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# Field measurements for evaluating the RZWQM and PESTFADE models for the tropical zone of Thailand

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ABSTRACT

Evaluation of the field scale agricultural non-point source (NPS) simulation model against field experimental data is an important step that must be considered before a model can be used as a management tool. Therefore, the present study focuses on the testing of two NPS models known as the RZWQM (Root Zone Water Quality Model) and the PESTFADE (PESTicide Fate And Dynamics in the Environment). These models are used to predict the soil water content, metribuzin fate, and transport in a sprinkler-irrigated soybean field located at the experimental farm of the Asian Institute of Technology (AIT) in the Pathumthani Province, Thailand. Field soil water content and metribuzin residue adsorbed at soil profile depths of 0–10, 10–20, and 30–40 cm at different time periods were intensively measured by the gravimetric method and Liquid Chromatography Tandem Mass Spectrometry (LC-MS/MS), respectively. When comparing the field measured data, it was observed that the RZWQM performed better in simulating the soil water fcontent, whereas the performance of the PESTFADE model was better at simulating the metribuzin residue in the soil. Specifically, a reasonable agreement existed between the measured soil water content and that predicted by the RZWQM for 0–10 and 30–40 cm soil depths. The model slightly overpredicted the metribuzin residue at 0–10 cm soil depth one day after herbicide application, whereas the prediction of metribuzin residue at 10–20 and 30–40 cm soil depths was in accordance with the measured values. The PESTFADE model performed relatively well in simulating the soil water content at 10–20 cm and metribuzin residue concentration at 0–10 and 10–20 cm soil profile depths. However, the model performed relatively poorly at 30–40 cm soil profile depth. These results indicate that when properly calibrated, both the RZWQM and PESTFADE models can be used to predict the movement of water and metribuzin residue in the soil of tropical zones.

## 1. Introduction

Agricultural non-point source (NPS) pollution is costly and difficult to control, and it calls for the development and use of several modeling and analytical tools to understand the dynamics of pollution for efficient management. Field research in agriculture has been largely empirical, site specific, and conducted without the active help of agricultural system models (Ma et al., 2000; Clemente, 2002; Nilufar, 2005; Rombke et al., 2008). Numerous agricultural system models can be used to evaluate the effectiveness of agricultural Best Management Practices (BMPs) to control NPS pollution. Each model has its own assumptions, strengths, and weaknesses. Model users need to recognize that in reality, models are more valuable as a heuristic tool than as a full surrogate because many gaps still exist in our understanding of the function of natural systems (Sinclair and Seligman, 1996; Walker et al., 2000; Ahuja et al., 2002; Ma et al., 2004; Ahmed et al., 2007; López-Piñeiro et al., 2013; Esmaeili et al., 2014). Once adequately verified and tested, these models can be used to explore the interactions and effects of agricultural management practices on surface and groundwater quality. It can provide valuable information for decision makers and registration agencies in fertilizer and pesticide use. In addition, models can be used to explore system behavior under a variety of scenarios that may be economically or technically impossible to investigate by individual experiments.

To investigate the fate and transport of agrochemicals in the environment, mathematical models can be used to predict multiple scenarios and evaluate their impacts; instead of collecting large

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volumes of field data over a long period of time. Recently, deterministic models based on a physical approach are gaining wider acceptance as a tool for NPS and water quality management (Asare et al., 2001). Models simulate processes which are relatively difficult to predict (e.g., chemical transport to groundwater) by the input of relatively easy determined parameters (e.g., field capacity, soil bulk density, rainfall quantity and intensity, irrigation, tillage, and chemical half-life). A comprehensive agrochemical fate and transport model integrates the major processes operating in agricultural ecosystems to simulate movement, persistence, transformation, and the potential impact of agrochemicals. Computer simulation modeling offers an alternative, cost effective approach to laboratory, lysimeter, and field experiments in assessing NPS pollution of water resources. These models are useful, partly because performing field experiments is often very expensive or difficult, and models enhance our understanding of water quality processes. However, to obtain accurate results and ensure that models are reliable, they should be tested and evaluated against field data.

NPS contaminant transport models have been developed to assess chemical transport over a wide range of topographies, soil types, climatic conditions, and management practices. The vast majority of pesticide fate investigations in soil have been conducted under temperate conditions; primarily in Europe and North America. However, approximately more than half of the earth's population and roughly one-third of its land mass are found in the tropics. Research on the fate of pesticides in the tropical region is sparse, spanning less than three decades. The countries in this zone, many of them developing, make substantial use of pesticides to increase agricultural production. NPS pollutants affect the major lakes and river systems in Asia (Clemente, 2002). Karlsson (2004) reported that the proportion of pesticides used in developing countries is one-third of the total value of the world pesticide market (e.g., US$ 26 billion). For example in 2011, 164,383 tonnes of agricultural hazardous substances were imported into Thailand where herbicides, insecticides, and fungicides accounted for the top three imports with values of 112,176, 34,672, and 12,178 tonnes, respectively (PCD, 2012). Pesticides are used without fully understanding their impact on human health and the environment (Matthews, 2008). The increase in imports and their uses signifies a greater threat of pesticide pollution to the receiving waters. Pesticides applied to the soil surface prior to and immediately after planting are particularly susceptible to loss through surface runoff or leaching to groundwater through the soil profile. Given the concerns in relation to both pest control efficacy and environmental risk, it is perhaps surprising that pesticide fate of soil in the tropics has not received more attention. In recent years there has been a shift in focus regarding risk assessment of agrochemicals from the temperate to tropical regions (Rombke et al., 2008; Sarkar et al., 2008).

Many models such as GLEAMS (Leonard et al., 1987), OPUS (Smith and Ferreira, 1986), PRZM (Carsel et al., 1984), DRAINMOD (Skaggs, 1980) are available today to simulate the fate of water, nutrient, and pesticide in the soil-crop environment. Among them, the RZWQM (Ahuja et al., 2000) and PESTFADE (Clemente, 1991) are agricultural system models developed as tools for assessing the environmental impact of alternative management strategies on a field-by-field basis and predicting the management effect on crop production. There have been several evaluations of the performance of the RZWQM and PESTFADE to simulate pesticide fate and transport in a range of environmental and cropping conditions. However, the RZWQM and PESTFADE models have not yet been evaluated to simulate soil water content and pesticide/herbicide transport in the tropical conditions of Thailand in Southeast Asia. Therefore, the objectives of this study were to: (i) investigate the soil water content and metribuzin residue in the soil profile; and (ii) evaluate and compare the performance of the RZWQM and PESTFADE models to simulate the soil water content and metribuzin residue using measured data from the soil profile of a soybean [*Glycine max* (L.) Merr.] field in the Pathumthani Province, Thailand. This is the first time ever that these models have been used to test for the fate and transport of herbicides under Bangkok clay soil. The decision to choose these models was driven by the special feature of the models for in-depth representation of the critical soil-pesticide process and the broad handling of the transport mechanisms in the vadose zone.

In this study, metribuzin has been used to test the model. Metribuzin is a triazinone (4-amino-6-tert-butyl-4,5-dihydro-3-methyltio-1,2,4-triazin-5-one) herbicide commonly used in Thailand on a wide range of sites, including vegetable and field crops and non-crop areas, to selectively control certain broadleaf and grassy weed species. Metribuzin functions as a herbicide through the inhibition of electron transport in the photosynthesis pathway. It is a white crystalline solid with a melting point of about 126 °C. Metribuzin is prone to runoff into surface waters due to its high solubility in water (1200 mg $L^{-1}$). Contamination of surface water by metribuzin could result from accidental discharge or direct application to watercourses, spray and vapor drift, precipitation, or surface runoff, and groundwater intrusion from treated land. Losses primarily occur through movement in the water phase, caused by soil runoff as opposed to translocation through soil sediment erosion.

## 2. General description of the RZWQM and the PESTFADE models

### 2.1. Brief overview of the RZWQM

The RZWQM is a process based model developed to assess the effects of different management options on the soil and water quality in crop production (Ma et al., 2000). It is a one-dimensional (vertical into soil profile), continuous (can simulate more than one event), and physically based model, designed for a unit-area basis (point scale). The model integrates the physical, chemical, and biological processes to simulate the effects of various agricultural management practices on plant growth, water and chemical movement within and through the soil profile (Ahuja et al., 2000).

A number of studies have investigated the sensitivity of the RZWQM (Singh et al., 1996; Ahuja et al., 2000; Ma et al., 2000). Walker et al. (2000) identified saturated hydraulic conductivity ($K_s$), Brooks and Corey parameters, soil macroporosity, and drain spacing as the key input factors affecting tile flow and surface runoff. They also observed that macropore size is critical in determining the distribution of pesticides and nutrients in the soil matrix.

#### 2.1.1. Physical processes

These include interrelated hydrological processes: infiltration, chemical transport during infiltration, transfer of chemicals to runoff during rainfall, water and chemical flow through macropore channels and their absorption by the soil matrix, soil hydraulic properties estimated using bulk density and 33 or 1500 kPa water content, heat flow, evaporation, root water-uptake, soil water redistribution, and chemical transport during redistribution between rainfall and irrigation events.

The model uses the Green and Ampt equation for infiltration into soil, Poiseuille's equation for macropore flow, and the extended Shuttle–Wallace equation (Farahani and DeCoursey, 2000) for evapotranspiration (ET). Redistribution of soil water following infiltration is modeled by a mass-conservative numerical