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Influence of flow concentration on parameter importance and prediction uncertainty of pesticide trapping by vegetative filter strips

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SUMMARY

Flow concentration is a key hydrologic factor limiting the effectiveness of vegetated filter strips (VFS) in removing pesticides from surface runoff. Numerical models, such as VFSMOD-W, offer a mechanistic approach for evaluating VFS effectiveness under various hydrological conditions including concentrated flow. This research hypothesizes that the presence of concentrated flow drastically alters the importance of various hydrological, sedimentological, and pesticide input factors and the prediction uncertainty of pesticide reduction. Using data from a VFS experimental field study investigating chlorpyrifos and atrazine transport, a two-step global sensitivity and uncertainty analysis framework was used with VFSMOD-W based on (1) a screening method (Morris) and (2) a variance-based method (extended Fourier Analysis Sensitivity Test, FAST). The vertical, saturated hydraulic conductivity was consistently the most important input factor for predicting infiltration, explaining 49% of total output variance for uniform sheet flow, but only 8% for concentrated flow. Sedimentation was governed by both hydrologic (vertical, saturated hydraulic conductivity and initial and saturated water content) and sediment characteristics (average particle diameter). The vertical, saturated hydraulic conductivity was the most important input factor for atrazine or chlorpyrifos trapping under uniform sheet flow (explained more than 46% of the total output variance) and concentrated flow (although only explained 8% of the total variance in this case). The 95% confidence intervals for atrazine and chlorpyrifos reduction ranged between 43% and 78% for uniform sheet flow and decreased to between 1% and 16% under concentrated flow. Concentrated flow increased interactions among the system components, enhancing the relative importance of processes that were latent under shallow flow conditions. This complex behavior warrants the need for processbased modeling to be able to predict the performance of VFS under a wide range of specific hydrological conditions.

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Introduction

Vegetation filter strips (VFS) reduce pesticide movement to water bodies by reducing runoff volumes through infiltration in the filter strip's soil profile, through contact between dissolved phase pesticide with soil and vegetation in the filter strip, and/or by reducing flow velocities to the point where eroded sediment particles, with sorbed pesticide, can settle out of the water. However, predicting VFS effectiveness has historically been a difficult, if not impossible, task due to the variability observed in different field conditions. For example, in ten specific VFS studies, Sabbagh et al. (2009) document reported pesticide reduction of 11–100% for VFS of widths ranging from 0.5 to 20 m. Past research has at-

* Corresponding author. E-mail address: garey.fox@okstate.edu (G.A. Fox). tempted to develop general statistical relationships between sediment and/or chemical trapping as functions of buffer physical characteristics such as width and slope, but cannot predict strong relationships between the variables due to a lack of consideration for hydrological processes (Fox and Sabbagh, 2009).

One of the key factors influencing VFS effectiveness is concentrated as opposed to shallow overland or uniform sheet flow (Dosskey et al., 2002; Krutz et al., 2005; Blanco-Canqui et al., 2004, 2006; Fox and Sabbagh, 2009; Poletika et al., 2009; Sabbagh et al., 2009). Departure from sheet flow reduces VFS effectiveness by decreasing infiltration and sedimentation of suspended particles as the grass stems become inundated and flow velocity is undiminished (Dillaha et al., 1989). Blanco-Canqui et al. (2006) demonstrated that narrow filter strips could filter sediment and remove nutrients for interrill flow but their performance for concentrated flow was diminished even on gentle slopes of less than 5%.





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Recent research has proposed that performance of VFS for pesticide trapping depends on hydrologic conditions (precipitation, infiltration and runoff) driven by the filter design (length, slope, and densities of vegetation cover) and characteristics of the incoming pollutants (sediment and pesticides) (Dosskey et al., 2002; Blanco-Canqui et al., 2004; Fox and Sabbagh, 2009; Poletika et al., 2009; Sabbagh et al., 2009). Sabbagh et al. (2009) developed and evaluated an empirical model for pesticide trapping with a foundation of hydrological, sedimentological, and chemical specific parameters:

$$\Delta P = a + b(\Delta Q) + c(\Delta E) + d\ln(F_{ph} + 1) + e(\% C)$$
(1)

where ΔP is the pesticide removal efficiency (%), *a*, *b*, *c*, *d*, and *e* are regression coefficients, ΔQ is the infiltration (%) defined as the difference between flow entering the VFS (i.e., inflow runon plus precipitation) minus the runoff from the VFS, ΔE is the sediment reduction (%), %*C* is the clay content of the sediment entering the VFS, and *F*_{ph} is a phase distribution factor, defined as the ratio of pesticide mass in dissolved form to pesticide mass sorbed to sediment:

$$F_{ph} = \frac{Q_i}{K_d E_i} \tag{2}$$

where Q_i and E_i are the volume of water (L) and mass of sediment (kg) entering the VFS, and K_d is the distribution coefficient defined as the product of KOC, the organic carbon sorption coefficient, and PCTOC, the percent organic carbon in the soil, divided by 100. They also proposed a procedure linking the VFS numerical model VFS-MOD-W (Muñoz-Carpena et al., 1993a,b, 1999; Muñoz-Carpena and Parsons, 2004, 2008) with the proposed empirical trapping efficiency equation that significantly improved predictions of pesticide trapping over conventional equations based solely on physical characteristics of the VFS.

VFSMOD-W, is a field-scale, mechanistic, storm-based numerical model developed to route the incoming hydrograph and sedigraph from an adjacent field through a VFS and to calculate the resulting outflow (based on the kinetic wave approximation of the Saint-Vennant's equations for overland flow), infiltration (based on the Green-Ampt equation for unsteady rainfall), and sediment trapping efficiency based on sediment transport equations (Muñoz-Carpena et al., 1993a,b, 1999; Muñoz-Carpena and Parsons, 2004, 2008). VFSMOD-W originated from GRASSF (Barfield et al., 1979). Muñoz-Carpena et al. (1999) improved upon GRASSF by including improved routines for flow through the filter, time-dependent infiltration, and spatial variability in surface conditions. Researchers have successfully tested the model in a variety of field experiments with good agreement between model predictions and measured values of infiltration, outflow, and trapping efficiency for particles (Muñoz-Carpena et al., 1999; Abu-Zreig, 2001; Abu-Zreig et al., 2001; Dosskey et al., 2002; Fox et al., 2005; Han et al., 2005), and phosphorus (particulate and dissolved) (Kuo, 2007; Kuo and Muñoz-Carpena, 2009). VFSMOD-W is currently used in conjunction with other watershed tools and models to develop criteria and response curves to assess buffer performance and placement at the watershed level (Yang and Weersink, 2004; Dosskey et al., 2005, 2006, 2008; Tomer et al., 2009; White and Arnold, 2009).

Poletika et al. (2009) reported a combined field/modeling study investigating the effect of runoff volume and flow concentration on removal of chlorpyrifos [O,O-diethyl O-(3,5,6-tricholoro-2-pyridyl) phosphorothioate] and atrazine [2-chloro-4-(ethylamino)-6-(isopropylamino)-s-triazine] by filter strips. The field experiments demonstrated that increased flow volume had a minor impact on removal efficiency while flow concentration reduced removal performance regardless of the drainage area ratio. Poletika et al. (2009) concluded that the lack of clear trends between flow volume and flow uniformity verified the necessity of hydrologic modeling within the VFS to capture the hydrologic conditions and response to different events, and showed that the uncalibrated VFSMOD-W was capable of predicting ΔQ ($R^2 = 0.79$), ΔE ($R^2 = 0.85$), and ΔP ($R^2 = 0.84$) for uniform sheet flow and concentrated flow.

Analyses of sensitivity (Muñoz-Carpena et al., 1999, 2007; Abu-Zreig, 2001) and uncertainty (Parsons and Muñoz-Carpena, 2001; Shirmohammadi et al., 2006; Muñoz-Carpena et al., 2007, 2010) of the VFSMOD-W model have been previously reported for numerous applications. However, the influence of flow concentration relative to input factor importance and prediction uncertainty of pesticide trapping has not been analyzed. When conducting model sensitivity analysis, often, local, "one-parameter-at-a-time" sensitivity analysis is performed by varying each input a small amount around a base value and considering all other inputs fixed. However, this approach is only valid for additive and linear output models. Instead, an alternative "global" sensitivity approach, where the entire parametric space of the model is explored simultaneously for all input factors, is needed. Global methods provide not only a ranking of input factor importance and the direct (first order) effect of the individual factors over the output, but also about their interactions (higher order) (Saltelli et al., 2004).

The objective of this study was to evaluate input factor importance and uncertainty in predicted ΔQ , ΔE , and ΔP under uniform sheet flow versus concentrated flow conditions. The research utilized modern global sensitivity and uncertainty analyses for modeling ΔP using VFSMOD-W. The analysis tools were applied to two different treatments in the field study by Poletika et al. (2009) investigating the role of uniform sheet flow versus concentrated flow on atrazine and chlorpyrifos reduction by a VFS. This research is critical to advance the role of VFS as a central component of environmental management plans related to pesticide application.

Materials and methods

VFS field study

The Poletika et al. (2009) field study was conducted in western Sioux County, Iowa, with 4.6-m long smooth brome and bluegrass strips. The soil was a moderately erodible Galva silty clay loam (fine-silty, mixed, mesic, Typic Hapludoll). Slopes were uniform within the study area and ranged from 5.0% to 5.5%. Artificial runoff was metered into the VFS plots for 90 min following a simulated rainfall of 63 mm applied over 2 h. The artificial runoff contained sediment and was dosed with chlorpyrifos and atrazine.

The Poletika et al. (2009) study investigated runoff volumes, corresponding to field:VFS ratios of 15:1 and 30:1 flowing across the strip, by adjusting the induced flow rate onto the VFS. Flow uniformity was investigated by applying runoff to either 100% of the plot area (i.e., uniform) or to only 10% of the plot area (i.e., concentrated). Data considered in this research for the uncertainty and sensitivity analyses included the average data from three blocks of two treatments: (1) 100% of the plot width or 4.60-m wide buffer with a 15:1 (VFS to field) drainage area ratio representing uniform sheet flow conditions and (2) 10% of plot width or 0.46-m wide buffer with a 15:1 drainage area ratio representing concentrated flow conditions. The VFS performed well when flow across the strips was uniform. Flow concentration reduced these measures of performance (Table 1). Infiltration (ΔQ) under uniform sheet flow versus concentrated flow was distinct and averaged 66% and 16%, respectively. Sediment reductions (ΔE) averaged 91% for uniform sheet flow and 33% for concentrated flow. As expected, chlorpyrifos and atrazine reductions (ΔP) were less for concentrated flow than uniform sheet flow: chlorpyrifos reduction averaged

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Table 1

Measured runoff reduction (ΔQ), sedimentation (ΔE), and pesticide reduction (ΔP) for atrazine and chlorpyrifos under both uniform and concentrated flow conditions. Data from Poletika et al. (2009).

Flow condition	Output	Average (%)	Range (%)
Uniform sheet flow	ΔQ	66	46–77
	ΔE	91	84–94
	ΔP (Atrazine)	70	55–78
	ΔP (Chlorpyrifos)	78	64–88
Concentrated flow	ΔQ	16	5-25
	ΔE	33	11-54
	ΔP (Atrazine)	7	1-13
	ΔP (Chlorpyrifos)	24	16-38

24% for concentrated flow compared to 78% for uniform sheet flow and atrazine reduction averaged 7% for concentrated flow compared to 70% for uniform sheet flow (Table 1).

Global sensitivity and uncertainty analysis methods

Two state-of-the-art global sensitivity and uncertainty methods were used: the screening method of Morris (1991) and a variancebased method, extended Fourier Amplitude Sensitivity Test (FAST) (Saltelli, 1999) based on the methods proposed by Cukier et al. (1973, 1978) and Koda et al. (1979). A brief summary of each method is given below with more details summarized by Muñoz-Carpena et al. (2007).

The Morris (1991) method is qualitative in nature and therefore can only be used to assess the relative importance of input factors. A simplified explanation of the method is that a number of local measures, called elementary effects, are computed for each input factor. The elementary effects are calculated by varying one parameter at a time across a discrete number of levels in the space of input factors. The absolute values of the elementary effects for each input factor produces a statistic named μ^* whose magnitude, when compared for all the model input factors, provides the order of importance for each factor with respect to the model output of interest (Campolongo et al., 2007). The standard deviation of the elementary effects, σ , can be used as a statistic indicating interactions of the input factor with other factors and of its non-linear effects (higher-order effects).

The extended FAST variance-based method provides a quantitative measure of sensitivity of the model output with respect to each input factor, using what is termed as a first-order sensitivity index, S_i , and defined as the fraction of the total output variance attributed to a single input factor. In the rare case of a perfectly additive model where the total output variance is explained as a summation of individual variances introduced by varying each parameter alone, $\Sigma S_i = 1$. In general, $\Sigma S_i < 1.0$, and when $\Sigma S_i < 0.6$, models are considered non-additive and the original FAST method (Cukier et al., 1973, 1978; Koda et al., 1979) is generally not applicable. Saltelli (1999) extended FAST to non-additive models with the calculation of the first (direct) and all higher-order effects (interactions) for a given input factor in what is called a total sensitivity index, S_{Ti} :

$$S_{Ti} = S_1 + S_{1i} + S_{1ik} + \dots + S_{1\dots n}$$
(3)

Based on Eq. (3), interaction effects can then be determined by calculating $S_{TI} - S_1$. It is interesting to note that μ^* of the Morris (1991) method is generally a close estimate to the total sensitivity index (S_{TI}) obtained through the variance-based global sensitivity analysis (Campolongo et al., 2007). Since the extended FAST method uses a randomized sampling procedure, it provides an extensive set of outputs that can be used in the global uncertainty analysis of

the model. Thus, probability distribution functions (PDFs), cumulative probability functions (CDFs), and percentile statistics can be derived for each output of interest.

In general, the proposed analysis procedure followed six main steps: (1) probability distribution functions, PDFs, were constructed for uncertain input factors; (2) input sets were generated by sampling the multivariate input distribution, according to the selected global method (i.e., Morris method for the initial screening and extended FAST for the quantitative refining phase); (3) model simulations were executed for each input set; (4) global sensitivity analysis was performed according to the selected method; (5) after some input factors were identified as important by the Morris method, steps 2-4 were repeated using FAST to quantify the results; and (6) uncertainty was assessed based on the outputs from the extended FAST simulations by constructing PDFs, cumulative distribution functions (CDFs), and statistics of calculated errors. The Monte-Carlo sampling software Simlab (Saltelli et al., 2004) was used for multivariate sampling of the input factors and postprocessing of the model outputs. Overall 60,668 simulations (190 Morris and 14,977 FAST simulations for each pesticide-flow scenario) were performed using the High-Performance Computing Center at the University of Florida.

Derivation of input PDFs and selection of model outputs

To avoid the subjectivity of judging a priori what parameters might be most important, all model input parameters, 18 in total, were selected in the analysis (Table 2). Input-PDF selection for the model's 18 input variables (Table 3) followed Muñoz-Carpena et al. (2007) and were based upon a combination of reported values for the study, literature reviews, and parameter databases. The model output parameters selected in the analysis were the infiltration or runoff reduction, ΔQ (%), sediment reduction, ΔE (%), and pesticide trapping efficiency, ΔP (%).

It should be noted that the specific ranges adopted for each parameter will affect the final results, but do not preclude the globality of the analysis. McKay (1995) recommended that, in absence of experimental values to inform a probability distribution, a uniform distribution could be used when the parameter range was considered to be finite. In fact, the use of uniform distributions for a given range constitutes a conservative assumption (Saltelli et al., 2008), since parameters that are not found to be important in the global sensitivity analysis with this type of distributions, will not be important if other centered or biased distributions on the same range are used. A variation range of $\pm 20\%$ around the mean is commonly used as default for parameters of moderate natural variability (Warrick, 1998; McBratney and Mulla, 2002).

Uniform distributions were used for several input factors due to the absence of specific information on their variability. Uniform distributions were utilized for the surface slope (SOA), with a range between 5.0% and 5.5%, and Green–Ampt's average suction at the wetting front (SAV), with a distribution range of $\pm 20\%$ of the base values reported by Poletika et al. (2009).

The effective flow width of the strip (FWIDTH) is the actual field width of the filter perpendicular to the primary flow direction under uniform sheet flow conditions, but becomes smaller than the actual field width when the flow concentrates. Abu-Zreig et al. (2001) found deviations from uniform sheet flow under field conditions that introduce uncertainty into this input factor. A uniform distribution was used for FWIDTH, with the distribution ranging between the width of the filter reported in each study (maximum value) and 10% below this maximum value to represent departure from uniform runoff across the filter. A similar strategy was employed in assigning a distribution to the length of the filter parallel to the primary flow direction (VL). For simplicity, VL is usually taken as the distance from the top to the bottom of the filter along

Table 2

Simulation input factors for VFSMOD-W explored in the sensitivity and uncertainty analysis.

#	Input factor	Units	Description
Hyd	rological in	outs	
1	FWIDTH	m	Effective flow width of the strip
2	VL	m	Length in the direction of flow
3	RNA(I)	s/m ^{1/3}	Filter Manning's roughness <i>n</i> for each segment
4	SOA(I)	m/m	Filter slope for each segment
5	VKS	m/s	Soil vertical saturated hydraulic conductivity in the VFS
6	SAV	m	Green-Ampt's average suction at wetting front
7	OS	m ³ /m ³	Saturated soil water content, θ_s
8	OI	m³/m³	Initial soil water content, θ_i
9	SCHK	-	Relative distance from the upper filter edge where check for ponding conditions is made (i.e., 1 = and
			0.5 = mid point, 0 = beginning)
Sedi	mentologica	ıl inputs	
10	SS	cm	Average spacing of grass stems
11	VN	s/cm ^{1/3}	Filter media (grass) modified Manning's n_m (0.012 for cylindrical media)
12	Н	cm	Filter grass height
13	VN2	s/m ^{1/3}	Bare surface Manning's <i>n</i> for sediment inundated area in grass filter
14	DP	cm	Sediment particle size diameter (d_{50})
15	COARSE	_	Fraction of incoming sediment with particle
			diameter >0.0037 cm (coarse fraction routed
			through wedge as bed load) [unit fraction, i.e.,
			100% = 1.0]
Pest	icide inputs		
16	KOC	-	Organic carbon sorption coefficient
17	PCTOC	%	Percentage of organic carbon in the soil
18	PCTC	%	Percentage clay in the soil
			- •

the maximum slope line, which is correct under theoretical, uniform, sheet flow conditions. However, it is likely that flow is not uniformly organized and could be sinuous, thereby creating uncertainty in this input factor. For VL, the uniform distribution ranged between the specific value reported in the study (minimum value) and 10% above this minimum value to represent possible sinuosity in the flow path.

The fraction of incoming sediment with particle diameters greater than 0.0037 cm (COARSE) was approximated as the sand fraction. The average sediment particle size diameter (DP) was

estimated based on the reported fraction of silt, sand, and clay (PCTC). The study did report single values of percent organic carbon (PCTOC), but no measurements of within field variability were available for deriving a statistical distribution. Therefore, uniform distributions were assumed for COARSE, DP, PCTC, and PCTOC with a range of $\pm 20\%$ around the reported base values.

The saturated hydraulic conductivity (VKS), saturated water content (OS), and initial water content (OI), which was assumed to be the field capacity, were adopted directly from recommended distributions by Meyer et al. (1997) and Carsel and Parrish (1988) based on the silty clay loam soil type (i.e., lognormal for VKS and normal for the OS and OI). Parameters of the distributions for OS and OI were taken directly from Meyer et al. (1997) and Carsel and Parrish (1988). The VKS distributions based on soil texture varied by three to four orders of magnitude. In order to develop more plausible site-specific values for this particular field site, the standard deviation was assumed equal to the mean (i.e., coefficient of variation, CV, of 100%), with the mean of log-values at the simulation value used originally by Poletika et al. (2009). Literature supports the assumed range in field-scale VKS (Giménez et al., 1999; Mertens et al., 2002). For example, Gupta et al. (2006) reported a variance that exceeded mean measured VKS by approximately one order of magnitude.

Triangular distributions with a $\pm 20\%$ range around the peak recommended values (based on the 90% smooth brome (*Bromus inermis*) and 10% bluegrass vegetation type, Haan et al., 1994) were assumed for the following vegetation and roughness parameters: the filter Manning's roughness *n* (RNA), microscale modified Manning's *n* for cylindrical media (VN), bare surface Manning's *n* for the sediment inundated area in the grass filter (VN2), and average spacing of grass stems (SS). A normal distribution was used to describe the filter grass height, H, with the mean as the maintained grass height (i.e., 10 cm) and standard deviations of the assumed normal distributions derived using a 15.5% CV (Muñoz-Carpena et al., 2007).

A triangular distribution was also used for the organic carbon sorption coefficient (KOC) for atrazine and chlorpyrifos. The triangular distribution was centered at the recommended KOC from the United States Department of Agriculture's (USDA) pesticide database (United States Department of Agriculture, 2006). However, instead of a $\pm 20\%$ range around the peak, this research used potential

Table 3

Base values and assumed statistical distributions for the input factors of the Poletika et al. (2009) study.

Input factor	Base value	Distribution ^b	Statistics
FWIDTH (m)			
Trt1 ^ª	4.60	Uniform	Min = 4.14; max = 4.60
Trt3 ^a	0.46		Min = 0.41; max = 0.46
VL (m)	4.60	Uniform	Min = 4.60; max = 5.06
RNA (s/m ^{1/3})	0.40	Triangular	Min = 0.3; peak = 0.4; max = 0.5
SOA (-)	0.0525	Uniform	Min = 0.05; max = 0.055
VKS (m/s)	3.022e-05	Lognormal	μ_y = -12.3; σ_y = 1.59; min = 3.35e-8; max = 6.19e-4
SAV (m)	0.4	Uniform	Min = 0.32; max = 0.48
OS (-)	0.43	Normal	μ_x = 0.43; σ_x = 0.0699; min = 0.21; max = 0.65
OI (-)	0.347	Normal	μ_x = 0.347; σ_x = 0.071; min = 0.13; max = 0.57
SS (cm)	1.5	Triangular	Min = 1.35; peak = 1.5; max = 2.2
VN (s/cm ^{1/3})	0.012	Triangular	Min = 0.0084; peak = 0.012; max = 0.016
VN2 (s/m ^{1/3})	0.05	Triangular	Min = 0.04; peak = 0.05; max = 0.06
SCHK (-)	0.5	Uniform	Min = 0; max = 1
COARSE (-)	0.171	Uniform	Min = 0.121; max = 0.221
DP (cm)	0.0010	Uniform	Min = 0.0008; max = 0.0012
H (cm)	10.0	Normal	$\mu_x = 10; \ \sigma_x = 1.5$
KOC (-)			
Atrazine	147	Triangular	Min = 38; peak = 147; max = 288
Chlorpyrifos	6070		Min = 5300; peak = 6070; max = 14;800
PCTOC (%)	2.58	Uniform	Min = 2.37; max = 2.78
PCTC (%)	28.9	Uniform	Min = 27; max = 30.7

^a Trt = treatment; Trt1 = 4.60-m wide buffer representing uniform flow conditions; Trt3 = 0.46-m wide buffer representing concentrated flow conditions.

^b Lognormal and normal distributions are truncated between (0.001, 0.999) except for H with (0.025, 0.975).

ranges in KOC reported by the USDA database for atrazine and chlorpyrifos.

Results and discussion

As proposed by Morris (1991), only input factors separated from the origin of the $\mu^*-\sigma$ plane were considered important (Figs. 1 and 2). In general, the number of important input factors for predicting ΔQ (i.e., approximately four for both uniform sheet flow and concentrated flow in Fig. 1a and b) decreased considerably from the full set of 18 model inputs. The Morris results appropriately indicated that ΔQ was not dependent on any sediment or pesticide inputs. The VKS was the dominant input factor for ΔQ for either the uniform sheet flow or concentrated flow scenarios and the four most important input factors were VKS, OI, OS, and FWIDTH (Fig. 1a and b). Muñoz-Carpena et al. (2010) also report VKS as the dominant input factor from sensitivity analyses for three uniform sheet flow field studies.

A slightly greater number of input factors were deemed important for ΔE than ΔQ , but was still much fewer than the full set of 18 model inputs. For the two flow treatments, ΔE was governed by hydrologic (VKS, VL, and FWIDTH) and sediment characteristics (DP), as shown in Fig. 1c and d. The VKS and DP were most important in impacting sedimentation for uniform sheet flow (Fig. 1). For concentrated flow, the most important input factors were DP, FWIDTH, and two inputs representing the vegetation characteristics (SS and VN). These results suggested that the importance of VKS decreased considerably in the rank of input factor importance when infiltration capacity was overloaded by excess flow under concentrated flow conditions. Although most regression-based models of VFS sedimentation performance are dependent specifically on VL and/or SOA, this study demonstrated that VL was of secondary importance and that SOA was one of the least important input factors. Muñoz-Carpena et al. (1993b) demonstrated that the effect of varying SOA, and correspondingly RNA, was only appreciable for less steep VFS conditions. Since SOA in this field study was relatively steep, ranging from 5.0% to 5.5%, this may have contributed to the lack of importance of this input factor. The analysis also showed that other input factors are important, especially for the concentrated flow scenario, and should be incorporated in any predictive or modeling efforts.

The ΔP was largely influenced by hydrologic variables for uniform sheet flow and sediment variables for concentrated flow, further verifying the model behavior based on the techniques proposed by Fox and Sabbagh (2009) and Sabbagh et al. (2009) (Fig. 2). Morris results were almost identical between atrazine and chlorpyrifos under the same hydrologic conditions. For uniform sheet flow. VKS dominated input factor importance in predicting atrazine and chlorpyrifos reduction. This result again was confirmed by recent sensitivity analyses reported by Muñoz-Carpena et al. (2010) for three different uniform sheet flow studies. In fact, the Morris results for ΔP under uniform sheet flow mimicked the results for ΔQ . Uniform sheet flow conditions allowed sufficient time for infiltration processes to occur within the VFS and contributed considerably to ΔP . A greater number of input factors were important for predicting ΔP under concentrated flow than uniform sheet flow (Fig. 2). Morris results for ΔP with concentrated flow more closely resembled results for ΔE than ΔQ . As expected, VKS decreased considerably in the rank of input factor importance when infiltration capacity was overloaded by excess flow.

Interestingly, pesticide-specific input factors were only ranked in the middle range of importance, less important than VKS, OI, OS, and PCTC for shallow flow and DP, PCTC, and VKS for concentrated flow. The PCTC was the most important input factor that arose in analyzing for ΔP compared to hydrology and sediment in all



Fig. 1. Global sensitivity analysis results obtained from the Morris (1991) screening method for the VFS hydrologic response (i.e., ΔQ = infiltration) and sedimentation (i.e., ΔE = sediment reduction) with uniform sheet flow and concentrated flow. Input factors separated from the origin of the μ^* - σ plane were considered important. Labels of unimportant input factors (close to the μ^* - σ plane origin) have been removed for clarity.



Fig. 2. Global sensitivity analysis results obtained from the Morris (1991) screening method for the VFS pesticide reduction (i.e., ΔP = pesticide trapping) for (a) atrazine and uniform sheet flow, (b) chlorpyrifos and uniform sheet flow, (c) atrazine and concentrated flow, and (d) chlorpyrifos and concentrated flow. Labels of unimportant input factors (close to the μ^* - σ plane origin) have been removed for clarity.

cases (Fig. 2). An input factor initially hypothesized to be important in the analysis was KOC; however, the Morris results suggested that the KOC value within a specific pesticide's KOC range was only of secondary importance to those representing ΔQ and ΔE . It was less important which value within the KOC range was utilized to simulate trapping of a specific pesticide; however, the pesticide being simulated and its KOC range were still important. The importance of KOC was greater when comparing the more soluble pesticide atrazine versus chlorpyrifos (Fig. 2). The KOC was important for the more soluble pesticide since uncertainty within this value shifted the transport characteristics towards flow-dominated (soluble pesticide) responses where infiltration controlled the filter efficiency. For chlorpyrifos, sediment input factors most likely already accounted for the sediment-bound transport of chlorpyrifos.

The Morris (1991) method indicated the presence of interactions between input factors in terms of predicted ΔQ , ΔE , and ΔP , as demonstrated by the σ values (Figs. 1 and 2). These results again suggested that simple linear or non-linear regressions based on VFS physical characteristics (e.g., SOA, VL, FWIDTH, and VN) are insufficient without interaction effects between variables considered. These results again support the need for non-linear, complex process-based modeling, as suggested by Fox and Sabbagh (2009) and Sabbagh et al. (2009) for pesticide runoff prediction.

Table 4 depicts the global sensitivity analysis results in terms of the total output variance explained by each input factor including the first-order effects (S_i) and higher-order effects or interactions, $S_{Ti} - S_1$. The percent of the total output variance for ΔQ , ΔE , and ΔP that was accounted for by first-order effects (ΣS_i) ranged between 48% and 64% for uniform sheet flow and 19% and 21% for concentrated flow (Table 4). The FAST results indicated that ΔQ controlled model response under uniform sheet flow with VKS accounting for approximately 49%, 46%, and 51% of the total output variance for ΔQ , atrazine reduction, and chlorpyrifos reduction, respectively. For concentrated flow, not one of the most important input factors (i.e., DP, PCTC, and VKS) explained more than 8% of the total output variance (Table 4). This confirmed that concentrated flow introduced unique processes compared to uniform sheet flow for the VFS.

In terms of input parameter importance, the FAST results confirmed Morris results for ΔQ for both the uniform sheet flow and concentrated flow scenarios with VKS dominating input parameter importance. The two methods uniformly predicted the importance of VKS and DP for ΔE and VKS for ΔP in the uniform sheet flow scenario. However, differences were observed between the two methods for ΔE and ΔP in the concentrated flow case. More specifically, DP was identified as the most important parameter in Morris for both ΔE and ΔP but this was not confirmed by the FAST results, which predicted VKS as the most important input parameter. In the concentrated flow case, interactions dominated the model response ($\Sigma S_i \approx 0.20$) and the limited sampling behind the Morris method did not seem to capture the interactions well. The larger sampling intensity of FAST made these results more reliable. However, the main benefit of the Morris method still persisted under these conditions. Note that μ_i^* is rather resilient against type II errors, i.e., if an input factor is deemed unimportant, it is unlikely to be identified as influential by another method (Saltelli et al., 2008). Notice that the factors quantified by FAST as important, although of lower importance to Morris, were among the group of parameters separated from the origin of the $\mu^*-\sigma$ plane, indicating their relative importance (Fig. 2). This illustrated the need to conduct the combined assessment of sensitivity with both screening and variance-based methods, especially for instances where interactions dominated the model response (i.e., concentrated flow through a VFS).

The global uncertainty analysis results shown in Fig. 3 and Table 5 illustrate the differences in PDFs and CDFs of ΔQ , ΔE , and

Table 4

Fourier Amplitude Sensitivit	v Test (FAST) results for the uniform s	heet flow and c	concentrated flow scenarios.
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Outputs	Input factors ^a										Total								
	VL	FWIDTH	RNA	SOA	VKS	SAV	OS	OI	SS	VN	VN2	SCHK	COARSE	DP	Н	КОС	PCTOC	PCTC	
First order index, S _i (% Uniform)																		
ΔQ	0	0	0	0	49	0	4	5	0	0	0	0	0	0	0	0	0	0	62
ΔE	1	3	0	0	24	0	4	5	1	0	0	0	0	8	0	0	0	0	48
ΔP – atrazine	0	0	0	0	46	0	4	5	0	0	0	0	0	0	0	1	0	1	59
ΔP – chlorpyrifos	0	0	0	0	51	0	4	5	0	0	0	0	0	0	0	0	0	1	64
Conc.																			
ΔQ	0	0	0	0	8	1	3	4	0	1	0	0	0	0	0	0	0	0	19
ΔE	0	1	0	0	8	1	2	3	1	1	0	0	0	2	0	0	0	0	21
ΔP – atrazine	0	0	0	0	8	1	2	3	1	1	0	0	0	0	0	1	0	1	20
ΔP – chlorpyrifos	0	0	0	0	8	1	2	3	1	1	0	0	0	0	0	1	0	1	20
Interactions, $S_{Ti} - S_i$ (% Uniform	8)																		
ΔQ	16	15	13	16	38	18	33	35	22	20	16	17	17	15	19	16	16	17	
ΔE	23	21	20	20	50	27	45	45	28	27	21	24	24	22	27	20	25	22	
ΔP – atrazine	18	16	15	18	40	19	35	37	23	22	17	19	18	16	21	17	17	18	
ΔP – chlorpyrifos	15	14	13	16	36	17	31	33	20	19	15	17	16	14	18	15	15	16	
Conc.																			
ΔQ	36	32	31	27	79	50	73	73	44	49	35	35	42	28	45	26	33	31	
ΔE	34	30	30	25	77	47	72	71	42	47	32	34	39	28	43	25	33	29	
ΔP – atrazine	36	31	31	26	79	49	73	73	43	49	34	36	41	28	45	26	33	30	
ΔP – chlorpyrifos	36	31	29	26	79	49	73	73	43	49	34	35	41	28	43	26	33	30	

^a Refer to Table 2 for a definition of the input factors. ΔQ = infiltration; ΔE = sedimentation; and ΔP = pesticide trapping.



Percent Reduction in Runoff (ΔQ), Erosion (ΔE) and Pesticide (ΔP)



Percent Reduction in Runoff (ΔQ), Erosion (ΔE) and Pesticide (ΔP)

Fig. 3. Global uncertainty analysis results obtained from the extended FAST variance-based method for infiltration (ΔQ), sedimentation (ΔE), and pesticide reduction (ΔP). Figures (a) and (b) are the PDF and CDF for the uniform sheet flow scenario. Figures (c) and (d) are the PDF and CDF for the concentrated flow scenario. The measured data are averages of three blocks of two treatments reported by Poletika et al. (2009).

 ΔP for uniform sheet flow versus concentrated flow. In general, the PDFs and CDFs from the global uncertainty analysis overlapped the ranges of measured data reported by Poletika et al. (2009), as shown in Table 1. The ΔQ , ΔE , and ΔP of the VFS depended consid-

erably on the hydrological conditions experienced by the buffer. For the concentrated flow scenario, the uncertainty (range in the PDF) narrowed (Table 5) due to the limited time for processes to occur in the filter with larger flow volumes and less opportunity

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Study	Output	Mean (%)	Median (%)	95CI ^b (%)	SD^{b} (%)	SE ^b (%)	Min ^b (%)	Max ^b (%)	Skew ^b (%)	Kurt ^b (%)
Uniform sheet flow	ΔQ^{a}	29.2	22.0	6.9–61.0 ^c	24.2	0.20	0.0	100.0	1.8	2.6
	ΔE^{a}	92.0	91.7	89.0–93.7 ^c	2.5	0.02	87.3	100.0	1.8	4.0
	ΔP^{a} (atrazine)	56.1	51.9	42.7–73.5 ^c	14.5	0.12	36.2	100.0	1.9	3.0
Concentrated flow	ΔP^{4} (chlorpyrifos)	61.9	58.0	49.0–78.3 ^c	13.3	0.11	44.1	100.0	1.7	2.3
	ΔQ	8.8	3.7	1.9–9.5 ^c	20.4	0.17	1.3	100.0	4.2	15.7
	ΔE	24.6	21.6	14.5–26. 3 ^c	17.0	0.14	9.8	100.0	4.0	14.9
	ΔP (atrazine)	10.0	5.7	1.2–10.1 ^c	20.1	0.16	0.0	100.0	4.2	15.8
	ΔP (chlorpyrifos)	15.9	11.9	7.5–15.9 ^c	18.8	0.15	4.3	100.0	4.2	15.8

Uncertainty analysis statistics for selected output probability distributions obtained from the extended FAST variance-based method.

^a ΔQ = infiltration; ΔE = sedimentation; ΔP = pesticide reduction (i.e., trapping efficiency).

^b 95CI = 95% confidence interval; SD = standard deviation; SE = standard error of the mean; Min = minimum; Max = maximum; Skew = skewness; Kurt = kurtosis.

 $^{
m c}$ 95Cl calculated by neglecting accumulation of values at the upper limit of 100% (second peak in the bimodal distribution).

for ΔQ , ΔE , and correspondingly ΔP (Fig. 3). Since the largest input uncertainties were associated with infiltration parameters (e.g., VKS in Table 3), the reduced importance of this process under concentrated flow propagated into a narrower range of output uncertainty. Another interesting trend was that ΔP for atrazine and chlorpyrifos consistently fell between the ΔQ and ΔE PDFs and CDFs, with a slight shift to the left (towards the ΔQ PDF or CDF) for the more soluble atrazine (lower KOC) and a slight shift to the right (towards the ΔE PDF or CDF) for the sediment-bound chlorpyrifos (higher KOC).

Summary and conclusions

Table 5

Concentrated flow provided less time for infiltration and sedimentation processes within a VFS and correspondingly less pesticide removal. Input factor importance for predicting VFS performance depended considerably on the hydrological conditions in terms of flow concentration. Attempts to rely explicitly on single input factors to predict VFS performance (i.e., hydraulic conductivity, buffer width, or slope) will fail unless one considers the flow conditions experienced by the VFS. In other words, the same buffer with equivalent characteristics may respond uniquely in terms of potential ranges in sediment and pesticide trapping efficiency depending on the hydraulic loading of a specific storm event.

The global sensitivity and uncertainty analyses suggested that the VFS hydraulic conductivity was the most important input factor for the hydrologic response of the buffer whether uniform sheet flow or concentrated flow conditions were prevalent. Average particle diameter and hydraulic conductivity were most important in predicting sedimentation. Input factors most important for hydrology and sedimentation were also the most important for ΔP . The hydraulic conductivity was the most important input factor for atrazine or chlorpyrifos trapping under uniform sheet flow, explaining approximately 46-51% of the total output variance (the sum of first-order effects was approximately 59-64%). The hydraulic conductivity was also the most important input factor under concentrated flow but explained no more than 8% of the total variance. The sum of first-order effects was approximately 20% for the concentrated flow conditions, suggesting a non-additive model behavior; i.e., process interactions dominated the model response. The KOC value within a specific pesticide's KOC range was less important than input factors representing infiltration and sedimentation. It was generally less important which value within the KOC range for a specific pesticide was used; however, it should be emphasized that the pesticide being simulated and its KOC range were still important. The importance of KOC was greater when comparing the more soluble pesticide atrazine versus chlorpyrifos. For chlorpyrifos, sediment input factors most likely already accounted for the sediment-bound transport of chlorpyrifos.

Global uncertainty analysis using the extended FAST technique demonstrated the commonly observed reduction in pesticide trapping efficiency under concentrated flow and narrowing of the output probability distribution function. For the flow concentration case studied, large decreases in median output values were obtained for runoff, sediment and pesticide reductions, and the uncertainty ranges were similarly reduced. Extended FAST results also suggested significant interaction effects among variables. Attempts to predict VFS effectiveness without including these implicit interactions will not have much statistical prediction power. Process-based methods are required to account for these interactions and therefore a program such as VFSMOD-W should be considered a powerful tool for such analyses, especially in terms of developing confidence in the scientific community's ability to predict pesticide surface runoff control by VFS.

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Appendix. Global sensitivity methods

Method of Morris

The screening method proposed by Morris (1991) (herein "Morris method" or "Morris") and later modified by Campolongo et al. (2007), was used in this study because it is relatively easy to apply, requires very few simulations, and its results are easily interpreted (Saltelli et al., 2004). Morris (1991) proposed conducting individually randomized experiments that evaluate the elementary effects (relative output differences) of changing one parameter at a time. Each input may assume a discrete number of values called levels that are selected within an allocated range of variation for the parameter.

For each parameter, two sensitivity measures are proposed: (1) the mean of the elementary effects, μ , which estimates the overall effect of the parameter on a given output and (2) the standard deviation of the effects, σ , which estimates the higher-order characteristics of the parameter (such as curvatures and interactions). Since sometimes the model output is non-monotonic, Campolongo et al. (2007) suggested considering the distribution of absolute values of the elementary effects, μ^* , to avoid the canceling of effects of opposing signs. The number of simulations (*N*) to perform in the Morris analysis is given by:

$$N = r(k+1) \tag{4}$$

where *r* is the sampling size for the search trajectory (*r* = 10 produces satisfactory results) and *k* is the number of factors. Although elementary effects are local measures, the method is considered global because the final measure μ^* is obtained by averaging the elementary effects and this eliminates the need to consider the specific points at which they are computed (Saltelli et al., 2004). Morris (1991) recommended applying μ (or μ^* thereof) to rank parameters in order of importance and Saltelli et al. (2004) suggested applying the original Morris measure σ when examining the effects due to interactions. To interpret the results in a manner that simultaneously informs about the parameter ranking and potential presence of interactions, Morris (1991) suggested plotting the points on a μ (or μ^*)- σ Cartesian plane. Because the Morris method is qualitative in nature, it should only be used to assess the relative parameter ranking.

Extended FAST

Variance-based methods can be used to obtain a quantitative measure of sensitivity. Such techniques decompose the total variance $(V = \sigma_Y^2)$ of the model output $Y = f(X_1, X_2, ..., X_k)$ in terms of the individual factors X_i , such that

$$V = \sigma_V^2 = V1 + V2 + V3 + \dots + V_k + R$$
(5)

where V_i is the part of the variance that can be attributed to the input factor X_i alone, k is the number of uncertain factors, and R is a residual corresponding to higher-order terms. The first-order sensitivity index, S_i , defined as a fraction of the total output variance attributed to a single factor, can then be taken as a measure of global sensitivity of Y with respect to X_i ; that is:

$$S_i = V_i / V \tag{6}$$

For a perfectly additive model with no interaction terms, $\Sigma S_i = 1$, but more complex models are generally not perfectly additive, and $\Sigma S_i < 1$.

One efficient variance-based method is the Fourier Analysis Sensitivity Test (Cukier et al., 1973, 1978; Koda et al., 1979), FAST. To calculate S_i , FAST uses a quasi-random sampling procedure to sample the *k*-dimensional space of the input parameters using closed sinusoidal trajectories of shifting phase. The number of model evaluations required by this method can be expressed as:

$$N = M(k+2) \tag{7}$$

where *M* is a number between 500 and 1000. For non-additive models where $\Sigma S_i < 0.6$, classical FAST cannot be used and Saltelli et al. (2004) extended the method to obtain the total order effects through the total sensitivity index, S_{Ti} , calculated as the sum of the first and all higher order indices for a given parameter X_i (Saltelli et al., 2004). For example, for X_1 :

$$S_{T1} = S_1 + S_{1i} + S_{1jk_1} + \dots + S_{1,\dots,n} \quad \text{and} \\ S_{T1} - S_1 = S_{1i} + S_{1jk_1} + \dots + S_{1,\dots,n} \quad (8)$$

For a given parameter X_i , interactions can be isolated by calculating $S_{Ti} - S_i$, which makes the "extended FAST" technique a powerful method for quantifying the individual effect of each parameter alone (S_i) or through interaction with others ($S_{Ti} - S_i$).

An additional benefit of the extended FAST analysis is that since the results are derived from a randomized sampling procedure, they can be used as the basis for the uncertainty evaluation by constructing cumulative probability functions (CDFs) for each of the selected outputs. This leads to a very efficient Monte-Carlo type of uncertainty analysis since only the sensitive parameters are considered as the source of uncertainty.

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