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Numerical modeling of diazinon transport through inter-row vegetative filter strips

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Abstract

A numerical simulation model of pesticide runoff through vegetative filter strips (PRVFS) was developed as a tool for investigating the effects of pesticide transport mechanisms on VFS design in dormant-sprayed orchard. The PRVFS model was developed applying existing theories such as kinematic wave theory and mixing zone theory for pesticide transport in the bare soil area. For VFS area, the model performs flow routing by simple mass accounting in sequential segments and the pesticide mass balance by considering pesticide washoff and adsorption processes on the leaf, vegetative litter, root zone and soil. Model sensitivity analysis indicated that pesticide transfer from surface soil to overland flow and pesticide washoff from the VFS were important mechanisms affecting diazinon transport. The VFS cover ratio and rainfall intensity can be important design parameters for controlling diazinon runoff using inter-row VFS in orchard. The PRVFS model was validated using micro-ecosystem simulation of diazinon transport for 0, 50 and 100% VFS cover conditions. The PRVFS model is shown to be a beneficial tool for evaluating and analyzing possible best management practices for controlling offsite runoff of dormant-sprayed diazinon in orchards during the rainy season.

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1. Introduction

Pesticide runoff from row, field, and orchard crops has been considered the primary cause of toxicity in rivers of the Central Valley of California (Foe and Connor, 1991). Thousands of hectares of deciduous fruit and nut orchards in the Central Valley are subject to dormant-season application of organo-phosphate insecticides such as diazinon. As a result of Mediterranean climate, pesticides were often found at toxic levels in the streams during the winter rainy season because of off-site movement of pesticides previously applied as dormant-sprays to orchards (Crepeau et al., 1991; Damagalski et al., 1997; Panshin et al., 1998; Kratzer, 1999).

Vegetative filter strips (VFS) are known to have potential for reducing pesticide runoff. Generally, VFS filter suspended soil particles by reducing runoff flow velocity and increasing infiltration rates, and can be effective in controlling some non-point source pollutants such as sediment and sediment-bound agricultural chemicals and pesticides (Dillaha et al., 1989). USDA (2000) reported

detailed practical applications such as design, installation, and maintenance of buffer strips. Watanabe and Grismer (2001) reported that total diazinon losses as percent of applied pesticide mass from the orchard floor following rainfall–runoff simulation were 8.6, 5.8 and 2.3%, respectively, for 0, 50, and 100% VFS cover treatments. Diazinon has moderate to high mobility based on its wide range of K_{OC} values and its solubility of 68.8 mg/l at 20 °C (Howard, 1989). The study by Watanabe and Grismer (2001) suggested that the principle mechanism for the reduction of diazinon runoff in VFS was reduction of runoff, the primary pesticide carrier. Runoff was reduced by diverging incoming runoff into lateral subsurface flow or interflow through the VFS rootzone and mainly movement below rootzone in VFS area. Therefore, the inter-row VFS installed between tree rows, can be effective in reducing diazinon runoff from dormant-sprayed orchards. Identifying and quantifying the design criteria such as optimum VFS coverage and rainfall intensity should contribute to a better conceptualization of the role of VFS in non-point source pollution control.

Simulation models can be used as tools for analyzing the mechanisms of pesticide transport and for evaluating possible best management practices (BMPs) in controlling

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Nomenclature			
Eq. (1)		v_c	the retarded velocity of the centroid of the contaminant plume
f	the infiltration rate (LT^{-1}) of the soil	λ	dispersivity (L)
T	the time (T)	ν	pore velocity (LT^{-1})
a and b	fitting parameters		
Eq. (2)		Eq. (10)	
θ	the volumetric water content for the soil layer (L^3L^{-3})	MC_{mWp}	the initial pesticide mass per area (ML^{-2})
f_i	the infiltration rate (L/T)	Eq. (11)	
d	the depth of the layer (L)	C_{mW0}	the initial soil–water mixing zone pesticide concentration (ML^{-3})
t	the time		
Δt	the time interval (T)	Eq. (12)	
Eq. (3)		MC_{LF}	the diazinon residue on the leaf during the simulation (ML^{-2})
t	time (T)	M_{ap}	the pesticide application rate (ML^{-2})
h	the depth of the overland flow (L)	$R, (= ri t)$	the rainfall depth (L)
m	the K-W exponent	a_{wof} and b_{wof}	the fitting constants
ri	the rainfall intensity (LT^{-1})		
x	the length of the slope on the plane	Eq. (13)	
$\alpha = C\sqrt{S}$	S is slope and $C = (1/n)R^{1/6}$ where n is the Manning's roughness coefficient and R is the hydraulic radius ($\cong h$ for the overland flow)	C_{wof}	the pesticide concentrations in washoff (ML^{-3})
Eqs. (4) and (5)		Eq. (15)	
C_r	the pesticide concentration in overland flow (ML^{-3})	C_{vr}	the diazinon concentration in the vegetative residues (MM^{-1})
C_m	the pesticide concentration in soil water in the mixing zone (ML^{-3})	M_{vra}	the mass of the vegetative residues comprising the thatch layer (ML^{-2})
k_f	the film transport coefficient (LT^{-1})	Eq. (16)	
θ_s	the volumetric water content at saturation (MM^{-3})	a_{vr} and b_{vr}	fitting parameter
ε	the mixing zone thickness (L)	Eq. (17)	
ρ_b	the bulk density of the soil (ML^{-1})	C_v	the diazinon concentration in runoff on VFS area (ML^{-3})
k_d	the soil/water partitioning coefficient of the pesticide (LM^{-1})	C_{vr}	diazinon concentration in runoff from upstream soil area (ML^{-3})
q	the excess rainfall and $q = ri - f$	w	the width of the VFS (L)
Eq. (8)		L_{vfs}	the length of the VFS (L)
C_{mW0}	the pesticide concentration in the soil–water mixing zone at the ponding time	Fq_{sl}	the runoff per unit width of the basin at the downstream edge of the baresoil area (L^2T^{-1})
Eq. (9)		$Fq_v(ndxv)$	the runoff per unit width at the downstream-end node ($ndxv$) of the VFS area (L^2T^{-1})
$C_{mW}(z, t_p)$	the chemical concentration distribution in the soil water at ponding (ML^{-3})	f_{dvrw}	the fraction of the runoff water depth for the runoff zone
M_a	the applied pesticide mass on the soil surface (ML^{-2})	d_{vr}	runoff zone depth in VFS (L)
z	the vertical coordinate taken as positive downwards (L)	Eq. (18)	
D	the hydrodynamic dispersion coefficient of the pesticide (L^2T^{-1})	C_{rzw}	the diazinon concentration in rootzone soil water (ML^{-3})

k_{drz}	the diazinon soil/water partitioning coefficient for the rootzone (L^3M^{-1})	$f_{vss}(i)$	the infiltration rate at the base of the soil layer for segment (i) (LT^{-1})
d_{rz}	the depth of the root zone (L)	Eq. (20)	
ρ_{brz}	the bulk density of the root zone (ML^{-3})	A	the area of the bare soil area
θ_{srz}	the saturated volumetric water content of the rootzone (L^3L^{-3})	h_k	the depth of the water at k th row and w is the width of the field
$Fq_{rz}(ndxv)$	the interflow per unit width of the rootzone at the downstream-end node $ndxv$ (L^2T^{-1})	VQ_{k-1}	the inflow from the previous row $k - 1$
$f_{vs}(i)$	the infiltration rate at the base of the rootzone for segment (i) (LT^{-1})	Eq. (21)	
Eq. (19)		C_{VFSP}	the pesticide concentration in overland flow (ML^{-3}) from the previous row VFS obtained from the combined inflow pesticide mass of runoff and interflow
C_{vsw}	the diazinon concentration in the soil water (ML^{-3})		

pesticide discharges from agricultural fields. Studies of the numerical modeling of VFS in the field are mainly related to sediment transport control (Tollner et al., 1977; Barfield et al., 1979; Hayes et al., 1979; Flanagan et al., 1989; Hayes and Dillaha, 1992; Munoz-Carpena et al., 1999). A few chemical transport models for VFS are available in the literature (Glick et al., 1992; Barfield et al., 1992; Chaubey et al., 1995). Glick et al. (1992) studied the effects of vegetative cover and filter width on water quality from urban vegetative buffers using a physically based model to simulate urban buffer zones. Their preliminary test studies showed that the simulated concentrations were very close to those at the entrance to the buffer, however, the model tended to overestimate concentrations of chemicals leaving the longer buffer strips. Barfield et al. (1992) studied water quality control aspects of natural riparian grasses and used a mass balance approach to partition the chemical transport pathways. Their analysis concluded that the major pathway of chemical transport in the vegetative buffer was infiltration of runoff containing dissolved chemicals. Chaubey et al. (1995) developed an event-based model to simulate nutrient transport in VFS. The performance of their model for predicting nutrient transport in VFS depends upon accurate prediction of infiltration and runoff. Srivastava et al. (1998) suggests that including nutrient removal mechanisms in the model component may improve its performance.

However, little information is available regarding modeling pesticide transport in VFS. For application of VFS in orchards for controlling runoff of dormant-sprayed diazinon during winter rains, design guidelines and methodology evaluating VFS performance need to be developed. In this study, we present the development of a numerical simulation model of pesticide runoff through vegetative filter strips (PRVFS) by focusing on the control of diazinon runoff from dormant-sprayed orchards. While an attempt is made to consider process-based models to describe each transport mechanism, such as adsorption

and pesticide washoff, PRVFS was developed as a decision support model for VFS design and serve as a starting point of future model development of similar transport phenomena. Therefore, existing theory and algorithms were applied from available models for each transport process.

2. Numerical model development

Pesticide transport in runoff is a combination of processes such as pesticide desorption from the surface soil and vegetation, overland flow of dissolved and sediment-adsorbed pesticide, infiltration of dissolved pesticide and dilution by rainfall. Pesticide detachment from the vegetative surface by rainfall can be a significant process when it is foliar applied. Detachment and washoff of pesticide from the vegetative surface depends on adsorption strength of the chemical to the vegetative surface, rainfall intensity and runoff volume. Lipophilic compounds such as organo-chlorine pesticides penetrate leaf surface waxes and become difficult to dislodge by rain, whereas polar compounds do not penetrate the leaf surface (Leonard, 1990). Shallow interflow also contributes dissolved chemicals into the runoff stream (Ahuja et al., 1981; Donigian et al., 1977). Interflow within macro-pores in the root zone may have significant effects on pesticide concentration in runoff, however, the overall contribution of pesticide transport from the VFS system may depend on the flow path of the dissolved pesticide.

In orchard, VFS can be installed on the edge of the field or between tree rows as inter-row VFS. The VFS coverage or the ratio of width of inter-row VFS over total length of the tree row depends on the farmer's management goals. In inter-row VFS, flow paths and consequent pesticide interaction between soil and VFS become unique as shown in Fig. 1. For the simulation of pesticide losses through overland flow from bare soil

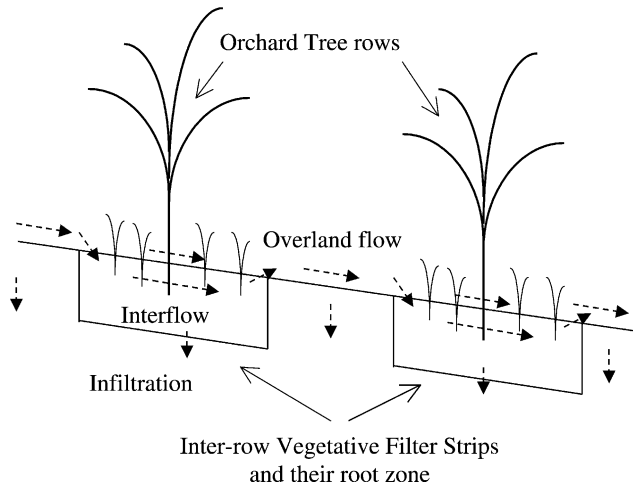


Fig. 1. Conceptual flow paths in inter-row vegetative filter strip system in dormant orchard.

area, the solute transport model developed by Havis et al. (1992) was used. For bare soil area, diazinon transport by overland flow was assumed to be the result of two processes: (1) chemical transport process of turbulent mixing in surface flow, and (2) mixing zone process of chemical transport by infiltration and chemical transfer between runoff and mixing zone. The model simulated the indoor laboratory and outdoor laboratory data for bromide tracer concentrations (Havis et al., 1992). For the pesticide transport within the VFS area, major chemical processes governing diazinon transport in VFS system were assumed to be diazinon washoff from plant leaf, diazinon adsorption on vegetative litter, diazinon adsorption in rootzone and underlying soil layers. Although filtering sediment-bound chemicals is a major importance of VFS's effectiveness on controlling non-point source pollution, we neglected the effect of sediment transport in order to simplify the initial model development. Therefore for the simulation of diazinon transport in VFS, a simple pesticide mass balance in each compartment such as plant leaf, vegetative litter, root zone and underlying soil layers were considered. PRVFS was first formulated for single VFS row case then, applied to multiple VFS row cases. Results of laboratory experiments consisting of three rainfall–runoff simulations on 0, 50 and 100% VFS cover treatments of a physical model (micro-ecosystem) for assessing diazinon transport in VFS (Watanabe and Grismer, 2001) were used for calibrations of pesticide transport parameters and validation of the model.

2.1. Hydrologic response on bare soil area

The bare soil infiltration rate was estimated using a power function fitted to infiltration rate data obtained from

the 0% VFS cover treatment of rainfall–runoff simulation by Watanabe and Grismer (2001). Havis et al. (1992) used a modified Philip's infiltration equation (Smith and Hebbert, 1983) for the estimation of ponding time. However, this equation did not satisfactorily replicate the micro-ecosystem simulation results; perhaps because the micro-ecosystem soil layer depth was limited to only 120 mm and it overlaid a sand layer. Therefore, the following fitted power function was used:

$$f = aT^b \quad (1)$$

where f is the infiltration rate (LT^{-1}) of the soil, T is the time (T) and a and b are fitting parameters obtained from the experimental data equal to 0.30 and -0.703 , respectively ($R^2 = 0.92$). The ponding time was obtained from the rainfall intensity and the infiltration rate from Eq. (1). A water balance for the soil layer (0–30 mm) was calculated as:

$$\theta_{t+\Delta t} = \theta_t + \frac{f_i \Delta t}{d} \quad (2)$$

where θ is the volumetric water content for the soil layer (L^3L^{-3}), f is the infiltration rate (LT^{-1}), d is the depth of the layer (L), and Δt is the time interval (T). Following saturation of the 0–30 mm soil layer, the water balance of the underlying 30–90 mm layer was also approximated using Eq. (2).

For overland flow initiated after ponding, the kinematic-wave (K-W) model was used and the equation can be written as:

$$\frac{\partial h}{\partial t} + \alpha m h^{m-1} \frac{\partial h}{\partial x} = ri - f \quad (3)$$

where t is time (T), h is the depth of the overland flow (L), m is the K-W exponent, ri is the rainfall intensity (LT^{-1}), x is the length of the slope on the plane, $\alpha = C\sqrt{S}$ where S is slope and $C = (1/n)R^{1/6}$ where n is the Manning's roughness coefficient and R is the hydraulic radius ($\cong h$ for the overland flow). Here it was solved using the Lax–Wendroff second-order scheme (Singh, 1996).

2.2. Pesticide runoff on bare soil area

For the pesticide losses through overland flow from bare soil without VFS, the model developed by Havis et al. (1992) was applied. The chemical transport in overland flow was simulated by considering the conservation of mass at each control volume of the runoff zone and the pesticide mixing zone. Havis et al. (1992) defined the mixing zone as the depth (ϵ) of soil layer that interacts with overland flow through turbulent mixing, where convection and diffusion contribute chemicals to surface water during rainfall events. Since it is a complex physicochemical process, chemical transport within the mixing zone is approximated as a completely mixed reactor having uniform, unsteady chemical concentrations separated from the overland flow zone as shown in Fig. 2.

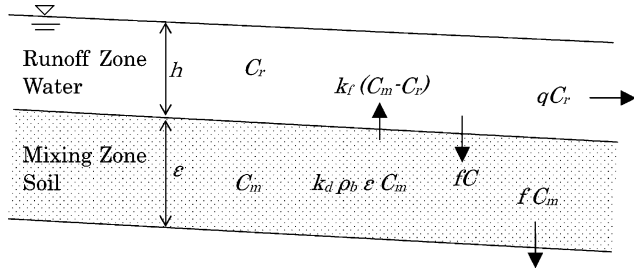


Fig. 2. Schematic of pesticide transport in runoff zone and mixing zone (refer to Eqs. (4) and (5) for terms).

The governing equation for pesticide transport in runoff on the bare soil is:

$$\frac{\partial(hC_r)}{\partial t} + \frac{\partial(qC_r)}{\partial x} = k_f(C_m - C_r) - fC_r \quad (4)$$

and that of the mixing zone is:

$$(\theta_s \varepsilon + \varepsilon \rho_b k_d) \frac{dC_m}{dt} = -k_f(C_m - C_r) + f(C_r - C_m) \quad (5)$$

where C_r is the pesticide concentration in overland flow (ML^{-3}), and C_m is the pesticide concentration in soil water in the mixing zone (ML^{-3}), k_f is the film transport coefficient (LT^{-1}), θ_s is the volumetric water content at saturation (L^3L^{-3}), ε is the mixing zone thickness (L), ρ_b is the bulk density of the soil (ML^{-3}), k_d is the soil/water partitioning coefficient of the pesticide (L^3M^{-1}), q is the excess rainfall and $q = r.i. - f$.

The depth of the mixing zone was assumed to be constant during simulations. Eqs. (4) and (5) can be simplified using the product rule on the left hand side, and substituting the derivative of the lateral runoff flux obtained from K-W equation. Also, the approximation of uniform chemical transport from soil to overland flow was applied such that there is no pesticide concentration variability along the surface plane. As a result, the chemical transport model consists of a pair of coupled, first order, linear, non-homogeneous ordinary differential equations having variable coefficients (Havis et al., 1992). The pesticide mass balance in the overland flow is given by:

$$\frac{dC_r}{dt} = \frac{k_f C_m}{h} - \frac{(k_f + ri)C_r}{h} \quad (6)$$

and the chemical mass balance in the mixing zone is given by:

$$\frac{dC_m}{dt} = \frac{(f + k_f)(C_r - C_m)}{Z_1} \quad (7)$$

where $Z_1 = \theta_s \varepsilon + \rho_b k_d \varepsilon$. Eqs. (6) and (7) were numerically solved using the Lax–Wendroff second-order scheme (Watanabe, 1999).

At the ponding time, t_p , the depth of overland flow, h , and excess rainfall, q , are assumed to be zero. In the absence of significant lateral flow at $t = t_p$, it is assumed to

be $\partial h/\partial t = ri - f$. Applying the above conditions on Eq. (4), the initial pesticide concentration at the ponding time, $C_{r(t=t_p)}$, can be approximated by:

$$C_{r(t=t_p)} = \frac{k_f C_{mW0}}{ri + k_f} \quad (8)$$

where C_{mW0} is the pesticide concentration in the soil–water mixing zone at the ponding time as described below in Eq. (11) (Watanabe, 1999). To estimate C_{mW0} , the pesticide infiltration process after initiation of rainfall until ponding ($t < t_p$) was considered as an instantaneous or pulse type point source problem by assuming there is no significant change in pesticide concentration after pesticide application until rainfall begins. The chemical concentration distribution is approximated using the Baetsle model for one-dimensional transport without pesticide decay (Domenico and Schwartz, 1997):

$$C_{mW}(z, t_p) = \frac{M_a}{\sqrt{4\pi t_p D}} \exp\left[-\frac{(z - v_c t_p)^2}{4D t_p}\right] \quad (9)$$

where $C_{mW}(z, t_p)$ is the chemical concentration distribution in the soil water at ponding (ML^{-3}), M_a is the applied pesticide mass on the soil surface (ML^{-2}), z is the vertical coordinate taken as positive downwards (L), D is the hydrodynamic dispersion coefficient of the pesticide (L^2T^{-1}), and v_c is the retarded velocity of the centroid of the contaminant plume which is described by the retardation equation (Domenico and Schwartz, 1997). The hydrodynamic dispersion coefficient is dominated by mechanical dispersion when the water flux is large (Wagenet and Rao, 1990), that is, $D = \lambda v$ where λ is the dispersivity (L) and v is the pore velocity (LT^{-1}). Values for λ range from 5.0 to 20 mm in packed laboratory columns and 50–200 mm in the field (Jury et al., 1991), and the value of 15 mm seemed appropriate for the micro-ecosystem simulations. At ponding time, the initial pesticide mass per area (ML^{-2}) in the mixing zone available for the transport is given by:

$$MC_{mWp} = \theta_s \int_0^\varepsilon C_{mW}(z, t_p) dz \quad (10)$$

where MC_{mWp} is the initial pesticide mass per area (ML^{-2}). The initial pesticide concentration in soil water of the mixing zone is approximated from the average pesticide concentration in the mixing zone:

$$C_{mW0} = \frac{MC_{mWp}}{\theta_s \varepsilon} \quad (11)$$

where C_{mW0} is the initial soil–water mixing zone pesticide concentration (ML^{-3}).

2.3. Hydrologic response in VFS

Runoff, interflow and baseflow routing in VFS was accomplished by taking water balances in sequential

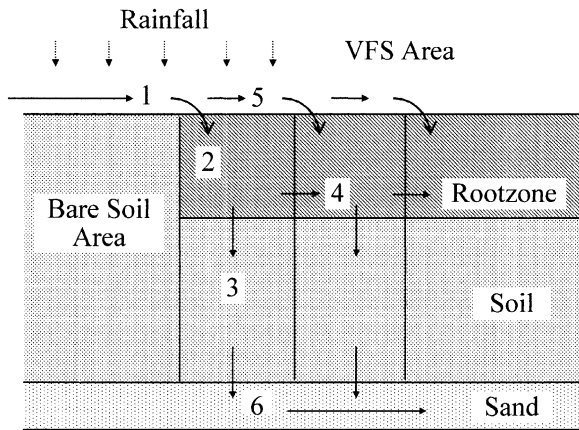


Fig. 3. Flow routing for the VFS area.

segments (user defined lengths) of root zone and underlying soil layer columns from upstream to the downstream outlet as shown in Fig. 3. Upon initiation of rainfall, rainwater is stored and increases water contents in the root zone segments. When the runoff from the upstream bare soil area (flow #1 in Fig. 3) begins, initially it flows into the first segment (flow #2) and is stored. When the water content reaches the estimated field capacity of the root zone, infiltration into underlying soil (flow #3) is initiated at a rate described by the infiltration function shown in Eq. (1). When inflow rate (flow #2) exceeds the infiltration rate (flow #3), lateral flow across the segment (flow #4) is initiated. Finally, when the root zone segment is saturated, runoff on the segment (flow #5) begins. This sequence was used for each column segment down to the outlet. Baseflow (flow #6) is initiated when estimated field capacity in the soil layer is exceeded. The water content values corresponding to field capacities in the soil layer were estimated to be $0.47 \text{ cm}^3 \text{ cm}^{-3}$ for the silt loam soil layer and $0.53 \text{ cm}^3 \text{ cm}^{-3}$ for the root zone soil based on the 100% VFS treatment of micro-ecosystem simulation. The infiltration function of the root zone and underlying soil layer interface used for flow #3 was obtained by fitting a power function to the result of the 100% VFS treatment of micro-ecosystem simulation. Infiltration rates at the rootzone–soil interface, f_{vs} , were estimated by subtracting runoff and interflow from rainfall in the micro-ecosystem simulations and easily fitted to Eq. (1) where the fitted values for a and b were 248 and -1.58 , respectively ($R^2 = 0.97$). This infiltration function is used until the soil layer below the rootzone is saturated. When saturated, the infiltration rate below the rootzone (flow #3) and the baseflow, f_{vss} (flow #6) are set to a constant. The value for f_{vss} was estimated as $0.00051 \text{ cm s}^{-1}$ from the final constant baseflow rate of the micro-ecosystem simulation for the 100% VFS cover treatment. The value of interflow flux (flow #4) was also calibrated using the result of the micro-ecosystem simulations.

2.4. Pesticide transport in VFS

Calculation of diazinon mass and its transport in VFS was simplified by taking a pesticide mass balance for the entire VFS plane. The spatial gradient of the diazinon concentrations over the VFS plane was neglected since the experimental results did not indicate such concentration gradients existed (Watanabe, 1999). Unanticipated, though significant processes considered for diazinon transport in the VFS included diazinon washoff from the leaf and diazinon adsorption on the leaf litter or thatch layer. Some studies reported that regardless of the pesticide fraction potentially dislodged, the amount washed off was a function of rainfall volume and independent of rainfall intensity (McDowell et al., 1984; Cohen and Steinmetz, 1986). The conceptualized diazinon transport processes considered in the VFS are shown in Fig. 4. For diazinon transport in the VFS area, four compartments, sod leaf, runoff zone (thatch layer), root zone and underlying soil layer were considered. For the sod leaf compartment, diazinon is washed off from the leaf and dissolved diazinon is released into the thatch layer. The diazinon washoff process was simulated using a diazinon-washoff function developed from the results of the micro-ecosystem simulation (Watanabe, 1999). The fraction of diazinon residues, as percent of applied mass on the leaf during the simulation, was plotted versus the rainfall depth and fitted to an exponential function given by:

$$\frac{MC_{LF}}{M_{ap}} = a_{wof} \exp[b_{wof}R] \tag{12}$$

where MC_{LF} is the diazinon residue on the leaf during the simulation (ML^{-2}), M_{ap} is the pesticide application rate (ML^{-2}), and $R(= \int r_i t)$ is the rainfall depth (L). The fitting constants a_{wof} and b_{wof} were 0.91 and -0.04 , respectively ($R^2 = 0.997$). The constant a_{wof} , which represents the initial fraction of applied diazinon on the sod leaf at the beginning of the simulation was less than 1.0. It suggested

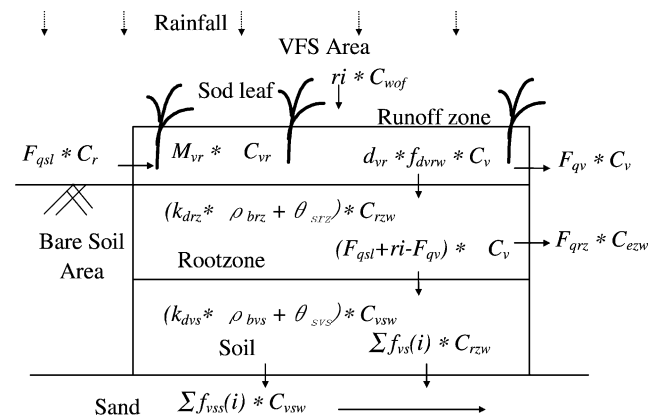


Fig. 4. Conceptualized diazinon transport processes in the VFS area (refer to Eqs. (17)–(19) for terms).

that the initial diazinon mass actually available for washoff was slightly less than the applied mass, perhaps as a result of spray drift and subsequent volatilization losses. The changes in pesticide residues on the leaf and pesticide concentration in washoff were assumed to have the relationship given by:

$$\Delta MC_{LF} = -ri C_{wof} \Delta t \quad (13)$$

where C_{wof} is the pesticide concentration in washoff (ML^{-3}). Rearranging and taking the limit on ΔMC_{LF} and Δt in Eq. (13), substituting MC_{LF} using relationship in Eq. (12), then differentiating with respect to t yields:

$$C_{wof} = -a_w b_{wof} M_{ap} \exp[b_{wof} ri t] \quad (14)$$

Now, C_{wof} is a function of applied diazinon mass and rainfall volume.

Diazinon adsorption phenomenon on the vegetative residues of the thatch layer is simulated using the diazinon concentration function developed from the diazinon concentration changes in vegetative residues in the micro-ecosystem during the rainfall–runoff simulations. Assuming adsorbed pesticide mass in the thatch layer is proportionally related to the mass entering the thatch layer, the diazinon concentration in the vegetative residues has the following relationship:

$$C_{vr} \propto \frac{ri t C_{wof}}{M_{vra}} \quad (15)$$

where C_{vr} is the diazinon concentration in the vegetative residues (MM^{-1}) and M_{vra} is the mass of the vegetative residues comprising the thatch layer (ML^{-2}). Measured diazinon concentration in the vegetative residue was plotted against the quantity on the right-hand-side of Eq. (15) and fitted to a logarithmic function to obtain:

$$C_{vr} = a_{vr} \ln\left(\frac{ri t C_{wof}}{M_{vra}}\right) + b_{vr} \quad (16)$$

where $a_{vr} = 1.499$ and $b_{vr} = 9.911$ ($R^2 = 0.73$) (see Watanabe, 1999).

The runoff zone in the VFS included a leaf litter layer of about 5 mm depth above the soil surface. Diazinon enters the VFS thatch layer as runoff from the upstream bare soil area and as washoff water from the sod leaf above. Diazinon is discharged from the thatch layer as surface runoff and as infiltration into the root zone (see Fig. 3). The diazinon mass balance in the VFS runoff zone can be written as:

$$\begin{aligned} \frac{dC_{vr}}{dt} M_{vra} w L_{vfs} + \frac{dC_v}{dt} d_{vr} f_{dvrw} w L_{vfs} \\ = C_r F_{qsl} w + C_{wof} ri w L_{vfs} - C_v F_{qv}(ndxv) w \\ - C_v [F_{qsl} w + ri w L_{vfs} - F_{qv}(ndxv) w] \end{aligned} \quad (17)$$

where C_v is the diazinon concentration in runoff on VFS area (ML^{-3}), C_{vr} is the diazinon concentration in the vegetative residue (MM^{-1}), C_r is diazinon concentration in runoff from upstream soil area (ML^{-3}), w is the width of

the VFS (L), L_{vfs} is the length of the VFS (L), F_{qsl} is the runoff per unit width of the basin at the downstream edge of the bare soil area (L^2T^{-1}), $F_{qv}(ndxv)$ is the runoff per unit width at the downstream-end node ($ndxv$) of the VFS area (L^2T^{-1}), f_{dvrw} is the fraction of the runoff water depth for the runoff zone depth, d_{vr} (L) in VFS.

Similarly, diazinon transport in the rootzone was estimated using a diazinon mass balance as:

$$\begin{aligned} \frac{dC_{rzw}}{dt} (k_{drz} \rho_{brz} + \theta_{srz}) d_{rz} w L_{vfs} \\ = C_v [F_{qsl} + L_{vfs} ri - F_{qv}(ndxv)] w \\ - C_{rzw} F_{q_{rzh}}(ndxv) w - C_{rzw} \left[\frac{\sum_l f_{vs}(i)}{ndxv} \right] w L_{vfs} \end{aligned} \quad (18)$$

where C_{rzw} is the diazinon concentration in rootzone soil water (ML^{-3}), k_{drz} is the diazinon soil/water partitioning coefficient for the rootzone (L^3M^{-1}), d_{rz} is the depth of the rootzone (L), ρ_{brz} is the bulk density of the root zone (ML^{-3}), and θ_{srz} is the saturated volumetric water content of the rootzone (L^3L^{-3}), $F_{q_{rzh}}(ndxv)$ is the interflow per unit width of the rootzone at the downstream-end node $ndxv$ (L^2T^{-1}), $f_{vs}(i)$ is the infiltration rate at the base of the rootzone for segment (i) (LT^{-1}) and $[\sum_l f_{vs}(i)]/ndxv$ is the averaged infiltration rate over the VFS plane.

As with the root zone, the diazinon mass balance in the soil layer below the rootzone can be approximated by:

$$\begin{aligned} \frac{dC_{vsw}}{dt} (k_{dvs} \rho_{bvs} + \theta_{svs}) d_{vs} w L_{vfs} \\ = C_{rzw} \left[\frac{\sum_l f_{vs}(i)}{ndxv} \right] w L_{vfs} - C_{vsw} \left[\frac{\sum_l f_{vss}(i)}{ndxv} \right] w L_{vfs} \end{aligned} \quad (19)$$

where C_{vsw} is the diazinon concentration in the soil water (ML^{-3}), $f_{vss}(i)$ is the infiltration rate at the base of the soil layer for segment (i) (LT^{-1}), and other parameters with subscript ‘vs’ are the same as those with subscript ‘rz’ in Eq. (18).

The diazinon partitioning coefficients for the soil below the root zone, root zone soil and vegetative residue were measured in the laboratory as 2.34, 4.36 and 23.01 kg^{-1} , respectively (Watanabe, 1999). As expected, the vegetative residue, comprised mostly of organic matter, had the largest partitioning coefficient. Diazinon concentrations in runoff water, C_v , root zone soil water, C_{rzw} , and soil water below the root zone, C_{vsw} , were solved using the backward approximation of Eqs. (17)–(19), respectively.

2.5. Application for the multiple inter-row case for the field scale simulation

In order to perform field-scale numerical simulations in orchards, model equations for simulating the multiple

inter-row VFS sequence were incorporated. For this case, inflow from the previous VFS row was considered using the continuity equation of overland flow and pesticide transport from the bare soil area. For the overland flow equation, the inflow from previous row was assumed to be a lumped volume of runoff and root zone interflow from the previous VFS (see Fig. 1). However, incorporation of inflow from the previous row created an instability problem associated with solution of the K-W equation. The numerical stability criteria is $\Delta x/\Delta t \geq \alpha h^{m-1}$ and the recommended length of the Δx is $\Delta x = L/N$, where $N \in (10, 20)$ (Singh, 1996). Nonetheless, changing the values of Δx , Δt , and Manning's roughness coefficients within their appropriate ranges did not eliminate the numerical instability of the model (Watanabe, 1999).

In order to bypass the numerical instability problem associated with incorporation of the inflow term, a simple continuity equation was used to estimate overland flow:

$$A \frac{dh_k}{dt} = VQ_{k-1} + A ri - Af - h_k w \alpha h_k^{m-1} \quad (20)$$

where A is the area of the bare soil area, h_k is the depth of the water at k th row and w is the width of the field. VQ_{k-1} is the inflow from the previous row $k - 1$. The last term of the Eq. (20) represents the outflow from the bare soil area and was estimated using Manning's equation. The depth of runoff was estimated by applying a second-order Taylor series expansion to Eq. (20) (Watanabe, 1999).

Similarly, for pesticide transport equation on the bare soil area, inflow from the previous row was considered. Eq. (4) was modified for the multiple row case as:

$$\frac{\partial(h_k C_{rk})}{\partial t} + \frac{\partial(q_k C_{rk})}{\partial x} = k_f(C_{mk} - C_{rk}) - fC_{rk} + \frac{VQ_{k-1}C_{VFSP}}{A} \quad (21)$$

where C_{VFSP} is the pesticide concentration in overland flow (ML^{-3}) from the previous VFS row, obtained from the combined inflow pesticide mass of runoff and interflow. Following the derivation approach for the single-row case, derive ordinary differential equation from above equation as:

$$\frac{dC_{rk}}{dt} = \frac{k_f C_{mk}}{h} - \frac{(k_f + ri)C_{rk}}{h} + \frac{(C_{VFSP} - C_{rk})VQ_{k-1}}{Ah} \quad (22)$$

This was again solved through application of the Lax–Wendroff second order scheme (Singh, 1996). The PRVFS model was coded in Fortran 77. The model first calculates the time-space average runoff depth that is used as a parameter for the pesticide transport simulation. Then the model starts the hydrologic and pesticide transport calculations for each time step. If the multiple row simulation flag

is 'on', Eqs. (20) and (22) are executed. Otherwise Eqs. (3) and (6) for the single row case are used.

2.6. Model sensitivity

Chemical transport parameters were calibrated using some of the experimental results obtained from micro-ecosystem experiments described by Watanabe and Grismer (2001). Table 1 lists major input parameters. Calibrated parameter values were found to be comparable to those from other similar studies (Watanabe, 1999). The model sensitivity with respect to estimation of diazinon losses was examined by changing the calibrated input parameter values within appropriate ranges (Table 2). Table 2 lists some parameter values and corresponding model output differences in percent of total pesticide losses from those in micro-ecosystem experiment for 0% VFS cover treatment. The depth of the mixing layer (ε), film transport coefficient (k_f), dispersivity (λ) and the soil/water partitioning coefficient of the pesticide (k_d) are sensitive parameters affecting model performance on pesticide transport simulation in bare soil area. Also, the model sensitivity analysis

Table 1
Major input parameters for the PRVFS model and their values for diazinon transport

Input parameter	Description	Unit	Value
L_{vfs}	The length of VFS slope	cm	80
θ_s	Saturated water content of mixing layer soil	$cm^3 cm^{-3}$	0.52
ri	Rainfall intensity	$cm s^{-1}$	0.0014
θ_i	Initial water content of the soil	$cm^3 cm^{-3}$	0.26
θ_{svs}	Saturated water content of the soil	$cm^3 cm^{-3}$	0.51
n	Mannings n coefficient for bare soil area	$s m^{-1/3}$	0.02
S	Slope	–	0.03
m	Kinematic Wave exponent	–	1.67
ε	Mixing layer depth	cm	0.15
M_{ap}	Pesticide application rate	$\mu g cm^{-2}$	28.02
λ	Dispersivity	cm	1.70
ρ_b	Soil bulk density	$g cm^{-3}$	1.40
k_d	Soil/water partition coefficient	$cm^3 g^{-1}$	2.41
k_f	Film transport coefficient	$cm s^{-1}$	0.0007
θ_{srz}	Saturated water content of the rootzone	$cm^3 cm^{-3}$	0.54
a_{wof}	Pesticide wash off fitting parameter	–	0.91
b_{wof}	Pesticide wash off fitting parameter	–	–0.04
a_{vr}	Pesticide adsorption process fitting parameter	–	1.50
b_{vr}	Pesticide adsorption process fitting parameter	–	9.91
M_{vra}	Leaf litter mass density	$g cm^{-2}$	0.29
ρ_{brz}	Bulk density of the rootzone	$g cm^{-3}$	1.27
k_{drz}	Soil/water partition coefficient of rootzone	$cm^3 g^{-1}$	4.47

Table 2
Results of model parameter evaluation

n	Value	0.02	0.1	0.45
	% Diff. ^a	-3	-3	-4
ε	Value (cm)	0.05	0.15	0.25
	% Diff.	-81	-3	70
k_r	Value (cm s^{-1})	0.0002	0.0007	0.0012
	% Diff.	-44	-3	9
λ	Value (cm)	0.5	1.7	3
	% Diff.	79	-3	-27
k_d	Value (1 kg^{-1})	2.7	10	20
	% Diff.	-3	202	290

% Diff.^a: percentage difference of total pesticide losses from observed values for 0% VFS cover treatment.

indicated that the pesticide washoff from the VFS were important mechanisms affecting diazinon transport in VFS area (Watanabe, 1999).

The effectiveness of inter-row VFS in controlling diazinon runoff losses depends on the rainfall intensity, VFS length and pesticide application rates. These three parameters are important especially in the evaluation of VFS design and the BMPs for controlling diazinon runoff from the orchard. We evaluated three significant parameters, the rainfall intensity, the VFS length that corresponds to VFS coverage over the orchard floor and pesticide application rate on inter-row VFS using the hypothetical field setting of a 60 m \times 60 m orchard having 10 tree rows spaced at a 6.0 m interval. The remaining model parameters were set to be the same values as described previously. We conducted 54 simulations that consisted of six VFS coverages (0, 10, 25, 50, 75, and 100%), three rainfall intensities (20, 35 and 50 mm h^{-1}) of a 1-h rainfall event and three pesticide application rates (100, 75, and 50% of the conventional rate).

Fig. 5 shows the diazinon losses as fractions (%) of applied diazinon mass from the different combinations of VFS coverage and rainfall intensity in the case of conventional application rate. Diazinon losses from 0% VFS coverage condition were always the greatest, accounting for 4.3, 6.6 and 7.9% of applied diazinon mass,

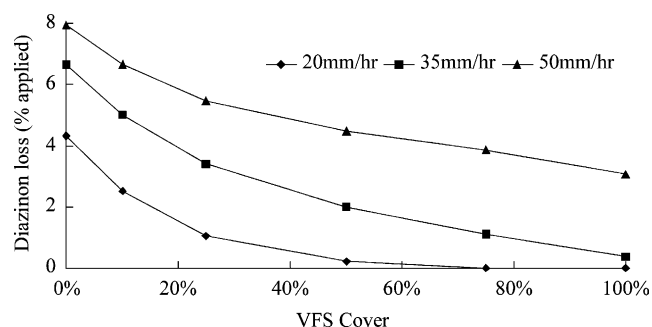


Fig. 5. Simulated diazinon losses from orchard with different VFS cover at different rainfall intensities.

respectively, for rainfall intensities of 20, 35 and 50 mm h^{-1} . Generally, diazinon losses decreased by increasing VFS coverage, while diazinon losses increased at greater rainfall intensities. Some studies indicated that runoff concentration and mass transport of nutrients and some metals (i.e. Cu) from poultry litter treated area exponentially decreased with increasing VFS length (Srivastava et al., 1996; Edwards et al., 1997). Not surprisingly, reduction of diazinon losses with respect to VFS coverage were more significant in smaller rainfall intensities, however, increasing VFS coverage may provide little additional diazinon runoff control. For example, at the 20 mm h^{-1} rainfall intensity, the 25% VFS cover treatment reduced more than 40% of total diazinon loss as compared to the treatment without VFS. On the other hand, VFS cover greater than 50% did not have further significant reduction in diazinon losses at the 20 mm h^{-1} rainfall intensity since most, if not all precipitation infiltrated through VFS. As expected, reducing the application rate reduced the diazinon losses. For 25% VFS cover, total diazinon losses were 1.1, 0.8 and 0.5% of applied mass, respectively for 100, 75 and 50% of the conventional application rate.

2.7. Validation of the PRVFS model

The PRVFS model validation was performed using the result of the micro-ecosystem experiments for 0, 50 and 100% VFS cover treatment discussed by Watanabe and Grismer (2001). Table 3 lists the experimental and simulated results for 0, 50, and 100% VFS cover conditions. For 0% VFS treatment, the model simulated runoff had a prediction error for the total runoff volume of -1.5% of the experimental value. Predicted diazinon concentration in runoff agreed well with experimental values with respect to the trend of decreasing concentrations with time. The PRVFS model predicted both total runoff and diazinon losses with errors less than 3%. Time series trends for runoff, diazinon concentration and its loss over the simulation period were also well predicted. For bare soil area, application of mixing zone model by Havis et al. (1992) was appropriate for approximating the potential solute transport into surface water under rainfall. However as discussed above, model parameters for the mixing zone are sensitive and require careful calibration for different pesticides and soil conditions.

For the 100% VFS cover condition, simple flow routing by sequential segments of runoff, root and underlying soil zones in VFS produced similar discharge hydrographs for runoff, interflow and baseflow with experimental results. However, total flow depths for the runoff, interflow and baseflow during the simulation period were overestimated by 22, 32 and 19%, respectively, from experimental results. As a comparison, Munoz-Carpena et al. (1999) reported that their model performance of total outflow volume resulted with prediction error ranging from -5 to 18% by solving physical equations for hydrological modeling of VFS.

Table 3
Experimental and numerical results for discharge, diazinon concentrations and diazinon losses

Period (min)	0% VFS treatment		50% VFS treatment						100% VFS treatment					
	Exp. runoff	Num. runoff	Experimental			Numerical			Experimental			Numerical		
			Runoff	Interflow	Base flow	Runoff	Interflow	Base flow	Runoff	Interflow	Base flow	Runoff	Interflow	Base flow
<i>Discharge (cm)</i>														
0–10	0.458	0.395	0.017	0.002	0	0	0	0.006	0	0	0	0	0	0
10–20	0.723	0.677	0.142	0.035	0.005	0	0.005	0.046	0	0	0	0	0	0
20–30	0.738	0.727	0.256	0.094	0.123	0.307	0.122	0.130	0	0	0	0	0	0
30–40	0.747	0.748	0.361	0.091	0.168	0.516	0.122	0.153	0.058	0.008	0.100	0.038	0.011	0.238
40–50	0.737	0.763	0.424	0.077	0.177	0.523	0.122	0.153	0.271	0.089	0.305	0.405	0.122	0.305
50–60	0.742	0.772	0.455	0.065	0.175	0.528	0.122	0.153	0.369	0.097	0.306	0.405	0.122	0.305
Total	4.15	4.08	1.654	0.363	0.648	1.874	0.493	0.641	0.698	0.194	0.710	0.848	0.255	0.848
% Diff. ^a	–	–1.5	–	–	–	13.3	35.7	–1.1	–	–	–	21.5	31.6	19.4
<i>Diazinon concentration (mg l⁻¹)</i>														
0–10	2.09	1.92	2.104	1.027	–	–	–	0.000	–	–	–	–	–	–
10–20	0.74	1.05	1.403	1.085	0.251	0.758	0.127	0.003	–	–	–	–	–	–
20–30	0.45	0.57	1.110	0.813	0.146	0.662	0.145	0.007	–	–	–	–	–	–
30–40	0.33	0.32	0.843	0.649	0.084	0.570	0.162	0.008	1.493	0	0	0.783	0.114	0.004
40–50	0.25	0.18	0.659	0.565	0.073	0.501	0.173	0.010	0.918	0	0	0.784	0.123	0.005
50–60	0.20	0.10	0.575	0.506	0.067	0.457	0.182	0.011	0.765	0	0.019	0.778	0.138	0.006
<i>Diazinon loss (mg)</i>														
0–10	4.67	3.69	0.178	0.010	0.000	0.000	0.000	0.000	0	0	0	0	0	0
10–20	2.62	3.47	0.983	0.183	0.007	0.000	0.003	0.001	0	0	0	0	0	0
20–30	1.60	2.01	1.263	0.404	0.073	0.992	0.086	0.004	0	0	0	0	0	0
30–40	1.19	1.16	1.437	0.297	0.063	1.437	0.096	0.006	0.454	0	0	0.145	0.006	0.005
40–50	0.91	0.67	1.345	0.213	0.058	1.280	0.103	0.007	1.165	0	0	1.551	0.073	0.008
50–60	0.74	0.39	1.267	0.159	0.055	1.176	0.108	0.008	1.348	0	0.108	1.539	0.082	0.010
Total	11.74	11.40	6.473	1.265	0.256	4.885	0.396	0.026	2.967	0	0.108	3.235	0.161	0.023
% Diff. ^a	–	–2.9	–	–	–	–24.54	–68.71	–89.84	–	–	–	9.03	–	–78.76

% Diff.^a: percentage difference of total from the observed total value.

The model prediction of diazinon concentrations in runoff underestimated the experimental value for the initial period however, the prediction towards the end of the simulation period was satisfactory. Also, predicted diazinon concentrations in interflow and baseflow ranged closely with experimental values, which were near or below the detection limits of the pesticide analysis. For model performance in VFS area, the accurate prediction of infiltration and runoff is also important for the accurate prediction of pollutant concentration and mass transport (Srivastava et al., 1998). As a result, the model overestimated the experimental value for the total runoff loss of diazinon by 9%. The net total diazinon losses by combining three discharges were overestimated by 11.2% of the experimental value.

For the 50% VFS cover condition, in which both the bare soil and VFS model compartments are executed, the model underestimated initiation of runoff and overestimated peak runoff. The total runoff volume was overestimated by 13.3% due to its overestimation in VFS area. The interflow had also significant overestimation by 36% of experimental value, however, its volume contribution in total discharge was

about 13%. The prediction error for the baseflow was insignificant. As micro-ecosystem experiment suggested, the diversion of runoff into interflow and baseflow is the most significant mechanism for reducing diazinon runoff in VFS (Watanabe and Grismer, 2001). Model parameter evaluation of VFS coverage and rainfall intensity in Section 2.6 also indicated the significant roll of infiltration on controlling diazinon runoff from inter-row VFS systems. However, PRVFS requires improvement in flow routing of runoff diversion in VFS compartment since the underestimation of runoff contributed to the underestimation of diazinon losses in earlier period.

Model prediction of diazinon concentration in runoff was underestimated. The experimental values and the rate of decrease in predicted diazinon concentration was not as great as that of experimental values. The above results were probably due to underestimation of diazinon concentration in runoff and also inability of the model to simulate decreasing trends of the diazinon concentration for VFS covered area. Predicted diazinon concentrations in interflow and baseflow were much less than those of experimental values. According to the micro-ecosystem experiment for

the 50% VFS cover treatment, the effect of diazinon washoff and desorption of adsorbed diazinon in runoff zone became predominant as the diazinon concentration in migrating runoff from bare soil area became small with time (Watanabe and Grismer, 2001). Therefore, it seems that the PRVFS model requires an improvement in the pesticide desorption process for better prediction of diazinon transport in VFS. In general, diazinon losses by runoff were underestimated in earlier periods however, they were well predicted in later periods. Predicted total diazinon losses by runoff were underestimated by 24.5%, and that of net total diazinon losses by combining three discharges were underestimated by 33.2% of the experimental value, respectively.

Overall, PRVFS has a potential to be a useful tool for evaluating VFS for controlling diazinon runoff from dormant-sprayed orchard. Model sensitivity analysis also indicated that the model is able to give some insight to the important design factors using inter-row VFS in the orchard towards BMPs for diazinon runoff control. However, the model evaluation with field data is still necessary for complete validation of PRVFS. The model application can be extended for the use of other pesticides in orchard production nevertheless, careful calibration of pesticide transport parameters such as washoff and adsorption is essential. Also, application of the model for VFS used in other fields rather than orchards is possible with proper parameter calibration. However, the model is limited for use where the sediment loss is not significant, since the model does not account for the pesticide transport affected by sediment transport.

3. Summary and conclusions

In this study, the development of a numerical simulation model of PRVFS for the control of diazinon runoff from dormant-sprayed orchards was presented. The PRVFS model was developed applying existing theories. The model developed by Havis et al. (1992) was applied for pesticide transport in the bare soil area. For VFS area, the model performs flow routing by simple mass accounting in sequential segments and the pesticide mass balance by considering pesticide washoff and adsorption processes on the leaf, vegetative litter, root zone and soil. Model sensitivity analyses indicated that pesticide transfer from surface soil to overland flow and pesticide washoff from the VFS were important mechanisms affecting diazinon transport. The VFS cover ratio and rainfall intensity can be important design parameters for establishing inter-row VFS controlling diazinon runoff in dormant orchards. The PRVFS model was validated using results of micro-ecosystem experiments described by Watanabe and Grismer (2001). The PRVFS model successfully predicted the micro-ecosystem simulated diazinon transport for the 0% VFS cover condition and the 100% VFS cover conditions. For the 50% VFS condition, the PRVFS model prediction was also

satisfactory, but depended on the particular time period considered. The prediction errors for the net total diazinon losses by net discharge of runoff, interflow and baseflow were -2.9 , -33.2 and $+11.2\%$ of experimental value for 0, 50, and 100% VFS cover treatment, respectively.

Although field-testing is necessary for complete validation, the PRVFS model can be a beneficial tool for evaluating and analyzing possible BMPs for controlling the offsite runoff of pesticides applied in orchard production.

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