EFFECT OF UNCERTAINTIES OF AGRICULTURAL WORKING SCHEDULE AND MONTE-CARLO EVALUATION OF THE MODEL INPUT IN BASIN-SCALE RUNOFF MODEL ANALYSIS OF HERBICIDES

Yoshihiko Matsui, Takanabu Inoue, Taku Matsushita, Takeshi Yamada, Masahiro Yamamoto, and Yasushi Sumigama

Department of Civil Engineering, Gifu University, 501-1193 Japan
Tel. +81-58-293-2429; Fax +81-58-230-1891; E-mail: y-matsui@cc.gifu-u.ac.jp

ABSTRACT
In the prediction of time-series concentrations of herbicides in river water with diffuse-pollution hydrological models, farming schedules (the dates of herbicide application and drainage of irrigation water from rice paddies) greatly affect the runoff behavior of the herbicides. For large catchments, obtaining precise data on farming schedules is impractical, and so the model input inevitably includes substantial uncertainty. This paper evaluates the effectiveness of using the Monte-Carlo method to generate sets of estimated farming schedules to use as input to a GIS-based basin-scale runoff model to predict the concentrations of paddy-farming herbicides in river water. The effects of using the Monte-Carlo method to compensate for uncertainty in the evaluated parameters for herbicide decomposition and sorption were also evaluated.

KEYWORDS: herbicide, runoff prediction, modeling, farming schedule, pollutograph

INTRODUCTION
Pesticides used in agriculture can enter hydrological catchment systems and contaminate rivers, which are primary sources of drinking water in many regions. Hydrological diffuse-pollution models are designed to simulate the movements of water and pollutants in river basins and thereby aid in assessing water quality. Several models for predicting pesticide concentrations in river water have been proposed and applied. The Hydrologic Simulation Program-FORTRAN (HSPF) (Johanson et al., 1983, 1997) is a comprehensive model of watershed hydrology and water quality that enables integrated simulations of runoff, sediments, and nutrient transport. Models can be applied to pesticide transport in basin-size areas (Moore et al., 1988, Laroche et al., 1996, Dabrowski, et al., 2002).

The application of these models for predicting pesticide movements in river basins requires accurate agricultural as well as hydrological, meteorological, and geographical data as input. Accurate hydrological, meteorological, and geographical data are collected throughout Japan and are available to researchers. For large target catchment areas, however, acquisition of precise data on farming schedules, including the amounts of pesticides used and the dates of application, is impossible; the data acquired inevitably involves substantial uncertainty. Moreover, many factors affect the processes of sorption and decomposition of pesticides in soil and water. Owing to a lack of information on the reaction environment, however, it is impossible to quantify specific reaction rates. Generally, reported values are subject to various kinds of uncertainties.

Accordingly, the purpose of our work was to study the effects of uncertain input data regarding agricultural work schedules on model-based predictions of herbicide concentrations in river water. This paper evaluates the effectiveness of using the Monte-Carlo method to create estimates of input data, using a river-basin model composed of a large area divided into small compartments. The effects of uncertainty in the input parameters for herbicide decomposition and sorption are also discussed.

MODEL DESCRIPTION
Compartment Model
A compartment model was used to describe the movement of herbicides in a river basin and to create herbicide pollutographs. In the model, a river basin was divided into a grid of 1 km × 1 km grid cells. Each grid cell was subdivided into 12 compartments: each compartment was defined as consisting mainly of a river-water compartment (R compartment), a river-bed compartment (S compartment), a paddy-field-water compartment (W compartment), 2 paddy-field-soil compartments (X and Y compartments), or others (Fig. 1). Water and herbicides from all compartments except the C compartment move laterally to the R compartment of one of the immediately surrounding 8 grid cells, specifically, to the cell along the steepest downhill slope from the source cell. Lateral movement from the C compartment goes to the R compartment of the next grid cell via the S compartment of that grid cell. The irrigation water in the W compartment comes from the R compartment of the same grid cell or from the grid cell that contains the intake gate (R compartment) for the paddy field. Vertical flows from all compartments except the R and S compartments are downward.

A set of differential mass-balance equations describing the dynamics of a solute (herbicide) and water in each compartment was formulated, based on the law of conservation of mass for the herbicides and the water. In the hydrology (water flow) part of the model, the rates of lateral water flow into ($Q_{W,in}$) and out of ($Q_{W,out}$) the W compartment are described as functions of the water level (h_W) in the compartment:

$$Q_{W,in} = A\,a_{W,in}\max\left(0, h_{W,0} - h_W\right) + A\,q_W \qquad (1)$$

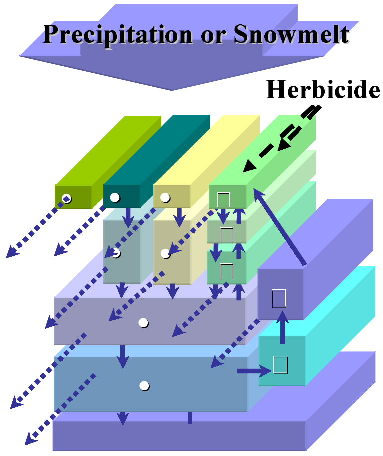

Fig. 1 Compartments in a grid cell
(R: river, S: river bed, W: paddy field, U: urban area, M: mountain, F: upland field)

$$Q_{\mathrm{W,out}} = A\, a_{\mathrm{W,out}} \max\left(0, h_{\mathrm{W}} - h_{\mathrm{W,0}}\right) \tag{2}$$

The water depth in the paddy field (h_{W}) is artificially controlled at various levels according to the growth stage of rice and the weather conditions. The desired water level in the rice paddy field ($h_{\mathrm{W,0}}$) and the spill-over irrigation flow rate (q_{W}) are input variables, which are determined by the rice farming schedules.

Vertical flow from W compartments ($Q_{\mathrm{W,V}}$) is described as a function of water level in the rice paddy field; this water goes into the X compartment beneath the W compartment in the same grid cell

$$Q_{\mathrm{W,V}} = a_{\mathrm{W,V}}\, A \left(\frac{h_{\mathrm{W}}}{h_{\mathrm{W,0}}}\right) \tag{3}$$

The rates of lateral flow (Q_{H}) from the M, F, and U compartments are described by the Manning equation:

$$Q_{\mathrm{H}} = \frac{A}{B} h \frac{1}{n_{\mathrm{M}}} h^{2/3} I^{1/2} \tag{4}$$

The rates of lateral interflow from X, Y, N, G, B, and C compartments are described as a function of the water level in the compartment and the slope of the compartment:

$$Q_{\mathrm{H}} = a_{\mathrm{H}}\, I \left(\frac{A}{B}\right) h \tag{5}$$

Vertical flows from the X, Y, M, N, F, G, B, and C compartments are described as percentages of each water contents, which is equivalent to the water level relative to the compartment height:

$$Q_{\mathrm{V}} = a_{\mathrm{V}}\, A \left(\frac{h}{h_0}\right) \tag{6}$$

The Manning equation is also used to describe the flow rate in the R compartment:

$$Q_{\mathrm{R}} = \frac{A}{L_{\mathrm{R}}} h \frac{1}{n_{\mathrm{M}}} h^{2/3} I^{1/2} \tag{7}$$

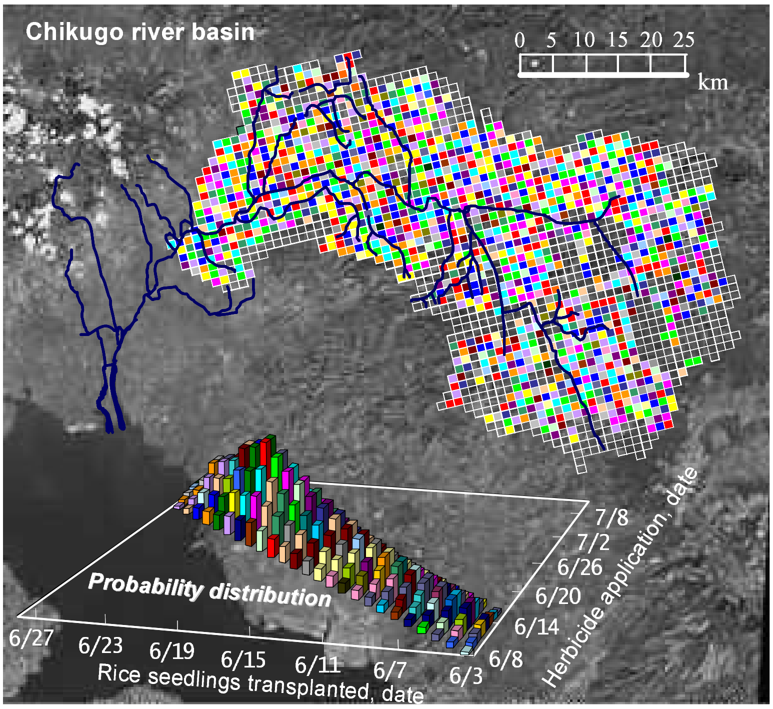

Fig. 2 Probability distribution of farming schedules (histogram) and an allocation pattern of farming schedules in a target river basin (each farming schedule shown as a colored bar in the histogram was allocated to compartments randomly)

For solute movement between compartments, advection and diffusion are considered. Solute advections are given as the product of the concentration and water flow rate calculated from equations 1–7. However, the maximum real concentration for each solute is limited by its solubility in water, so any amount of herbicide over the solubility limit must exist in the solid phase and is not subject to movement. The rate of solute movement by diffusion between compartments is given by the linear driving force model:

$$q_{\mathrm{D}} = A\frac{D}{L}\left(C_1 - C_2\right) \qquad (8)$$

Within a compartment, both the solute concentration and the water level are assumed to be uniform, each represented by a single variable. For example, rainfall is assumed to mix completely and uniformly with herbicides in the paddy-field-water compartment (W compartment). If a compartment consists of multiple subelements (soil–solid and soil–water), a dynamic equilibrium exists between the dissolved and sorbed fractions at the solid–water interface. These phases are assumed to be in equilibrium at all times; sorption processes are considered to be instantaneous and are described by a single constant (the solid–water partition coefficient) in the linear equilibrium relationship. Hence, once the concentration in one phase is known, the concentration in the other phase can be calculated. Degradation of herbicides in each compartment follows first-order kinetics. The processes of herbicide uptake by plants and herbicide evaporation into the atmosphere were not considered in this model. The flow rate coefficient in each type of compartment (W, X, etc.) is assumed to be a single value (for each compartment) throughout the entire set of grid cells in the basin. These assumptions were made to reduce the total number of hydrologic parameters, even though the target river basin was divided into numerous grid cells, which contributed to preventing too much uncertainty in determining the model parameter values.

SITE DESCRIPTION AND MODEL APPLICATION

Two river basins were selected to test the model and to analyze the effects of uncertainties in agricultural work schedules on modeled predictions of herbicide concentrations: the Chikugo River basin (1884 km^2; Fig. 2) and the Oirase River basin (667 km^2, Matsui *et al.*, 2002). The Chikugo basin includes rice paddy fields (261 km^2) cultivated by 22860 farmers, and the Oirase basin includes rice paddy fields (92 km^2) cultivated by 3400 farmers. The Oirase River basin was divided into 667 grid cells (each 1 km^2), for a total of 8004 compartments. A set of 16008 equations was solved to describe the movements of water and herbicides in the river basin. The Chikugo River basin was divided into 1884 grid cells. Because the Chikugo River basin includes several dams, where river flow rates are artificially controlled, model calculations were conducted for the catchment area of each dam. The model equations were solved as a system of ordinary differential equations by Gear's stiff method from the IMSL MATH/LIBRARY.

Application of the compartment model to the river basin requires geographic data: the altitude of each compartment was determined from Geographic Information System (GIS) data (The Geographical Survey Institute, Japan, 1999), and water flow directions between compartments were determined based on the direction of the steepest gradient. The GIS data (The

Geographical Survey Institute, Japan, 1990) were also used to calculate the areas of the compartments (paddy field, river, forest, etc.) in each grid. However, the GIS data available were old and may not reflect current land utilization. The area of paddy fields, which is the most important geographical information in this research, was corrected with data published by the local governments (Census of Agriculture Japan, 1995 and 2000), which include data on the percent of rice paddy area

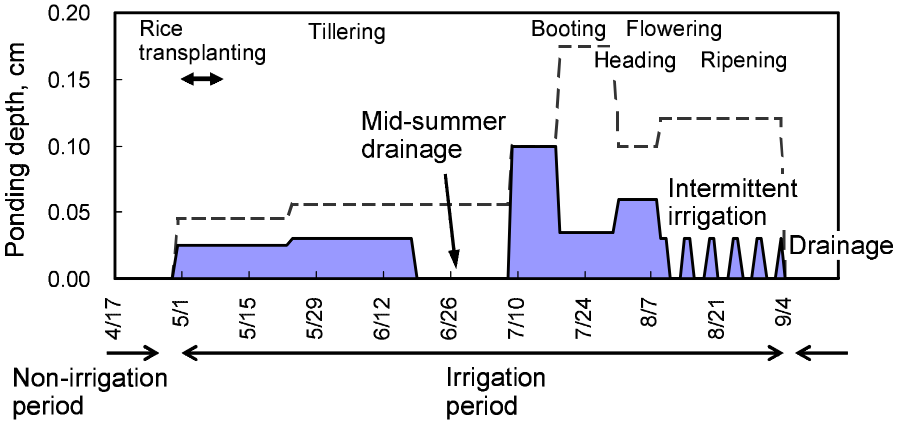

Fig. 3 A pattern of irrigation (solid line for ordinary temperature and dashed line for high temperature)

removed from cultivation due to compulsory adjustments in production. The fallow paddy fields were regarded as upland field compartments.

HYDROLOGIC MODEL INPUTS AND SYSTEM PARAMETERS

The amount of precipitation in each grid cell was estimated by interpolating the observed data from observation points in and around the target area and applying three-dimensional corrections for variations in altitude and location. Evapotranspiration was estimated by the method of Brutsaert and Stricker (1979) from data on air temperature, wind velocity, duration/intensity of sunshine, and celestial declination. For the Oirase river basin, the effects of snowfall and snowmelt were estimated by a temperature index method (Ikebuchi *et al.*, 1984, 1985).

The hydrologic (water flow) model requires 11 parameters optimized. The values of the vertical flow rate coefficients in the W and X compartments ($a_{W,\ V}$) were determined to be a typical value for the field percolation rate of water in paddy fields, 0.01 m s^{-1}. The spill-over flow rate (q_W) was estimated to be 0.02 m s^{-1}. Irrigation and drainage rate coefficients of rice paddy fields ($a_{W,\ in}$ and $a_{W,\ out}$) were inputs as 5 and 2 d^{-1}, respectively, after talking with a farmer, considering the structures and dimensions of outlets of several rice paddy fields, and also actually measuring the drainage flow rate of a paddy field. The values of the remaining parameters were seached by iteration to give the best fit to the observed river flow rate within the minimum error. In addition to this best-fit criterion, the parameters were set so as to give no annual long-term water loss in the C compartment. The hydrologic parameters of the model were successfully calibrated, with the result that they fit the observed stream flow data to the model simulation with reasonable accuracy.

MONTE-CARLO GENERATION OF RICE CULTIVATION SCHEDULE

Fig. 3 shows the irrigation schedule recommended by a local government, which was used to determine the input data for water depth and irrigation rate. The irrigation schedule is set according to the rice-transplanting date. To maintain the water depth in a field during various periods of rice growth, the water consumed due to evapotranspiration and percolation is replaced by irrigation. The irrigation and drainage schedule can be adjusted for herbicide dusting and ambient temperature. For example, after herbicide dusting, drainage is halted for 5 days. The water depth is also changed according to whether the ambient temperature is high (>20 °C) or not. Therefore, the input rice farming schedule can be based on the dates of rice transplanting and herbicide dusting. For a large paddy field cultivated by numerous farmers, however, the schedule of agricultural tasks in the entire paddy field is not homogeneous: rice transplanting and herbicide dusting are not each performed on a single date. The transplanting season continues for several weeks, and each herbicide is dusted once within a certain period after transplantation is finished. For example, dusting with the herbicide mefenacet is done once, between 5 and 15 days after transplantation.

Modeling the agricultural schedules of each farmer after detailed data acquisition is ideal but too troublesome to be feasible. However, due to the large scale of the study area and its cultivation by many farmers, it should be possible to consider agricultural tasks as random events within defined periods of time, which can be estimated from data published by local governments. Two hundred farming work schedules (combinations of dates for rice transplanting and herbicide dusting) were created for each herbicide; the probability of occurrence of each work schedule is indicated by the histogram in Fig. 2. For example, in about 5% of the rice paddy fields, rice seedlings were transplanted on June 23 and herbicide was dusted on July 2. Farming schedules were allocated to the paddy field compartments of the grid cells in the river basin randomly, within an expected occurrence probability (the histogram in Fig. 2 shows an allocation pattern for the herbicide mefenacet). A total of 100 schedule-allocation patterns for each herbicide were created and used as input to the modeling. For comparison, model predictions with deterministic input were also conducted, for which a single farming schedule for rice transplanting and herbicide dusting was used throughout the entire river basin (the dates of the highest bar in the histogram in Fig. 2). The amounts of herbicides consumed in the target river basin were estimated from marketing information on the sales of commercial herbicide products.

MONTE-CARLO GENERATION OF DEGRADATION RATES AND SOIL–WATER PARTITION COEFFICIENTS OF HERBICIDES

Many factors (aerobic/anaerobic conditions, soil-sediment organic content, etc.) affect herbicide decomposition and its partition between soil and water. Because of a lack of information regarding the reaction environment in the field, however, it is impossible to quantify the specific decomposition rate and sorption equilibrium in each grid cell of the model, so these values are subject to various kinds of uncertainties. Although some reports include values for the decomposition rates or half-lives, the reported ranges of these rate coefficients are very wide, partly owing to variability in the reaction conditions. Therefore, a single reported value is not appropriate for representing decomposition rates in a whole area. It is more reasonable to assume that all rate parameter uncertainties are random. Using the Monte-Carlo method, a degradation rate coefficient for each herbicide in each compartment was randomly selected from values in the ranges of the reported values. The solid–water sorption coefficient of each herbicide was treated the same way. For comparison, we repeated the model calculation using the average of reported values as deterministic parameter value inputs.

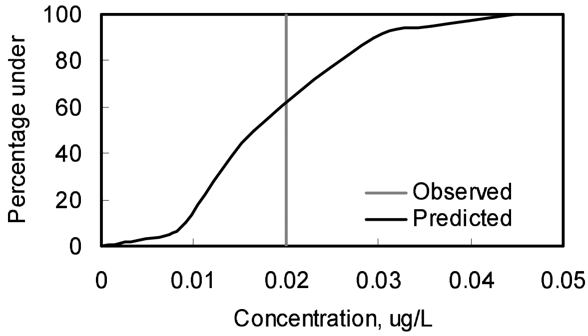

Fig. 4 Probability distribution of predicted pretilachlor concentration on June 9, 1999

PREDICTING HERBICIDE CONCENTRATIONS

Herbicide concentrations were measured 5 days a week during 1999 and 2000 in the Chikugo River and once a week during 1995 and 1996 in the Oirase River. After the hydrological system parameters were calibrated, the hydrological and solute models were solved simultaneously by substituting solute input data, yielding predicted concentrations of herbicides in the river waters. Model-based predictions from the Monte-Carlo inputs were made, starting with each of the 100 schedule-allocation patterns. Fig. 4 shows the probability distribution for the concentration of the herbicide pretilachlor on one day in 1999 in the Chikugo River. The predicted concentrations are distributed broadly, due to the Monte-Carlo generation of the farming schedules and herbicide parameters. The highest 95th percentile concentration was 7 times the lowest 5 percentile concentration. Fig. 5 shows time variations in the pretilachlor concentration. About half the observed data points are within the 1%–99% probability range of the predicted concentrations. Although the herbicide dusting date and the amount applied are important factors in predicting the concentrations, our modeling did not consider the amount and date of herbicide dusting by individual farmers. Moreover, the simulations were conducted without optimizing the herbicide decomposition/sorption parameters. In light of these limitations, we consider the model prediction for pretilachlor to be reasonably successful. As shown in Fig. 5, compared with the prediction using Monte-Carlo inputs, the prediction obtained with deterministic input yielded a rather discrete concentration variation with improper peaks .

Although prediction of pretilachlor concentration with the Monte Carlo method was good, the results for other herbicides were less successful. For example, the predicted concentration of dimethametryn was lower than that observed (Fig. 6). These discrepancies could be due to poor estimates of herbicide consumption (from the sales volume) and/or of the herbicide decomposition parameter. A precise evaluation of local herbicide sales would improve the prediction. Nonetheless, use of the Monte-Carlo method for generating input farming schedules and decomposition/sorption parameters improved predictions of herbicide runoff (Figs. 7 and 8). More than 60% of the predictions based on Monte-Carlo inputs were within 0.1 to 10 times the observed values, and the Monte-Carlo method reduced the percentage of 'bad' predictions (shown in yellow). Fig. 9 summarizes the prediction performance for the Oirase River, again showing the effectiveness of the Monte-Carlo method in alleviating input data uncertainties.

CONCLUSIONS

The effectiveness of the Monte-Carlo method for creating input data for agricultural work schedules and pesticide decomposition/sorption parameters was studied. The Monte-Carlo method was used to randomly allocate 200 patterns of farming work schedules to each paddy field in grid cells of a GIS-based basin-scale pesticide runoff model. The degradation rate and sorption coefficient for each herbicide in each compartment were also randomly selected from values in the ranges of reported values. Prediction of pesticide concentrations in river water by the runoff model was better with Monte-Carlo input than with deterministic input. The Monte-Carlo method alleviates the difficulty of obtaining precise data on individual farming schedules (including pesticide dusting dates) and on individual degradation rates and sorption coefficients in each soil. Once better values are available for the amounts of pesticides applied and for pesticide degradation rates and sorption parameters under actual field conditions, the GIS-based basin-scale runoff model should successfully predict river water pesticide concentrations.

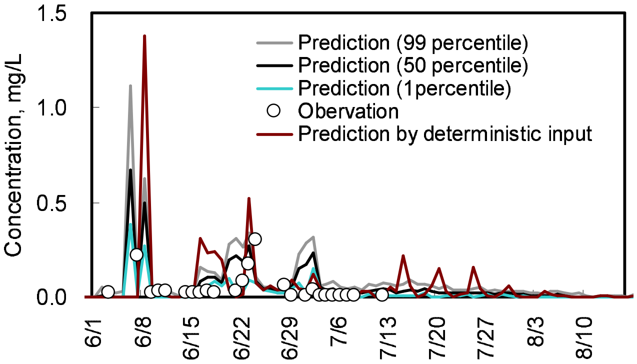

Fig. 5a Predicted and observed pretilachlor concentrations in Chikugo River in 1999

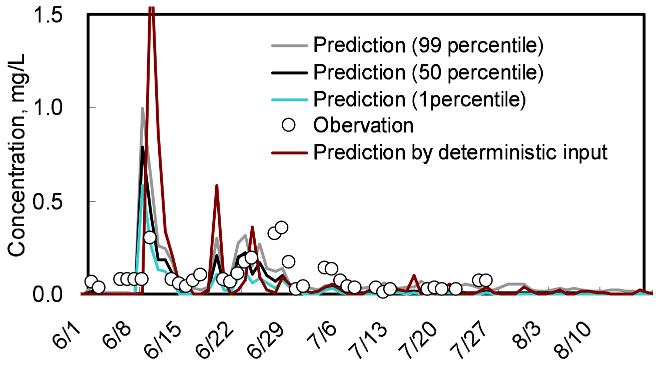

Fig. 5b Predicted and observed values of pretilachlor concentration in Chikugo River in 2000

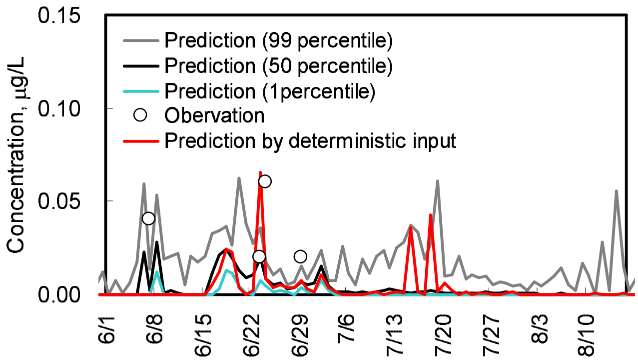

Fig. 6a Predicted and observed dimethametryn concentrations in Chikugo River in 1999

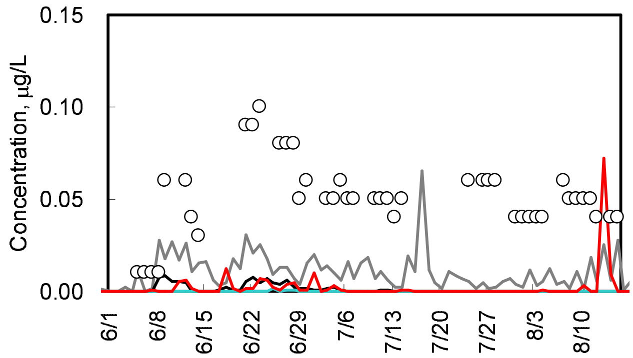

Fig. 6b Predicted and observed dimethametryn concentrations in Chikugo River in 2000

ACKNOWLEDGMENTS

We thank Satoshi Tsutsumi and Eikichi Shima for their assistance in field survey and the Science and Technology Agency and the Ministry of Education, Science, Sports and Culture of the Government of Japan for funding this research.

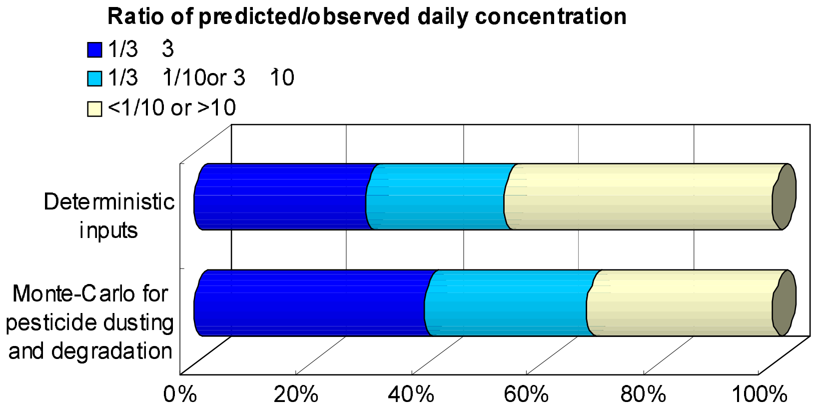

Fig. 7 Comparison of model predictions with inputs generated by Monte-Carlo and deterministic methods (Chikugo River)

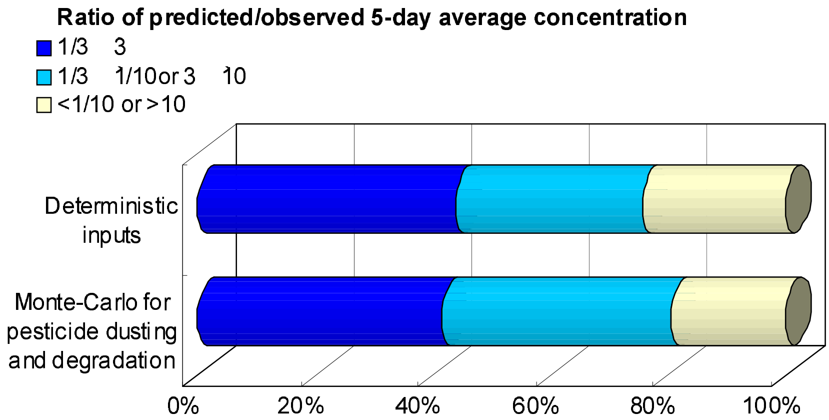

Fig. 8 Comparison of model predictions with inputs generated by Monte-Carlo and deterministic methods (Chikugo River)

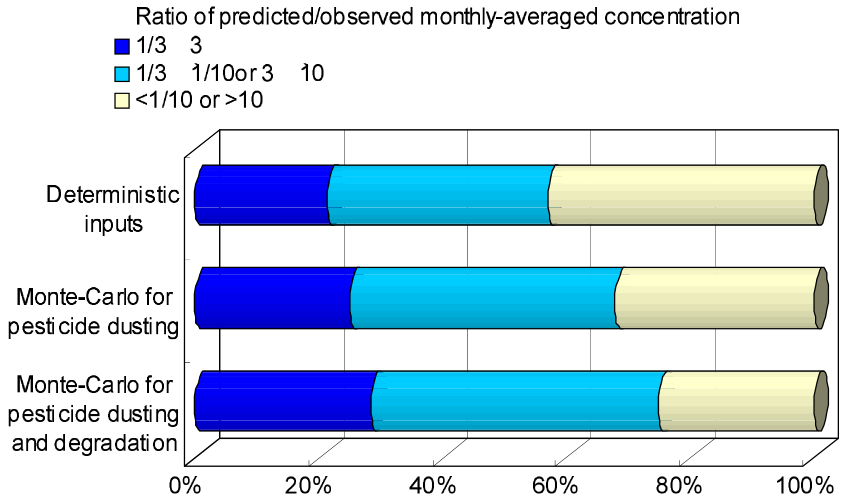

Fig. 9 Comparison of model predictions with inputs generated by Monte-Carlo and deterministic methods (Oirase River)

REFERENCES

Brutsaert, W. and Stricker, H. (1979) An advection-aridity approach to estimate actual regional evapo-transpiration. *Water Resour. Res*, 15(2), 443-450.

Census of Agriculture Japan 1995 and 2000, Association of Agriculture & Forestry Statistics, Tokyo, Japan

Dabrowski, J. M., Peall, S. K. C., Niekerk, A. V., Reinecke, A. J., Day, J. A., and Schulz, R. (2002) *Water Res.* 36, 4975-4984.

Geographical Survey Institute (1990) *Detailed Digital Information KS-200-1*, CD-ROM, Japan Map Center, Tokyo, Japan.

Geographical Survey Institute (1999) *Digital Map 50m Grid (Elevation)*, CD-ROM, Japan Map Center, Tokyo, Japan.

Ikebuchi, S., Takebayashi, S., and Tamomura, M. (1984) Snowfall-melt-runoff analysis of Lake Biwa-Ohura river basin. *Proc. 28th Japanese Conference on Hydraulics*, pp.441-446 (in Japanese).

Ikebuchi, S., Takebayashi, S., and Tamomura, M. (1985) Snowfall-melt-runoff analysis of Lake Biwa-Ohura river basin-II. *Proc. 29th Japanese Conference on Hydraulics*, pp.155-160 (in Japanese).

Johanson, R. C. (1983) A new mathematical modeling system In *Fate of Chemicals in the Environment: Compartmental and Multimedia Models for Predictions* (ACS symposium series; 225), R. L. Swann (ed.), American Chemical Society, Washington, D.C. pp.125-147.

Johanson, A. S., Imhoff, J. C., Kittle, J. L., and Donigian, A. S. (1997) *Hydrologocal simulation program-Fortran (HSPF): user's manual for Release 10.0*. EPA-600, USEPA, Washington, D. C.

Laroche, A.-M., Gallichand, J., Lagacé, R, and Pesant, A., (1996) Simulating atrazine transport with HSPF in an agricultural watershed. *J. Envir. Engrg., ASCE*, 122(7), 622-630.

Matsui, Y., Itoshiro, S., Buma, B., Hosogoe, K., Yuasa, A., Shinoda, S.,, Matsushita, T., and Inoue, T. (2002) Predicting Pesticide Concentrations in River Water by Hydrologically Calibrated Basin-Scale Runoff Model, *Water Science & Technology*, 45(9), 141–148.

Moor, L. W., Matheny, H., Tyree, T., Sabaniti, D., Klaine, S. J. (1988) Agricultural runoff modeling in a small west Tennessee watershed. *J. Water Pollution Control Federation*, 60(2), 242-249

Verschueren, K. (1996) *Handbook of Environmental Data on Organic Chemicals*, Van Nostrand Reinhold, New York, NY.

NOMENCLATURE

$a_{W,V}$: infiltration rate coefficients of the rice paddy field (m/s).
$a_{W,in}$ and $a_{W,out}$: irrigation and drainage rate coefficients of the rice paddy field, respectively (s^{-1})
a_V: vertical flow rate coefficient (s^{-1})
a_H: lateral flow rate coefficient (m/s)
A: area of the compartment (m^2)
B: length on a side of a square grid (m)
C_1 and C_2: concentration in each compartment (kg/m^3).
D: a diffusion coefficient (m^2/s)
L: a distance between compartments (m)
L_R: river length in a compartment (m)
h: water level of the compartment (m)
h_0: depth of the compartment (m)
h_W: water depth of the rice paddy field (m)
$h_{W,0}$: objective water depth of the rice paddy field (m)
I: slope (dimensionless)
n_M: Manning coefficient ($m^{2/3}$ s/m^3)
q_D: a solute diffusion rate between compartments (kg/s)
q_W: flow rate of spill-over irrigation divided by the paddy area (rate of continuous irrigation in order to keep a certain water depth and to prevent hot water damage: extra amount of irrigated water spill over from the outlet of the paddy, m/s)
Q_V: vertical flow rate (m^3/s)
Q_R: river flow rate (m^3/s)
Q_H: lateral flow rate (m^3/s)
$Q_{W,in}$: irrigation rate (flow rate of water to the paddy field, m^3/s)
$Q_{W,out}$: drainage rate (flow rate of water from the paddy field, m^3/s)