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Research paper

Development and application of a dynamic in-river agrochemical fate and transport model for simulating behavior of rice herbicide in urbanizing catchment

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ABSTRACT

This study aimed to develop and validate a Dynamic in-River Agrochemical Fate and Transport (DRAFT) model simulating one-dimensional advective and dispersive pesticide transport processes under unsteady flow regime in a riverine system. The DRAFT model was coupled with two other modeling components, the PCPF-B model and the land use based tank model, which simulated hydrological/pesticide process in paddy fields and hydrological process in other land uses such as city, agricultural field and forest, respectively. The PCPF-B/DRAFT model was fed with the spatial information of the target catchment by incorporating the Geographical Information System (GIS). For the model validation, a full catchment monitoring data of a rice herbicide, mefenacet, along the Kose River, Fukuoka, Japan was utilized. After model calibration, hourly river discharge and daily mefenacet concentration were simulated by the PCPF-B/DRAFT model at individual observed points of the Kose River and model performance was evaluated by graphical assessment and multiple statistical indices (e.g. Nash-Sutcliffe efficiencies were 0.84–0.86 for streamflow and 0.16–0.72 for herbicide, respectively). The predicted mefenacet concentrations were strongly affected by: (1) water managements practiced in rice fields and (2) intensive rainfall events. The former concentrations were characterized by broad peak while for the latter the peak concentration was sharp and narrow. We used the PCPF-B/DRAFT model to further evaluate the applications of 7 days of water holding period after herbicide application in paddy fields, which was shown to effectively reduce the total loss of mefenacet from 18.9 to 12.8% of applied mass. Consequently, the broad peak concentrations of mefenacet in the Kose River decreased remarkably while the water management practice was less effective to reduce the sudden and sharp peak concentration resulting from intensive rainfall events.

1. Introduction

In Japan, like in many other East Asian countries, paddy fields cover nearly half of the total agricultural land use and about 34% of total pesticide shipment was used for rice cultivation (Japan Crop Protection Association, 2016). Pesticide contamination of surface waters in Japan was reported to be mainly caused by rice cultivation (Watanabe et al., 2008). Indeed, a number of monitoring studies have reported that pesticides used in rice cultivation, including herbicides, insecticides and fungicides as well as their metabolites, were frequently detected during the recommended application periods of those formulated products (Iwafune et al., 2010; Phong et al., 2010). Therefore, assessing the concentration level of rice pesticide in water released from paddy fields is a key component for the evaluation of environmental risk of pesticide in Japan and to develop appropriate management practices to prevent the contamination of public water by pesticide.

In exposure assessment process, mathematical models have been widely applied to simulate, at various scales, the environmental fate and transport of rice pesticides (Karpouzas and Capri, 2006; Luo et al., 2011). In Japan, the PADDY model (Inao et al., 2001; Inao and Kitamura, 1999) and the PCPF-1 model (Boulange et al., 2016; Watanabe et al., 2006) have been developed for predicting pesti-

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cide fate and transport processes in rice paddy plots. The PCPF-1 model was extended to a block-scale model, the PCPF-B (Phong et al., 2011) and the PADDY model was also extended to a basin scale model, the PADDY-Large model (Inao et al., 2003). However, there are difficulties in developing the model for larger scale due to complex hydrological processes within catchments, especially in the urbanizing catchment where agricultural field and other types of land use are heterogeneously distributed (MAFF, 2012).

Recently, simulation models often rely on Geographical Information System (GIS) to effectively summarize input as well as to visual predictions. Incorporating GIS-processed data into simulation models ensures the implementation of more realistic hydrological simulation for urbanizing catchment. For paddy fields, three GIS-based models, the diffuse pollution hydrological model, the PADDY-Large model and the PCPF-1@SWAT model, have been developed and applied in Japan (Boulange et al., 2014; Iwasaki et al., 2012; Matsui et al., 2006).

However, these models adopt simplified hydrological and pesticide processes in river by compromising the energy conservation on the flow simulation and the dispersion term for the pesticide transport simulation. The accurate accounting of these processes in watershed modeling is particularly important in small catchments where the occurrence of pesticides in the river is highly dynamic (Holvoet et al., 2007).

Various studies have reported that the use of a dynamic in-river water quality model based on one dimensional advective and dispersive transport equation coupled with unsteady flow regime would ensure more realistic water quality simulations (Roshanfekr et al., 2008; Zhang et al., 2008) as well as pesticide transport (Kilic and Aral, 2009; Mossman and Mulki, 1996) by considering the hydrodynamic conditions in the riverine systems. Nevertheless, to our knowledge, no study applying such models to the issues on fate and transport of rice pesticides released from paddy fields in Japanese catchments has been reported.

This study aims to develop a new one-dimensional dynamic in-river pesticide fate and transport model. The applicability of the developed model coupling with the PCPF-B model and the tank model designed for other land use types was then evaluated using rice pesticide monitoring data conducted in the urbanizing catchment in Japan. The spatial variation of complicated land use and other parameters was fed into the model using the GIS-processing and the literature survey, respectively. Finally, the effect of different water management practices in paddy fields within the target catchment was evaluated based on the validated result.

2. Description of dynamic in-river pesticide fate and transport model

We developed a new simulation model, named as the DRAFT (Dynamic in-River Agrochemical Fate and Transport) model, for simulating the fate and transport of pesticide in riverine system. The DRAFT model is a one-dimensional dynamic model both in space and time solving the advective and dispersive transport equation under unsteady flow regime along the flow direction. This model aims to simulate the pesticide fate and transport processes at a catchment scale. By coupling the DRAFT model with other models, water and pesticide flows from various land uses and pathways can be effectively computed. The algorithms of the DRAFT model are coded and implemented under the environment of Visual Basic for applications software with spreadsheet inputs in Microsoft Excel®.

2.1. Unsteady flow computation

Water flow in a riverine system was simulated by the one dimensional dynamic wave model which describes unsteady gradually varied flow. The governing equations of dynamic wave model are referred to as the St. Venant equations and expressed as (Cunge et al., 1980):

$$\frac{\partial A}{\partial t}+\frac{\partial Q}{\partial x}=0 \quad (1)$$

$$\frac{\partial Q}{\partial t}+\frac{\partial}{\partial x}\left(\frac{\beta Q^2}{A}\right)+gA\frac{\partial h}{\partial x}+gA\left(S_f-S_0\right)=0 \quad (2)$$

where A is the cross-sectional area [L^2], Q is the volumetric flow rate [L^3/T], t is the time [T], x is the distance along the flow direction [L], β is the correction factor (=1 in this study) [−], g is the gravitational acceleration [L/T^2], h is the flow depth [L], S_f is the friction slope [−] and S_0 is the bed slope [−]. The friction slope was approximated by the Manning formula:

$$S_f=\frac{n^2Q|Q|}{A^2R^{4/3}} \quad (3)$$

where n is the Manning roughness coefficient [−] and R is the hydraulic radius [L]. At the upstream boundary conditions ($x=0$), the observed or calculated hydrograph, $Q(0,t)=Q_U(t)$; where subscript U represents upstream, were imposed. At the downstream boundary ($x=L$; where L is the length of river), a loop rating curve that estimates boundary discharge using Manning formula and modified momentum equation (Fread, 1993) was applied and expressed as:

$$Q(L,t)=\frac{1}{n}AR^{2/3}S_f^{1/2} \quad (4)$$

$$S_f=-\frac{1}{gA}\frac{\partial Q}{\partial t}-\frac{1}{gA}\frac{\partial\left(Q^2/A\right)}{\partial x}-\frac{\partial h}{\partial x} \quad (5)$$

where all parameters were previously defined. Above equations were numerically solved by four-point implicit finite difference (Preissmann) scheme (Cunge et al., 1980; Szymkiewicz, 2010). The advantages of this scheme are the unconditional stability regardless of the limitation of time step Δt and the flexible selection of space step Δx since the scheme is implicit and box type finite difference structure. In this study, weighting parameter, θ was selected to be 0.55.

In addition to the abovementioned basic conditions, several hydraulic structures were considered as the internal boundary conditions that were distinguished from external boundary conditions such as upstream or downstream boundary. At a river confluence where two or more flows merge and at the inflow directly released from other land use, continuity and energy equations are required to be satisfied as the junction internal boundary (Fig. 1a). The continuity equation is expressed as:

$$Q_d=\sum_{i=1}^{m}Q_i \quad (6)$$

where subscript d represents the lower-junction node and m is the number of the upper-junction node. Note that the effect of storage is not considered in Eq. (6). The energy equation can be simplified by assuming that the head loss and the other local energy loss are negligible (Akan and Yen, 1981), resulting in:

$$h_i=h_d \quad i=1,2,\cdots,m \quad (7)$$

It is noteworthy that the proposed river routing model is applicable only for branched river network and not able to simulate looped river networks. The numerical stability of Preissmann scheme as described above is not valid for the case of simulating the transition of the flow condition from subcritical flow to transcritical- and supercritical flow in channels where the slope is steep This problem can be solved by explicit solution scheme such as two-step Lax-Wendroff scheme (Wongtragoon et al., 2009),