_yl”, etc. The chemical name is not really used in the

model simulation, but as an index for data management and also shown in the report of modeling results.

(a)



(b)

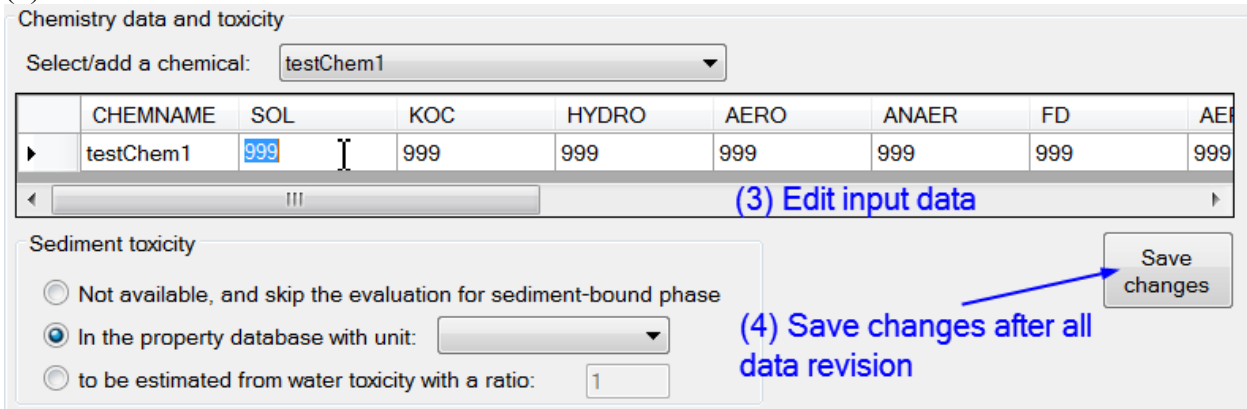
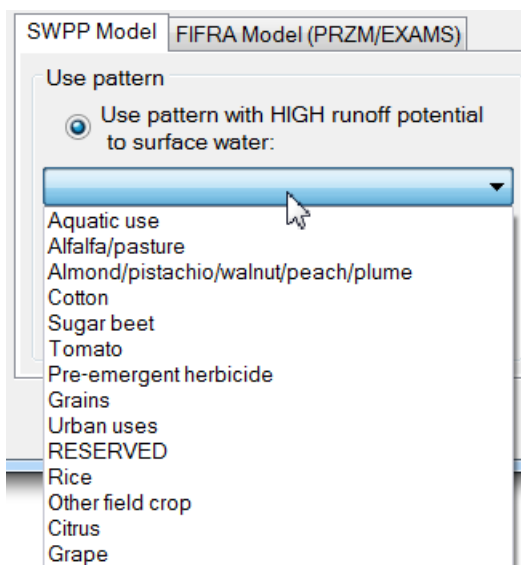


Figure 5. Creation of a new chemical in the database

## MODELING SCENARIOS

Carefully inspect the application instructions on the product label. If the pesticide product is associated with the listed high-risk use patterns (Figure 6), select the use pattern as modeling scenario. If more than one listed high-risk use patterns are involved in the product label, each of them needs to be modeled separately. Water-holding time is required for rice pesticides.



**Figure 6. Use patterns with high runoff potential to surface water**

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



Some unlisted use patterns may have potentials to release pesticides to a field with high-risk runoff potential. Those use patterns may be simulated by the modeling scenario of the receiving fields if the effective application rate (i.e., the mass of the pesticide AI that settles on terrestrial or aquatic surfaces per unit area) is provided in the label or can be estimated by a reviewer. Such use patterns include but not limited to:

- Aerial or ground-based spray over agricultural areas. Example: label amendment of Zenivex E4 RTU (Tracking ID #262552) containing etofenprox to add use as an adult mosquito insecticide in agricultural areas. The effective application rate was estimated based on USEPA AGDISP model ([http://em/localdocs/pubs/rr\\_revs/rr1432b.pdf](http://em/localdocs/pubs/rr_revs/rr1432b.pdf), DPR internal webpage).
- Seed treatments. Example: Remark-A 17960B (#247450) and A17960A (#247451) seed treatments containing cyantraniliprole. The effective application rate was estimated based on seed planting density ([http://em/localdocs/pubs/rr\\_revs/rr1427.pdf](http://em/localdocs/pubs/rr_revs/rr1427.pdf), DPR internal webpage).

It’s proposed to include some of the above use patterns in the next version of the model as additional modules or options. Meanwhile, effective application rates are determined case by case with label information, external models, and assumptions.

## APPLICATION RATES

Application rates and related data may be specified in two formats of (1) annual/seasonal maximum rate or (2) information for individual applications including maximum label rate, minimal application interval, maximum number of applications, and date of the first application (Table 3). Please note that the required **unit of application rate is kg[AI]/ha**. A rate calculator is

provided for the conversion from product-based label rates (Figure 7). Date of the first application is only required for urban uses, and agricultural uses with PRZM/EXAMS models. If this parameter is not specified in the label, “January 1st” is set as a default value.

Table 3. Input data for application rates

Use pattern	Annual/seasonal maximum rate (kg[AI]/ha)	Individual applications	
		Max label rate (kg[AI]/ha), min application interval, max number of applications	Date of the first application
Aquatic uses	Not used	Not used	Not used
Rice pesticides	OK	Recommended	Not used
Agricultural uses (non-rice), SWPP model	OK	Recommended	Not used
Agricultural uses (non-rice), PRZM/EXAMS		Required	Required
Urban uses		Required	Required

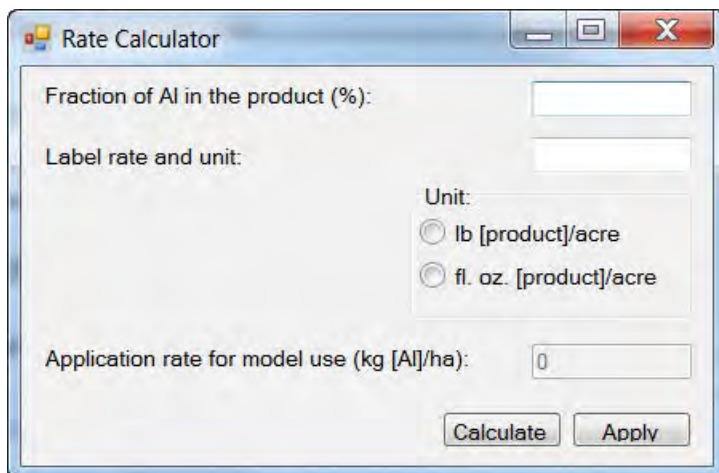


Figure 7. Rate calculator for pesticide applications

## ADDITIONAL DATA FOR URBAN EVALUATION

Additional data including detailed use pattern, product formulation and application method are required for evaluating urban uses (Figure 8). Those data are used to estimate treated areas (in fraction), by which the effective application rate to each component of the urban environment can be derived.

The model can handle either **predefined or customized** application methods:

- (1) Predefined application methods can be specified by “use pattern” and “application method” in the urban module interface (Figure 8). For residential and commercial/industrial uses, four application methods are predefined in the model (Table 4). For urban rights-of-ways applications, USEPA settings are used (pesticide applications to 10% pervious surface and 0.1% impervious surface) (USEPA, 2007b).



Table 4. Predefined pesticide application methods for residential and commercial/industrial uses

Application method	Description
Broadcast application (lawn)	All lawns in a lot will be treated, with 5.68% overspray to adjacent impervious surface
Broadcast application (paved area)	All paved area in a lot will be treated
Perimeter treatment (including wall treatment)	Perimeter treatment around a building. Widths of application are required in this case (Figure 8)
Crack & crevice treatment	5% of the lot area will be treated, with 2.5% on pervious surface and 2.5% on impervious surface

(2) If the proposed application method in the product label cannot be represented by the above predefined options, customized application methods can be defined by manually specifying the treated area fractions in the urban module interface (Figure 8). Please refer to the document for urban module (Luo, 2014) for details on the landscape scenarios in characterizing urban environment in California.

The screenshot shows a software interface for defining pesticide application parameters. It is divided into two main sections: 'Label information for urban uses' and 'Suggested parameters (in area fraction) for effective rate calculations'.

**Label information for urban uses:**

- Use pattern:** Radio buttons for Residential (selected), Commercial/industrial, and Rights-of-way.
- Product formulation:** Radio buttons for Liquid (selected) and Granular.
- Application method:** A dropdown menu.
- Width of application (ft), if applicable:** Input fields for [1] ground= 0 and [2] wall= 0, with an Update button.

**Suggested parameters (in area fraction) for effective rate calculations:**

	Maximum	Suggested	Adjusted
[1] treated pervious surface, without dry-weather runoff	5 %	0 %	0 %
[2] treated impervious surface, without dry-weather runoff	74 %	0 %	0 %
[3] treated pervious surface, with dry-weather runoff	12 %	0 %	0 %
[4] treated impervious surface, with dry-weather runoff	9 %	0 %	0 %

Note: for [4] it's possible that [treated area]>[maximum area] with wall treatment. Submit

Figure 8. Interface for urban module

**The general procedure** to characterize urban pesticide uses is to:

- (1) Read the proposed label and summarized the product formulation, use pattern, and application method.

- (2) In the urban module interface, select urban environment type (residential, commercial/industrial, or rights-of-way areas).
- (3) Select product formulation (liquid or granular).
- (4) Check the predefined application methods in the pull-down menu. If the proposed application method can be represented by the predefined ones, continue with step (5); otherwise, go to step (6).
- (5) Select application method, and specify widths of application (for perimeter treatment only). Confirm the inputs by clicking “update” button.
- (6) Manually adjust the treated area fractions as needed. This is applied to customize a new application method which is not predefined in this model.
- (7) “Submit” the data in the urban module interface to the main program.

## ADDITIONAL DATA FOR PRZM/EXAMS



When to use PRZM/EXAMS models? As summarized in Table 1, PRZM/EXAMS models are only used for evaluating agricultural uses. **SWPP model should be conducted first.** If SWPP modeling results suggest to deny the product registration, PRZM/EXAMS models may be conducted to further refine the results by considering additional reduction of pesticide concentrations in a receiving water body.

According to the identification of high-risk use patterns (Luo et al., 2012b) and the availability of Tier-2 modeling scenarios (USEPA, 2013b), 10 scenarios for agricultural uses are provided in the SWPP registration evaluation (Figure 9).

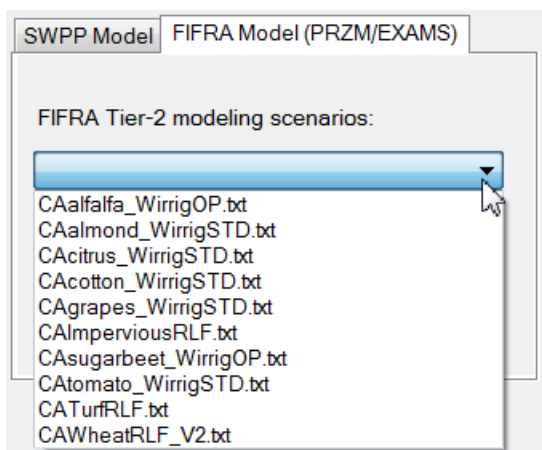


Figure 9. Modeling scenarios for PRZM/EXAMS modeling approach

With PRZM/EXAMS models, a reviewer is required to understand and adjust more modeling parameters (Figure 10). Pesticide application method and incorporation options can be retrieved from the product label. For the PRZM parameters, USEPA default values (USEPA, 2007c) are listed in the dialog window. Use those values unless field data are available and approved by the chemistry review. In August 2014, USEPA released the next generation of the models as PRZM5 and VVWM (Variable Volume Water Body Model). The new models will be incorporated as an option in the next version of SWPP evaluation model.

The screenshot shows a software interface for the PRZM/EXAMS models. It is divided into three main sections:

- Application method:** Three radio buttons are present: "aerial spray" (unselected), "ground spray" (selected), and "orchard air-blast" (unselected).
- Interception and incorporation:** Three radio buttons are present: "(CAM=1) applied to soil, DEPI=4cm" (unselected), "(CAM=2) applied to foliage with interception proportional to crop development, DEPI=4cm" (selected), and "(CAM=4) applied to soil, user-defined DEPI" (unselected).
- PRZM parameters:** A blue text box above the inputs reads "Use USEPA default values unless field data are available." Below this are several input fields:
  - Incorporation depth (cm) DEPI: 4
  - Application efficiency (decimal) APPEFF: 0.99
  - 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

A "Submit" button is located at the bottom right of the interface.

Figure 10. Interface for PRZM/EXAMS models

## MODELING RESULTS AND EVALUATION REPORT TEMPLATE

The model will generate a text file as modeling results by summarizing model inputs, outputs, and model-based registration recommendations. If the urban module or PRZM/EXAMS models are used, another text file will be provided for the daily pesticide concentrations in water and in bed sediment of the USEPA standard farm pond. It's suggested to print those modeling results in monospaced font (e.g., Consolas).

Attach modeling results as an appendix to the evaluation report. Approved evaluations (including a mixture of those that are model-aided and those conducted based on best professional judgment) are posted at: [http://em/localdocs/pubs/rr\\_revs/rr-rev.htm](http://em/localdocs/pubs/rr_revs/rr-rev.htm). A blank MS WORD version of an evaluation report is available in the share drive: <\\dprhq01\SurfaceWater\Registration Evaluation>. The report is typically organized into four sections: background, evaluation, conclusion, and references. Some considerations for each section of the report include:

- (1) **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.

- (2) 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 the SWPP model. If so, follow subsequent guidance below. If not, you can engage in an open discussion of anticipated impacts to California aquatic environments using a best professional judgment approach.
  - a. Explain that the SWPP model will be relied upon using data from chemistry and fish & wildlife reports that have been approved by Pesticide Registration Branch. Provide references for these data sources, and other documents that you deemed important for your evaluation.
  - b. If the values for model input parameters are taken directly from the chemistry or fish & wildlife review reports or their summary tables, it's not necessary to disclose them in this section of the evaluation. You should, instead, note that these values are documented in the modeling output file. If the value for a model input parameter is derived by a reviewer, otherwise, 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 calculation should be specified.
  - c. 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).
  - d. If there are multiple products or use patterns, you should consider summarizing their model results in a table in this section. The key columns to show are the products, modeled use patterns, application rates, risk quotient, and model-based recommendations. Example: various cyantraniliprole insecticide products ([http://em/localdocs/pubs/rr\\_revs/rr1404.pdf](http://em/localdocs/pubs/rr_revs/rr1404.pdf), DPR internal webpage). Individual modeling output files should also appear in the appendix of the evaluation report.
  - e. When applicable, consider highlighting and discussing important information not addressed by the model simulations, such as (but not limited to) label languages, proposed mitigation practices, buffers, use restrictions, and degradates. Consider these factors together with the modeling results to arrive at the final registration recommendation.
- (3) Conclusion: Present your final registration recommendation and briefly summarize how you arrived at your conclusion. Be as clear and succinct as possible.
  - a. For support, state that the data support the registration of the product.
  - b. For conditional registration, the registrant is required 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 (<http://www.cdpr.ca.gov/docs/emon/surfwtr/review/report2.pdf>, page 8, and associated reference of "Segawa, 1995"), 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). Data requirements should be reasonable in nature.

- c. 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. The reviewer may provide suggestions on:
    - i. potential label changes that will prevent or mitigate potential risks to surface water
    - ii. additional data to refine the registration evaluation
- (4) **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, DPR document numbers, and DPR tracking I.D. number.

## REFERENCES

- Luo, Y. (2014). Methodology for evaluating pesticides for surface water protection III. Module for urban scenarios (<http://www.cdpr.ca.gov/docs/emon/surfwtr/review.htm>), California Department of Pesticide Regulation (CDPR), Sacramento, CA.
- Luo, Y. and X. Deng (2012a). Methodology for evaluating pesticides for surface water protection, I: initial screening (<http://cdpr.ca.gov/docs/emon/surfwtr/review.htm>). Sacramento, CA, California Department of Pesticide Regulation.
- Luo, Y. and X. Deng (2012b). Methodology for evaluating pesticides for surface water protection, II: refined modeling (<http://cdpr.ca.gov/docs/emon/surfwtr/review.htm>). Sacramento, CA, California Department of Pesticide Regulation.
- USEPA (2007a). Data requirements for pesticide registration (<http://www2.epa.gov/pesticide-registration/data-requirements>, accessed 07/2014), U.S. Environmental Protection Agency, Washington, DC.
- USEPA (2007b). Effects Determination for Carbaryl and the California Red-legged Frog (<http://www.epa.gov/espp/litstatus/effects/redleg-frog/carbaryl/determination.pdf>), U.S. Environmental Protection Agency, Washington, DC.
- USEPA (2007c). Tier I Rice Model v1.0 for estimating pesticide concentrations in rice paddies. Washington, DC, U.S. Environmental Protection Agency.
- USEPA (2013a). SUPERSEDED Guidance for Selecting Input Parameters in Modeling the Environmental Fate and Transport of Pesticides, version II (updated on 4/16/2013), Office of Pesticide Programs, U.S. Environmental Protection Agency.
- USEPA (2013b). USEPA Tier 2 crop scenarios for PRZM/EXAMS Shell (<http://www.epa.gov/oppefed1/models/water/index.htm>). Washington, DC, U.S. Environmental Protection Agency, Office of Pesticide Programs.

## APPENDIX 1. GUIDELINE OF DATA PREPARATION IN THE REGISTRATION EVALUATION FOR SURFACE WATER PROTECTION

### INTRODUCTION

The SWPP model for pesticide registration evaluation requires only one value for each model input parameters, while multiple data values may be submitted by registrants and subject to the data review and approval by the Pesticide Registration Branch (PRB). This document is designed to answer the questions: which data to be used for model input parameters and how to calculate the value for each parameter.

The previous version of the data preparation guideline was released on January 29, 2013 in a memorandum format on DPR internal website (<http://em/localdocs/pubs/reviews/em1301.pdf>). The guideline is updated here for additional data requirement for urban module and PRZM/EXAMS models.

### DATA SOURCES

It's assumed that the registration data reviews by PRB in the areas of product chemistry, residue chemistry, environmental fate, and fish & wildlife toxicity have been developed before this (surface water) evaluation. Those reports are available in the Registration Tracking System (<http://registration/track/trackreps/trackreps.htm>). There may be **multiple volumes** available, and each adds or replaces values to the previous one. In this case, the latest data should be used in the data preparation.

### SUMMARY OF REQUIRED DATA

Table 5 lists potential model input parameters for the evaluation. According to their data sources and availability, the parameters can be categorized into 4 groups:

- Group 1, including KOC, SOL, AERO, ANAER, FD, and HYDRO. Experimental data for those parameters are usually available in the registrant-submitted package. In addition, their representative values or ranges are also summarized for the comparison with groundwater leaching criteria, in a table at the end of the review reports for “product chemistry, residue chemistry, environmental fate”;
- Group 2 (AERO\_W and ANAER\_W). Data for the two parameters could be retrieved from the results of soil metabolism studies;
- Group 3 (HLW and HLD). Overall dissipation half-lives in aquatic system are required for pesticides associated with aquatic applications, such as rice pesticides;
- Group 4 (MWT, AQPHOT, VP, and HENRY). Parameters for chemical fate simulation in a receiving water body.
- Group 5 (toxicity values in water and in sediment). Those values are reviewed and summarized in the review reports for “fish and wildlife toxicity”.

Table 5. Summary of required chemistry data, environmental fate data, and toxicity data

Description	Parameter in the model	Unit	Notes
organic carbon (OC)-normalized soil adsorption coefficient	KOC	L/kg[OC]	usually available in the registrant-submitted data, and summarized in the review reports for “product chemistry, residue chemistry, environmental fate”.
water solubility	SOL	mg/L	
aerobic soil metabolism half-life	AERO	day	
anaerobic soil metabolism half-life	ANAER	day	
field dissipation	FD	day	
hydrolysis half-life	HYDRO	day	
aerobic aquatic metabolism half-life	AERO_W	day	could be available from soil metabolism studies.
anaerobic aquatic metabolism half-life	ANAER_W	day	
aquatic dissipation half-life in water	HLW	day	only required for aquatic applications such as rice pesticides.
aquatic dissipation half-life in sediment or in water-sediment system	HLD	day	
molecular weight	MWT	g/mol	only required for urban module and PRZM/EXAMS models
aqueous photolysis half-life	AQPHOT	day	
vapor pressure	VP	torr	
Henry’s law constant	HENRY	atm*m <sup>3</sup> /mol	
soil photolysis half-life	SPHOT	day	only required for urban module
lowest toxicity value	TOX, TOXSED	TOX ( <b>µg/L</b> ) for water toxicity and TOXSED (µg/g[OC] or µg/kg[dry sediment]) sediment toxicity	

## DATA PREPARATION

### GROUP 1 PARAMETERS

For the parameters of KOC, SOL, AERO, ANAER, FD, and HYDRO, their representative values or ranges have been summarized for the comparison to groundwater leaching criteria, in a table at the end of the chemistry review reports. An example of such table is illustrated in Figure 11. The following procedures are proposed to prepare model input data.

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

<sup>1</sup>Photolysis in water

Figure 11. Example of data summary table in the chemistry review reports

[1] if a **single representative value** is provided in the summary table for a parameter, use that value as model input. In Figure 11, for example, water solubility (SOL) is set as 0.1 ppm.

[2] for a “**stable**” degradation process, a numerical value significantly larger than 100 days should be used (e.g., 999 days). The value of 100 days was taken from the critical value for defining a “high” persistence of a chemical in the model development (Luo et al., 2012a).

[3] if a parameter is presented with a **data range** in the summary table (e.g., field dissipation = 26-83 days, Figure 11), or a parameter is **not summarized** in the table, review of the individual data is required. Individual data are usually summarized in a table, such as the data table for field dissipation demonstrated in Figure 12.



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

Figure 12. Example of experimental results reported in the chemistry review reports, demonstrated for field dissipation studies.

[3.1] for degradation studies (including hydrolysis study, soil metabolism study, and field dissipation study), 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  $T_{1/2}$ )**.

[3.2] for degradation studies (including hydrolysis study, soil metabolism study, and field dissipation study), reported half-lives associated with **small coefficients of determination ( $R^2$ )** should be excluded. In this case, the chemistry review reports may include comments for the data reliability, such as “*reduced correlation ( $R^2=0.11\sim0.29$  and  $0.20\sim0.44$ ) of best fit in loam soil did not provide reliable values for half-life or DT50.*”

[3.3] if there were experiments performed under **California field conditions**, results from those experiments should be used.

[3.4] if test studies were conducted under various pH values, the results under neutral pH conditions (pH=7 or around 7) should be used.

[3.5] generally, the model parameter will be set to the **median values** of retrieved data. Taking Figure 12 as an example, the field dissipation half-life is set as 44 days, as the median of all reported  $T_{1/2}$  values.

---

## GROUP 2 PARAMETERS (AERO\_W, ANAER\_W)

Anaerobic and aerobic aquatic metabolism half-lives are not summarized for groundwater risk assessment in the chemistry review. The data may be available in the tables for soil metabolism studies. Please refer to the procedures in [3.1] to [3.5] for data preparation.

---

### GROUP 3 PARAMETERS (HLW, HLD)

Aquatic dissipation half-lives are only required for aquatic uses such as rice pesticides. The same procedures in [3.1] to [3.4] should be applied for data preparation.

---

### GROUP 4 PARAMETERS (MWT, SPHOT, AQPHOT, VP, HENRY)

Group 4 parameters are only required for urban evaluation or PRZM/EXAMS models. SPHOT is used to simulate pesticide persistence on impervious surfaces, while other parameters in the group are for the prediction of pesticide fate and distribution in a receiving water body. Those parameters are usually summarized in a table for chemistry discussion in the chemistry review report. For vapor pressure and Henry's law constant, unit conversion may be required between the unit in the data sources and that required by the model (Table 5).

---

### GROUP 5 PARAMETERS (TOXICITY)

Toxicity values are usually summarized at the end of the review report on fish and wildlife toxicity, and an example is shown in Figure 13.

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 <sub>50</sub> < 3.1 µg/L NOEC	Extremely toxic
Brown shrimp	Water exposure (96 hrs)	15 µg/L LC <sub>50</sub>	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 <sub>50</sub> 2.9 µg/l NOEC	Extremely toxic
Sheepshead minnow	Water exposure (96 hrs)	43 µg/L LC <sub>50</sub> 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 <sub>50</sub> 20.4 µg/l NOEC	Extremely toxic

Figure 13. Example of toxicity data summarized in the review report for fish and wildlife toxicity

[4] toxicity data from all relevant tests should be retrieved from the summary table, with the following considerations:

[4.1] for water toxicity, **LC50 or EC50** from **acute** (usually 48-hour or 96-hour) toxicity tests on **fishes and invertebrates in freshwater and saltwater** are considered to be appropriate data for surface water evaluation. Values should be converted into the unit of **µg/L**.

[4.2] evaluations on sediment toxicity are required for chemicals with **KOC>1000**. If so, all reported data for **sediment-dwelling organisms** could be considered for sediment toxicity. Units of toxicity values should be converted to µg/L[pore water] or µg/kg[dry sediment].

[4.3] if toxicity data were reported for both technical and formulated product, the **technical toxicity** should be used.

[4.4] if a toxicity value is reported as "larger than (>)" or "less than (<)" a certain value, the provided value will be used.

[5] the **lowest value of the retrieved toxicity data** is assigned to the model as TOX (for water toxicity) or TOXSED (sediment)