Department of Pesticide Regulation
Environmental Monitoring Branch
1001 I Street
Sacramento, California 95812

Study 293: Protocol to Develop a California-Based Water Quality Model for Pesticide Registration Evaluation

Yina Xie
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1. Introduction

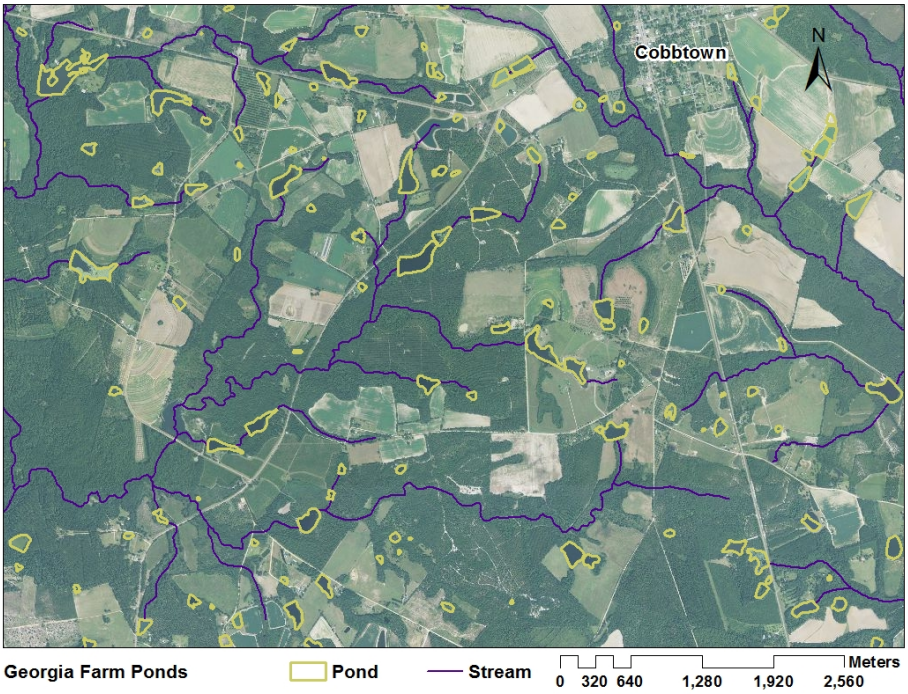
Water quality modelling is a crucial component to evaluate the environmental risk of pesticides. It accounts for different physical, chemical, and microbial processes associated with the fate of pesticides in surface water, and provides estimations of pesticide concentration in the receiving water body (Holvoet et al., 2007). Water quality models are usually combined with the field-scale models to provide screening tools for pesticide registration evaluation (Guo, 2002). For example, the Pesticide Root Zone Model and Variable Volume Water Body Model (PRZM-VVWM) toolset, also referred to as the Surface Water Concentration Calculator (SWCC) (Fry et al., 2014), is developed by the USEPA Office of Pesticide Programs (OPP) and recommended for pesticide registration screening in the US (Young, 2014). The SWCC calculates the fluxes of water, sediment and pesticides from a field, and assumes the field runoff enters a standard edge-of-field water body, where exposure can be measured and risk quotient can be computed.

The VVWM model, the successor of the Exposure Analysis Modeling System (EXAMS) model (Burns, 2000), in particular, is an important water quality model to assess the fate, transport, exposure, and persistence of pesticides in aquatic systems. According to the VVWM model, the hypothetical receiving water body is divided into two compartments – the littoral zone and the benthic zone, which are coupled by a completely-mixing (with dispersive and advective transports) and first-order mass-transfer process (Sato and Schnoor, 1991; Burns, 2000; Young, 2014). Typical processes, such as pesticide adsorption and desorption, photolysis, hydrolysis and redox, biolysis, and volatilization are involved and simulated in the model. The most important difference between the VVWM model and the previous EXAMS model relies on the assumption of the water volume of the receiving water body. The EXAMS model assumes constant water volume whereas the VVWM model allows water volume to vary in response to precipitation, runoff, evaporation, and overflow.

In order to conceptually represent the receiving water body in the model, two generic modeling scenarios were pre-defined in the VVWM model. They are the standard OPP farm pond scenario derived from a Georgian farm pond and the index reservoir scenario derived from a drinking water reservoir in Illinois. These scenarios are recommended by the USEPA OPP as national standards for aquatic risk and human health risk evaluation, respectively (Young, 2014). Although the VVWM model itself is a sophisticated screening tool to assess the behavior of

pesticides in a receiving water body, the application of the generic modeling scenarios to California can be problematic. The receiving water body essentially defines a dilution factor. The estimated pesticide concentrations in the receiving water body, thereby, can be significantly affected by the dimension of the water body, the size of the drainage area, and the physicochemical characteristics of the system. These factors can vary from site to site and a generic definition may result in failure to capture the variation. As such, it is practical to establish a state-specific definition of receiving water body for risk evaluation and modeling.

However, neither of the available modeling scenarios are associated with California nor can they be considered representative of the field conditions in California. Figure 1 demonstrates typical receiving water bodies on the landscape of central Georgia and California, respectively. In central Georgia, farm ponds, as highlighted in yellow polygons in the upper panel of Figure 1, are typically scattered around the farmlands, while open ditches (e.g., artificial ditches and canal ditches in the lower panel of Figure 1) are common structures that receive field runoff in California. The landscape from which the pre-defined VVWM farm pond scenario was derived appears to be significantly different from the actual field conditions in California. The application of the pre-defined standard scenarios to California, therefore, can result in inaccurate estimations of pesticide concentrations. The absence of an appropriate modeling scenario to define receiving water body in local conditions limits the application of the VVWM model to California.



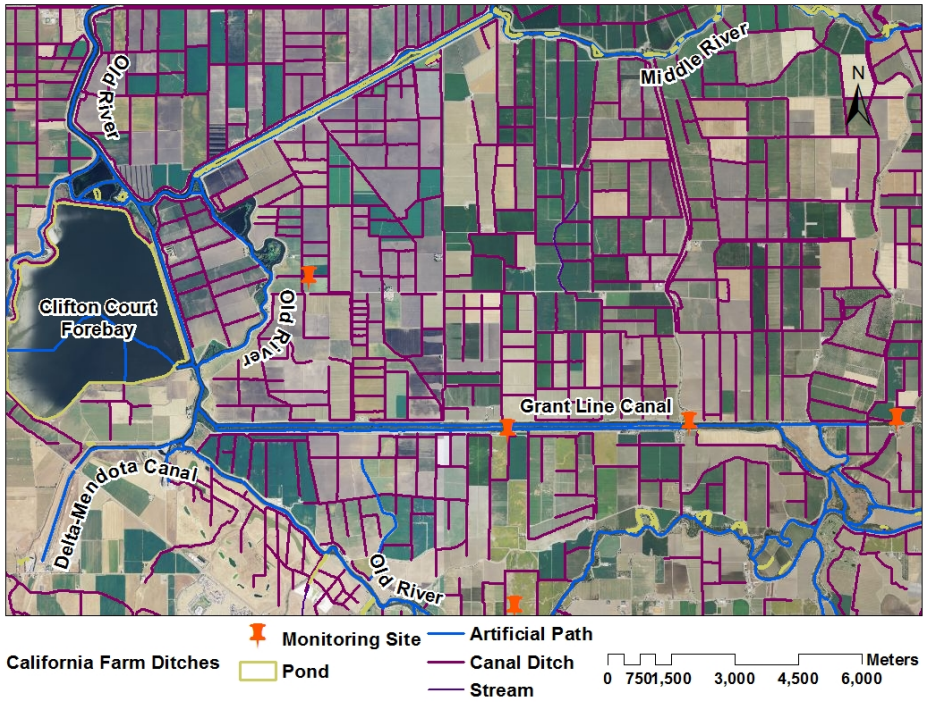


Figure 1: Comparison of typical receiving water bodies between Georgia (upper panel) and California (lower panel). Background map was derived from the National Agriculture Imagery Program (NAIP) Image, while stream lines, ditches, and ponds were derived from the National Hydrology Database (NHD). Aerial photos were taken over farmlands near Cobbtown of central Georgia and farmlands near the Clifton Court Forebay in San Joaquin County of California, respectively.

In addition to the VVWM model, at least two popular water quality models are available for pesticide screening. The European Surface Water FOCUS (FOrum for the Coordination of pesticide fate models and their USe) workgroup recommends the use of the TOXSWA (TOXic substances in Surface WAters) model, in conjunction with the PRZM and MACRO (non-steady state water and solute transport in MACROporous field soils) drainage model, for pesticide screening and ecotoxicological risk assessment (FOCUS, 2001). The TOXSWA model defines three types of receiving water bodies – ditch, pond, and stream – based on the conservative, worst-case assumption. For each type of receiving water body, the model specifies the dimensions, the size of the drainage area, and the physicochemical characteristics associated with pesticide fate in the receiving water body.

Another popular screening-level water quality model is the Canadian Environmental Modelling Centre (CEMC)'s AGRO modeling system (AGRO), which is Microsoft Excel worksheet-based application that predicts the environmental fate of chemicals in a variety of water bodies (CEMC, 2007). The model consists of the Quantitative Water Air Sediment Interaction (QWASI) Fugacity model (Mackay, 2001) and the Food Web Model (Arnot and Gobas, 2004). It accounts for chemical mass exchange between water column, benthic layer, and air, and is applied with the PRZM model to compute the estimated environmental concentrations. Similar

to the VVWM model, the AGRO model uses the USEPA OPP standard farm pond and the index reservoir as default receiving water body scenarios.

These three screening-level water quality models together provide the basis to develop a California-based water quality model for pesticide registration evaluation. The Surface Water Protection Program of the California Department of Pesticide Regulation (CDPR) is currently developing a systematic methodology for product registration evaluation, namely, the RegEval model (Luo and Deng, 2012a; Luo and Deng, 2012b; Luo, 2014). The RegEval model evaluates the aquatic risk of pesticides based on their aquatic toxicity, runoff potential, persistence, use pattern, and risk quotient. However, due to the lack of California-specific water quality model, the current version of the RegEval model only employs the standard farm pond scenario with the EXAMS model for receiving water body simulation. The development of the California-based water quality model will help to refine the receiving water body component of CDPR's RegEval model.

2. Objectives

Given the lack of appropriate receiving water body modeling that is suitable to California; the proposed study attempts to fill the gap through addressing the following objectives:

1. Review three water quality models (VVWM, TOXSWA, and AGRO) available for pesticide exposure evaluation and registration screening. Compare and contrast the methodology of defining the fate of pesticides in the receiving water body among the models. Make model application recommendations based on the review.
2. Derive receiving water body scenarios from the California field conditions for the appropriate model(s). Different scenarios will be developed separately for agricultural and urban areas given the landscape difference.
3. Validate the California-based water quality model by comparing the simulation results to monitoring data and to the results from pre-defined scenarios.

3. Personnel

This study will be conducted by Environmental Scientist Yina Xie under the supervision of Senior Environmental Scientist Nan Singhasemanon and the guidance of Research Scientist III Yuzhou Luo.

Questions regarding this protocol should be directed to project leading Yina Xie at 916-324-4111 or by email at Yina.Xie@cdpr.ca.gov.

4. Study Plan

4.1 Model review

A comprehensive review will be performed to compare and contrast among the three candidate pesticide-screening water quality models – the VVWM model, the TOXSWA model, and the AGRO model. The review will be primarily focused on two aspects of the models. First, we will examine the methodology used by the models to simulate the processes associated with the fate of pesticides in the receiving water body. That will involve comparison among the models in terms of the processes being simulated, theoretical basis employed to mathematically define the processes, and the associated equations and key parameters.

Second, we will specifically compare and contrast the approach among the models to define the receiving water body and the different scenarios. For example, the receiving water body is specified by the VVWM model with a set of parameters regarding the watershed and water body dimensions, and physical characteristics of the water column and benthic region, as illustrated in Table 1. The two pre-defined scenarios (i.e., the standard OPP farm pond and the index reservoir) are represented by two different sets of parameter values, also shown in Table 1.

Table 1: Parameters required for defining the receiving water body in the VVWM model

Parameter	Unit	Description	USEPA Pond	USEPA Reservoir
Watershed and Water Body Dimensions				
Field Area	m^2	Area of watershed draining to the receiving water body	100,000	1,728,000
Water Body Area	m^2	Surface area of receiving water body	10,000	52,600
Initial Depth	m	Initial depth of water column	2	2.74
Maximum Depth	m	Maximum depth of water column	2	2.74
Hydraulic Length	m		356.8	600
Cropped Area Fraction	-	Fraction of croplands in the watershed	1.0	1.0
Water Body Physical Parameters – Water Column				
DFAC	-	EXAMS-defined distribution factor associated with photolysis	1.19	1.19
Water Column SS	mg/L	Concentration of suspended sediment in water column	30	30
Chlorophyll	mg/L	chlorophyll concentration in water column	0.005	0.005
Water Column foc	-	Fraction of organic carbon in water column	0.04	0.04
Water Column DOC	mg/L	Concentration of dissolved organic carbon in water column	5	5
Water Column Biomass	mg/L	Concentration of planktonic biomass in water column	0.4	0.4
Water Body Physical Parameters – Benthic Region				
Benthic Depth	m	Average vertical depth of benthic region	0.05	0.05
Benthic Porosity	-	Volumetric water content (liter/liter) in benthic region	0.5	0.5
Bulk Density	g/cm^3	Fresh weight per unit volume of benthic sediments	1.35	1.35
Benthic foc	-	Fraction of organic carbon in benthic region	0.04	0.04
Benthic DOC	mg/L	Concentration of dissolved organic carbon in benthic region	5	5
Benthic Biomass	mg/L	Concentration of benthos in benthic region	0.006	0.006
Mass Xfer Coeff.	m/s	1st order water column-to-benthic mass transfer coefficient	1E-08	1E-08

Note: this table was adapted from Fry et al., 2014 and Young, 2014.

The standard OPP farm pond is a one-hectare by two-meter depth pond, fed by a ten-hectare agricultural watershed. The pond dimension was originally derived from a Georgian farm pond size, in accordance with USDA guidance for pond construction (i.e., approximately 2 acres of drainage per acre-ft of storage in central Georgia) (Young, 2014). The index reservoir is an 82.2-meter width by 640-meter length by 2.74-meter depth water body, fed by a 172.8-hectare watershed. Definition of the index reservoir was based on a drinking water reservoir in Illinois called Shipman City Lake, which was considered representative of a number of reservoirs in the central Midwest that were known to be vulnerable to pesticide contamination (USEPA, 2000). The approach involved in the VVWM model to define receiving water body will be compared and contrasted to that adopted by the TOXSWA and the AGRO model. We will not only compare the set of parameters employed to define a receiving water body among the models, but the values of parameters used to define the scenarios as well.

Based on the two aspects examined, we will summarize the applicability and limitations of the models, and make suggestions on model application for the purpose of pesticide registration evaluation in California.

4.2 Model development

This study will create California-based receiving water body scenarios for water quality models to facilitate pesticide registration evaluation in California. Considering that the runoff pattern and the receiving water network can be significantly different between the agricultural and urban areas, the receiving water body scenarios will be defined separately for them. The first stage of model development will primarily focus on agricultural areas, and the second stage will focus on urban areas. The development of new receiving water body scenarios will consist of a determination of the values of parameters required by the models to define the receiving water body.

Three methods will be used to help determine the values of parameters. First, a literature review will be performed to collect data from field studies in California. Data sources will include journal articles, engineering handbooks, government guidelines and codes, university extension factsheets and reports, etc. The review will provide a summary of the range of values reported for the set of parameters of interest. Second, GIS-based spatial data analysis will be performed to help explore the spatial pattern of the receiving water bodies throughout the State. Several data sources, as illustrated in Table 2, will be used to support the analysis. We will first map the surface drainage ditches in agricultural areas based on the NHD, CDL and NAIP, with which we will then explore the spatial patterns of ditch design and spatial distribution across agricultural regions, crop types, and other appropriate factors. With the spatial data, we will also be able to determine the relationship between the receiving water body and the adjacent watershed (e.g., flow direction and overland runoff direction) and ultimately determine the size of the drainage area. Similarly, GIS-based analysis will be performed for the urban areas to abstract spatial patterns of the receiving water body and the drainage area. Finally, we will obtain information directly via informal surveys or interviews with professionals in CDPR, university extension, and other relevant agencies.

The proposed California-based receiving water body scenarios will be incorporated into the selected water quality models to complete the simulation of receiving water body in California

conditions. According to preliminary review, both the VVWM model and the AGRO model have the feature of allowing users to define receiving water body by using customized values.

Table 2: Spatial data available for GIS analysis of receiving water body in California

Spatial Data	Resolution	Source
National Hydrology Dataset (NHD)	1:24,000	US Geological Survey (USGS)
Watershed Boundary Dataset (WBD)	1:24,000	US Geological Survey (USGS)
Cropland Data Layer (CDL)	30 meters	US Department of Agriculture National Agricultural Statistics Service (USDA-NASS)
National Agriculture Imagery Program (NAIP) Image	1 meter	US Department of Agriculture Farm Service Agency (USDA-FSA)
Digital Elevation Model (DEM)	10 and 30 meters	US Geological Survey (USGS)
Maps of City Storm Drainage Pipes	-	City and County Government

4.3 Model validation

The proposed California-based receiving water body scenarios will be validated through the following means. First, because the proposed water quality model is intended to be used for registration evaluation, the modeling results should be conservative enough to capture worst-case conditions. As such, the proposed receiving water body scenarios will be calibrated and validated by comparing the simulation results to worst-case conditions throughout the State. Worst-case conditions will be determined by using available field monitoring data, following the approach demonstrated by Luo (2014). Second, the simulation results from the proposed California-based modeling scenarios will be compared to that from the USEPA pre-defined scenarios to test the effectiveness of the new scenarios in predicting worst-case conditions.

5. Timelines and Expected Deliverables

The proposed study will last two years. Detailed timelines are demonstrated in Table 3. The final deliverable will be a review of screening-level water quality models and a set of California-based receiving water body scenarios (agricultural and urban) for the models, which will be appropriate for evaluating aquatic risk of pesticides under California conditions.

Table 3: Study timelines

8/2014	10	12	2/2015	4	6	8	10	12	2/2016	4	6	8
I												
II												
	III											
		IV										
								V				

Explanations:

I. Protocol reviews and discussions
II. Model review
III. Literature review of California field studies and data collection from professionals
IV. Use GIS-based spatial data analysis techniques to abstract desired information from the available spatial datasets

V. Model validation

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