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Study 260
Protocol to Evaluate Three Models for Simulating Pesticide Transport and Fate at Field Edge

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Introduction

Exposure modeling to evaluate potential fate and transport of pesticides in the environment has been adopted by regulatory agencies as a tool to assist in the evaluation of pesticide product registration. Models predict the expected environmental concentration of a specific chemical using data collected on their physiochemical properties, application rates and methods, and the use environment. For regulatory purposes, models often run under hypothetical conditions of weather, soil and crop (standard scenarios) that are determined as representative of the regulated area. For example, in order to aid in the evaluation of surface runoff potential, the U.S. Environmental Protection Agency (U.S. EPA) has developed a procedure using the PRZM-EXAM model to evaluate standard scenarios that are representative for a national assessment (U.S. EPA, 2009).

The U.S. EPA procedure may not be suitable for evaluating runoff potential under California's regulatory system and agronomic conditions. With respect to regulatory concerns, current water quality regulations in California are based on instantaneous water sampling designed to reflect the peak concentrations. These concentrations are compared to water quality criteria to determine if a violation has occurred. Therefore, a model must be able to predict peak pesticide concentrations at field edge that occur soon after rainfall or irrigation events. The PRZM-EXAM model may not be appropriate because predictions are averaged over a daily time step and, consequently, may fail to mimic peak concentrations.

With respect to agronomic conditions, the standard scenarios used by U.S. EPA are not representative of California's unique combination of climate and cropping patterns, many of which are not found in the rest of the nation. Also, wide-spread use of irrigation for California crops presents a challenge for exposure modeling because existing models may not have valid mechanisms that simulate irrigation water applications and subsequent runoff from a field.

A few models have been preliminarily selected according to their capabilities of predicting expected environmental concentrations of pesticides at field edge: the PRZM model, RZWQM (Root zone water quality model) and the OPUS model. All the models predict pesticide concentrations in dissolved and adsorbed forms and allow degradation. But they differ in many aspects, especially the hydrology component. PRZM simulates soil water movement based on a tipping-bucket approach and predicts daily runoff based on the curve number method. The most recent version of PRZM (PRZM3.12.3) uses Richard's equation based approach for water flow in deeper soil layers (Carsel *et al.,* 1998). RZWQM solves the Richard's equation to simulate soil water movement and predicts runoff as the part of rainfall/irrigation exceeding soil infiltration capacity (Ahuja *et al*., 1999). The OPUS model has the flexibility of simulating soil moisture using both tipping-bucket and Richard's type approaches depending on the availability of break-point rainfall data (Smith, 1992). Both PRZM and OPUS simulate sediment transport while RZWQM currently does not. The differences of the three models in hydrology as well as other components result in their relative strength and weakness while applied for predicting pesticide runoff in California conditions.

Objectives

The objective of this study is to evaluate the usefulness of the three models in predicting pesticide concentrations in runoff water under California climatic and agronomic conditions. The specific goals are threefold.

1) Calibrate the models using experiment data from California agricultural fields;
2) Simulate a list of pesticides with a wide range of physiochemical properties;
3) Investigate the usefulness of the three models for simulating pesticide transport and fate under California conditions.

Personnel

This study will be conducted by Environmental Scientist Xuyang Zhang under the supervision of Senior Environmental Scientist Sheryl Gill and the guidance of Research Scientists III Frank Spurlock, John Troiano and Bruce Johnson.

Project Leader: Xuyang Zhang

Research Scientist III: Frank Spurlock, John Troiano, Bruce Johnson

Study Plan

(1) Scenario description

This study will use data from two field experiments conducted in Fresno and Winters of California.

Experiment 1: Pre-emergent herbicide application in a citrus grove with rainfall simulator; conducted in Fresno, CA in August1995 (Troiano and Garretson, 1998)

Experiment 2: Dormant organophosphate (OP) application in a peach orchard with nature rainfall; conducted in Winters, CA in January1996 (Ross *et al.*, 1997).

Detailed information on the designs of the two experiments is summarized in Table 1.

Table 1: Experimental design and site information of the two datasets used for model calibration

	Experiment 1: Fresno site	Experiment 2: Winters site
Crop	Citrus	Peach
Plot / field size	0.00167 ha	0.89 ha
Water application	Simulated rainfall: 2 events 22 mm/hr for 1.5 h totally 32 mm	Natural rainfall: 2 events 38 mm in 15h, 15 mm in 10h
Soil	Hanford sandy loam, sand (73%), silt (19%), clay (8%)	Yolo silty loam, sand (37%), silt (38%), clay (25%)
	Organic carbon content: 0.4%	Organic carbon content: 1.2%
	Bulk density: 1.71 g/cm^3	Bulk density: 1.42 g/cm^3
	Infiltration rate: 0.0024 mm/s, Slope: 1-2 %	Slope: 1-2 %
Pesticide application	Simazine: 2.2 kg/ha AI	Diazinon, chlorpyrifos and methidathion 1.12 kg/ha AI using a mini air-blast sprayer
Management practices	Mechanical incorporation vs. conventional	Cover crop with clover mix and oats

(2) Data preparation

Input data such as daily/hourly meteorological data, soil properties and management practices will be prepared and formatted according to specific requirements for each of the three models.

(3) Sensitivity analysis and calibration

Sensitivity analysis and calibration will potentially be carried out using PEST shell (Doherty, 2002). Simulated results on runoff flow, sediment and pesticide concentration will be compared with measured data from field experiments. Parameters will be modified until the best set was found that simulates the closest results to the field measurements.

(4) Simulation of pesticides with varying physiochemical properties

The calibrated model will be used to simulate a list of pesticides with a wide range of variations in physiochemical properties. The predicted runoff concentration will be evaluated to determine whether the differences in model prediction are comparable with observation.

(5) Model comparison

The models will be compared on the basis of (1) ease of use including data preparation, documentation of model, ability to retrieve, display and analyze output (2) reasonableness of output in terms of simulating pesticides with different physicochemical properties (3) sensitivity of model to various inputs (4) ability to be calibrated to the monitored field data. The models will be compared using statistical measures such as Root Mean Square Error, Coefficient of Efficiency, Index of Agreement, and other measures as deemed appropriate (Legates and McCabe, 1999).

Time Table

Task	Tentative Schedule
Task 1:Model setup and test run	September, 2009 – November, 2009
Task 2: Input data preparation	December, 2009 – January, 2009
Task 3: Sensitivity analysis and calibration	February, 2010 – April, 2010
Task 4: Simulation of pesticides with varying physiochemical properties	May, 2010 – June, 2010
Task 5: Data analysis	July, 2010 – August, 2010
Task 6: Report writing	September, 2010 – October, 2010

Literature Cited

Ahuja L.R. Rojas K.W., Hanson J.D., Shaffer M.J. and Ma L. (eds.). 1999. Root zone water quality model – Modeling management effects on water quality and crop production. Water Resources Publications LLC, Colorado, USA. 360 pp.

Carsel R.F., Imhoff J.C., Hummel P.R., Cheplick J.M. and Donigan A.S.J. 1998. PRZM3, A model for predicting pesticide and nitrogen fate in the crop root and unsaturated soil zones: User manual for release 3.0, National Exposure Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Athens, Georgia, USA

Doherty, J. 2002, PEST: Model-independent parameter estimation user manual (5th ed.): Watermark Numerical Computing, Brisbane, Queensland, Australia.

Legates, D.R., and McCabe Jr. G.J. 1999. Evaluating the use of "goodness-of-fit" measures in hydrologic and hydroclimatic model validation. Water Resour. Res. 35:233–241.

Ross, L.J., Bennett, K.P., Kim, K.D., Hefner, K. and Hernandez, J. 1997. Reducing dormant spray runoff from orchards. EH97-03. State of California, Environmental Protection Agency, Department of Pesticide Regulation, Environmental Monitoring and Pest Management Branch, Environmental Hazards Assessment Program, Sacramento, California 95814-5624. http://www.cdpr.ca.gov/docs/emon/pubs/ehapreps/eh9703.pdf

Smith, R.E. 1992. OPUS, An integrated simulation model for transport of nonpoint source pollutants at the field scale: Volume I, Documentation. U.S. Department of Agriculture, Agricultural Research Service, ARS-98, 120pp.

Troiano, J. and Garretson, C. 1998. Movement of simazine in runoff water from citrus orchard row middles as affected by mechanical incorporation. J. Environ. Qual. 27: 488-494. (PDF, 102 kb). Reprinted with the permission of the American Agronomy Society. http://www.cdpr.ca.gov/docs/emon/pubs/ehapref/movesim.pdf

U.S. EPA. Water Models http://www.epa.gov/oppefed1/models/water. Last updated on Monday, June 1st, 2009