JOURNAL OF THE KOREAN SOCIETY OF AGRICULTURAL ENGINEERS, MAR. 2008, pp. 3-10

한국농공학회논문집
제50권 제2호

Calibration and Sensitivity Analysis of the RICEWQ Model

RICEWQ 모형의 보정 및 민감도 분석

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Abstract

The main objectives of this study are to calibrate the RICEWQ model with Korean field data and then analyse the sensitivity of the parameters to identify sensitive parameters. The RICEWQ is widely used to predict pesticide fate in a paddy plot. An experimental paddy plot of 0.2 ha(100 × 20 m) at Seobyeon-dong, Daegu, Korea was selected, and field observations for water and pesticide balance were performed from 4 June to 2 September 2006. The molinate, which is a herbicide widely used for weed control in rice culture, was selected. The RICEWQ model was successfully calibrated both for the water and pesticide mass balance. The calibrated model showed a RMSE of 0.537 cm for ponded water depths and a RMSE of 0.036 mg/L for the molinate concentrations in the ponded water. The most sensitive parameters for molinate concentrations in ponded water were the metabolism degradation rate in water, volatilization coefficient, and release rate for slow release formulation. In contrast, the RICEWQ model was not sensitive to parameters such as hydrolysis degradation rate in water and degradation rate in unsaturated soil.

Keywords : RICEWQ, Paddy, Pesticide, Molinate, Sensitivity analysis

I. Introduction

Rice culture presents a unique problem with respect to pesticide runoff because of the high seasonal rainfall, water management practices, and proximity of cropland to surface-water bodies typical of rice-growing areas.

In Korea, several researchers have monitored the pesticides introduced into the adjacent water ecosystems from rice paddies and have found that most pesticides in the receiving water system came from surface runoff due to rainfall or improper water management(Kim, et al., 1997; Lee, et al., 1983). In particular, in the investigation of the environmental concentrations of pesticide at 38 stream sampling points, molinate has been detected in more than 73.7% of samples and to the maximum concentration of 40 μg/L(Park et al., 1998). Molinate is a selective, thiocarbamate herbicide widely used in rice culture and was selected as a test pesticide in this study.

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Approximately 800 M/T of molinate active ingredient(a.i.) were used in Korea in 2004(KCPA, 2005).

The mathematical model for pesticide fate and transport in rice paddies should evaluate dissipation in an aquatic system and predict the runoff losses of pesticides to receiving waters. At present, no single model has been evaluated and validated in Korea but there are several models which are already in use for the assessment of the environmental behaviour of pesticides in other countries, including the USA, the European Union, Australia and Japan.

Most of the existing pesticide fate models are not configured to simulate the flooding conditions, overflow, and controlled release of water that are typical under rice culture. Only few models deal with rice paddy fields : RICEMOD(Rice Computer Simulation Model, McMennamy and O'Toole, 1983) ; PADDY(Pesticide Paddy Field Model, Inao and Kitamura, 1999) ; RICEWQ(Pesticide Runoff Model for Rice Crops, Williams et al., 2004), and PCPF(Pesticide Concentration in Paddy Field, Watanabe et al., 2006).

The RICEWQ model was assessed by Christen et al.(2006) and the Mediterranean-Rice group of the EU). It was found to be the most suitable model of those named above for the assessment of the exposure risk of surface waters neighbouring rice paddies(Karpouzas and Capri, 2004).

The main objectives of this study are to calibrate the RICEWQ model with Korean field data and then analyse the sensitivity of the parameters to identify sensitive parameters.

II. RICEWQ model

The fate of a pesticide and the potential for its movement from the site of application, are affected by factors such as the chemical and physical properties of the pesticide, site characteristics, weather conditions, and the pesticide handling practices. Individual pesticides vary widely in their response to environmental processes.

The latest RICEWQ version 1.7.2 is used in this study. The water balance algorithms account for precipitation, evaporation, seepage, irrigation, releases and overflow from various paddy outlet configurations, and controlled drainage prior to harvest. The pesticide application algorithms accommodate a single parent pesticide with up to four metabolites, multiple applications, pesticide losses from drift, and foliage and water interception. The crop algorithms include plant growth from emergence to maturation, associated pesticide washoff and degradation on foliage, and deposits of pesticide residues on foliage after harvest. The water quality algorithms include dilution, volatilization, partitioning between water and the bed sediments, decay in water and sediment, settling and resuspension from bed sediments.

The water balance and pesticide fate algorithms in the RICEWQ model are detailed in elsewhere (Williams et al. 2004; Chung et al. 2005; and Park 2007).

III. Model calibration

1. Field experiment

This study targets sites with the potential for aquatic environmental impacts due to pesticide exposure. An experimental paddy plot of 0.2 ha (100×20 m) at Seobyeon-dong, Daegu, Korea was selected. Field observation was performed from 4 June to 2 September 2006. The soil(0-30 cm) was characterized as clay loam according to the USDA soil-texture classification(37.2%

sand, 30.8% silt, and 32.0% clay) with 2.5% organic carbon content.

The experimental paddy plot was irrigated about 8.0 cm deep to puddle by a rotary plough, and leveled for cultivation before transplanting. The rice crop, seeded on 29 April, was transplanted on 27 May 2006 with a 15 cm × 30 cm spacing. The outlet weir height was set at 8 cm. The water balance was daily monitored for ponded water depth, irrigation, surface runoff/drainage, and seepage. The ponded water depth during the experimental period was monitored continuously by two automatic water level recorder, and inflow and outflow were measured using a flow meter and weir at the inlet and outlet of the paddy plot, respectively.

Molinate was applied at a rate of 1.5 kg/ha active ingredient on 5 June in 2006, ten days after transplanting. Water samples were collected for molinate analysis at two sampling points near the inlet and outlet. Water samples were taken 0, 1, 5, 12, and 21 days after pesticide application. Water samples were collected in 1 L amber bottles. The samples were stored in an insulated box filled with ice for transport to a commercial laboratory.

In this study, meteorological data were collected from the Daegu weather station, located about 5 km south of the experimental plot. The daily mean temperature and total precipitation during 4 June to 2 September 2006 were 25.4℃ and 759.7 mm, respectively. The daily mean and total actual evapotranspiration during the experimental period were 4.1 mm and 368.6 mm, respectively. The daily precipitation and actual evapotranspiration during the simulation period are shown in Fig. 1.

2. Water balance calibration

The model was calibrated in two steps: firstly, the water balance and then the molinate concentration in ponded water. The model was calibrated for the water depth in the rice paddy from 4

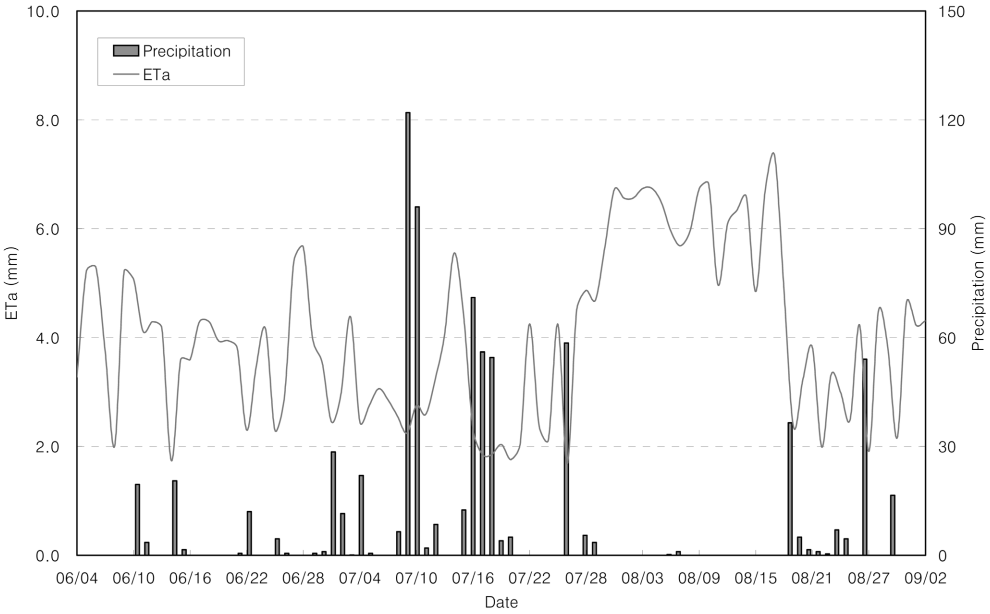


Fig. 1 Daily precipitation and actual evapotranspiration in 2006

Table 1 Input parameter values used for water balance calibration

Parameter Name	Value	Source/ comment
Date simulation begins and ends	5/24～9/2	field data
Date to start and stop irrigations	5/24～9/2	field data
Type of irrigation	fixed volume	field data
Height of drainage outlet	20 cm	field data
Maximum drainage rate	5 cm/day	field data
Surface area of paddy	0.2 ha	field data
Seepage	0.18 cm/day	calibrated
Evaportranspiration	daily	Daegu data
Field capacity of sediment	0.27	field data
Wilting point of sediment	0.13	field data

June to 2 September 2006. Table 1 shows the input parameter values selected for the water balance calibration. The calibrated model predicted water depths were well matched to the observed water depths(Fig. 2). The ponded water depths had a root mean square error(RMSE) of 0.537 cm.

3. Mass balance calibration

After the water balance was calibrated, the pesticide balance was calibrated. The pesticide calibration was undertaken to match the model predicted pesticide concentrations with observed concentrations. This was done by varying the settling velocity value. The settling velocity in the water column was varied across a range between 0.0 m/day to 2.3 m/day. The 0.2 m/day settling velocity was selected. Following the calibration of the settling velocity, the mixing depth of the sediment for direct partitioning was varied across a range between 0.001 cm to 0.500 cm. The mixing depth 0.01 cm was selected.

The model predicted molinate concentrations were well matched with the observed molinate concentrations in ponded water(Fig. 3). Molinate concentrations in ponded water had a RMSE of 0.036 mg/L. The molinate concentration in the paddy water reached maximum concentration (1.450 mg/L) on one day after application, thereafter, decreased rapidly until 4 days after treatment (DAT). On 5 DAT, the dissipation rate slowed down ; molinate was found to be reduced by 99% within 21.2 DAT.

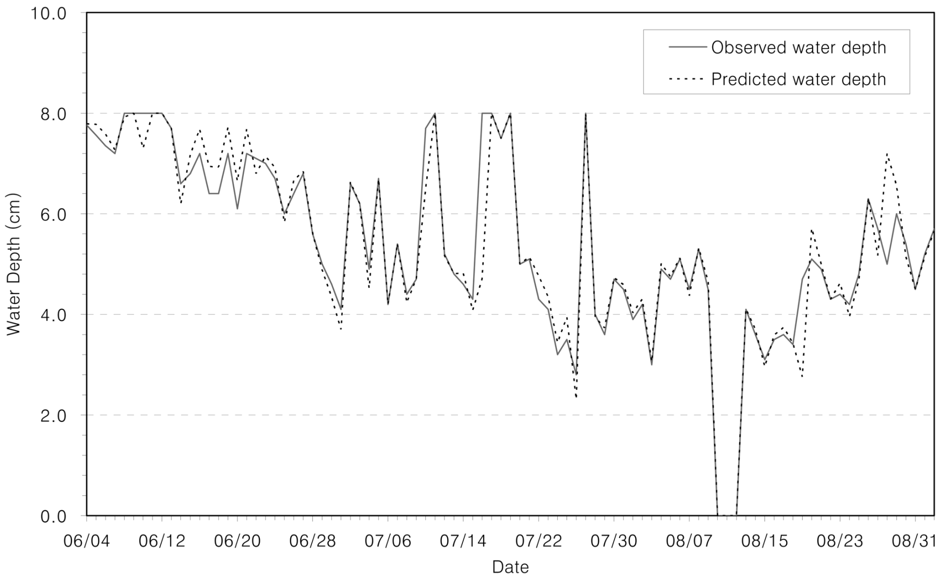


Fig. 2 Comparison of observed and predicted water depths in 2006

Table 2 Input parameter values used for the pesticide mass balance calibration

Parameter Name	Value	Source/comment
Depth of active sediment layer	2.0 cm	field data
Initial soil moisture of sediment	0.55	field data
Bulk density of sediment	1.35 g/cc	field data
Porosity of sediment	0.43 v/v	field data
Suspended sediment concentration	28 mg/L	field data
Application date	6/5/2006	field data
Application rate	1.5 kg/ha	field data
Incorporation depth	0 cm	field data
Application efficiency	1.0	field data
Aqueous metabolism decay rate	0.034 /day	US EPA(2005)
Aqueous hydrolysis decay rate	0.0004 /day	PAN(2006)
Aqueous photolysis decay rate	0.000 /day	PAN
Saturated sediment decay rate	0.017/day	PAN
Unsaturated sediment decay rate	0.007/day	PAN
Foliar decay rate coefficient	0.034/day	Neitsch et al.(2002)
Wash off coefficient	0.5	Neitsch et al.(2002)
Water-sediment partition coefficient	0.224 cc/g	Chapra(1997)
Volatilization coefficient	0.011 m/day	Bird et al.(1960)
Settling velocity	0.2 m/day	calibrated
Mixing depth for direct partition to sediment bed	0.01 cm	calibrated
Mixing velocity	0.0023 m/day	Di Toro et al.(1981)
Solubility	800 mg/L	Karpouzas and Capri(2004)

IV. Sensitivity analysis

Sensitivity analysis is the study of how the variation in the output of a model can be apportioned, qualitatively or quantitatively, to different sources of input variation ; it also makes clear how a given model depends upon the information fed into it.

A sensitivity analysis of the RICEWQ model was carried out for main parameters. The simulation results of the molinate concentrations in ponded water were analysed on 1, 4, 11, and 28 days after pesticide application, as the impact of a parameter change may occur early or late in the simulation. A number of parameters have been identified which may affect the molinate concentration in ponded water. Of the many parameters, thirteen primary factors were identified as critical in describing the sensitivity of the molinate concentration in ponded water(Table 3). The parameter value ranges were set through the available data, the literature, and suggestions from the RICEWQ User's Manual(Williams et al., 2004).

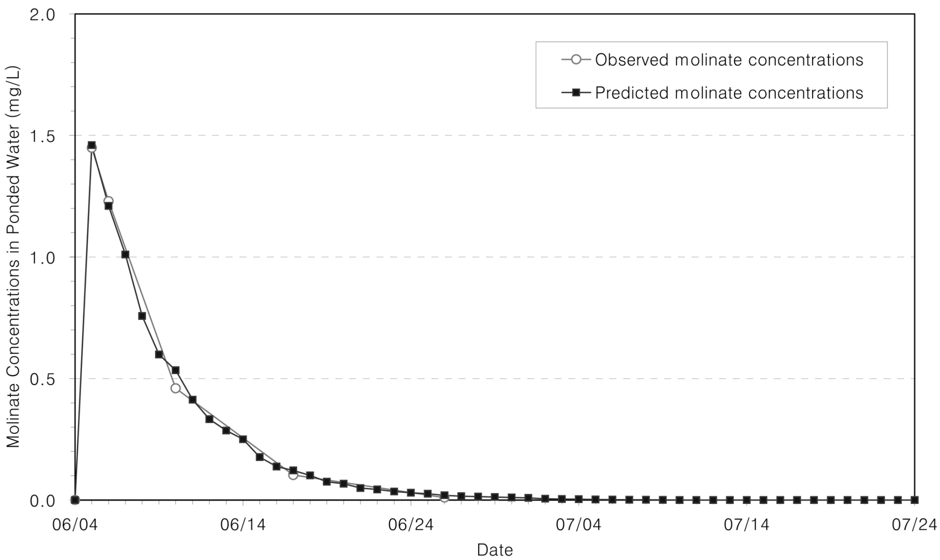


Fig. 3 Comparison of observed and predicted molinate concentrations in ponded water

Table 3 Ranges of physicochemical parameter values for sensitivity analysis

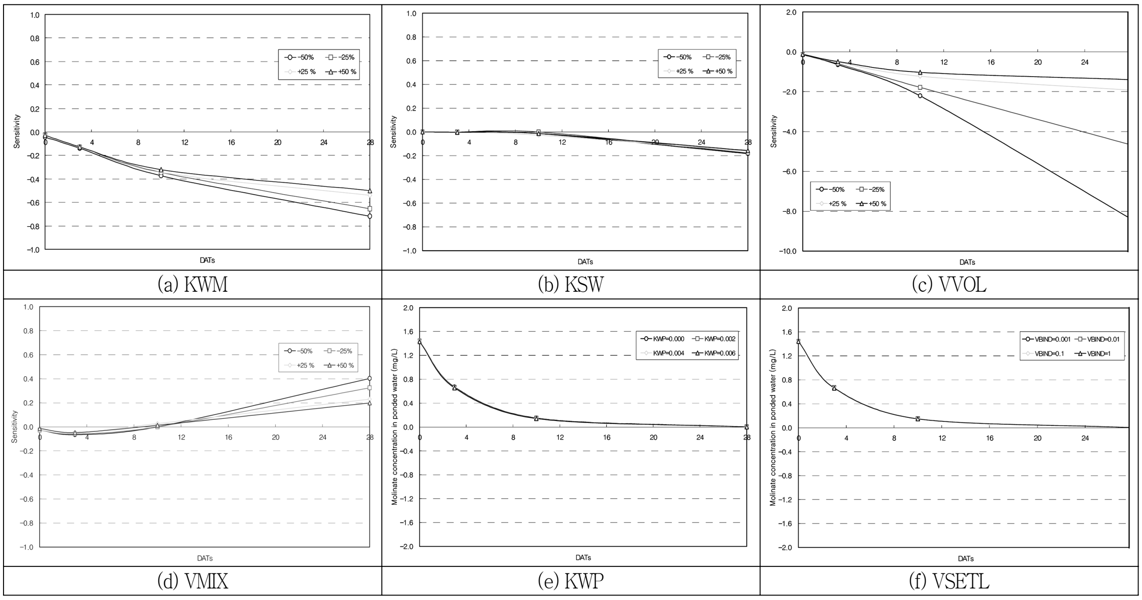
Parameters	Ranges	Description
KWM (0.034)※	0.017-0.051	Metabolism degradation rate in water
KWH (0.0004)	0.0002-0.0006	Hydrolysis degradation rate in water
KWP (0.0000)	0.0000-0.0008	Photolysis degradation rate in water
KSW (0.017)	0.0085-0.0255	Degradation rate in saturated sediment
KSD (0.007)	0.0035-0.0105	Degradation rate in unsaturated sediment
KF (0.034)	0.017-0.051	Degradation rate on foliage
KD (0.0224)	0.0112-0.0448	Water/sediment partition coefficient
VVOL (0.011)	0.0055-0.0165	Volatilization coefficient
VSETL (0.2)	0.1-2.0	Settling velocity
VBIND (0.01)	0.005-0.200	Mixing depth to allow direct partitioning to bed
VMIX (0.0023)	0.00115-0.00345	Mixing velocity(diffusion)
SOLUB (800)	700-900	Pesticide solubility in water
RREAC (0.0)	0.0-1.0	Release rate for slow release formulation

※ ( ) : basic value

In order to assess the relative sensitivity of the model to the various input parameter values a series of simulations were conducted using the calibrated fixed volume irrigation input file ; each parameter value was varied by ±50% of its original value. The results of the sensitivity analysis for 9 parameters are shown in Fig. 4, the other 5 parameters had near zero sensitivities. The most sensitive parameters for molinate concentrations in ponded water were the metabolism degradation rate in water(KWM), volatilization coefficient(VVOL), and release rate for slow release formulation(RREAC). In contrast, the RICEWQ model was not sensitive to parameters such as hydrolysis degradation rate in water(KWH) and degradation rate in unsaturated soil(KSD).

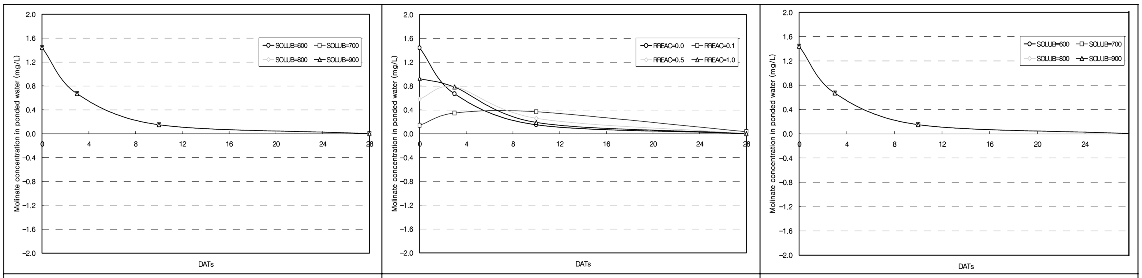
IV. Conclusions

In this study, the RICEWQ model was calibrated and the sensitivity of the input parameters was analysed. Field experiment was performed at a paddy plot in Daegu, Korea in 2006. Results of this study are summarized as follows :



(a) KWM (b) KSW (c) VVOL

(d) VMIX (e) KWP (f) VSETL



(g) VBIND | (h) SOLUB | (i) RREAC

Fig. 4 Relative sensitivity of the main input parameters

1. The RICEWQ model was successfully calibrated using field data from a Korean paddy plot. The calibrated model showed RMSE of 0.537 cm for ponded water depth and RMSE of 0.036 mg/L for the molinate concentrations in the ponded water.

2. The most sensitive parameters for molinate concentrations in ponded water were the metabolism degradation rate in water(KWM), volatilization coefficient(VVOL), and release rate for slow release formulation(RREAC). In contrast, the RICEWQ model was not sensitive to parameters such as hydrolysis degradation rate in water(KWH) and degradation rate in unsaturated soil(KSD).

This work was supported by the Korea Research Foundation Grant funded by the Korean Government(MOEHRD-2005-041-D00971).

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