Parameter Importance and Uncertainty in Predicting Runoff Pesticide Reduction with Filter Strips

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Vegetative filter strips (VFS) are an environmental management tool used to reduce sediment and pesticide transport from surface runoff. Numerical models of VFS such as the Vegetative Filter Strip Modeling System (VFSMOD-W) are capable of predicting runoff, sediment, and pesticide reduction and can be useful tools to understand the effectiveness of VFS and environmental conditions under which they may be ineffective. However, as part of the modeling process, it is critical to identify input factor importance and quantify uncertainty in predicted runoff, sediment, and pesticide reductions. This research used state-of-the-art global sensitivity and uncertainty analysis tools, a screening method (Morris) and a variance-based method (extended Fourier Analysis Sensitivity Test), to evaluate VFSMOD-W under a range of field scenarios. The three VFS studies analyzed were conducted on silty clay loam and silt loam soils under uniform, sheet flow conditions and included atrazine, chlorpyrifos, cyanazine, metolachlor, pendimethalin, and terbuthylazine data. Saturated hydraulic conductivity was the most important input factor for predicting infiltration and runoff, explaining >75% of the total output variance for studies with smaller hydraulic loading rates (~100–150 mm equivalent depths) and ~50% for the higher loading rate (~280-mm equivalent depth). Important input factors for predicting sedimentation included hydraulic conductivity, average particle size, and the filter's Manning's roughness coefficient. Input factor importance for pesticide trapping was controlled by infiltration and, therefore, hydraulic conductivity. Global uncertainty analyses suggested a wide range of reductions for runoff (95% confidence intervals of 7–93%), sediment (84–100%), and pesticide (43–100%) . Pesticide trapping probability distributions fell between runoff and sediment reduction distributions as a function of the pesticides' sorption. Seemingly equivalent VFS exhibited unique and complex trapping responses dependent on the hydraulic and sediment loading rates, and therefore, process-based modeling of VFS is required.

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A vegetated filter strip is a dense vegetation area designed to intercept surface runoff located at the down slope field border and is commonly recommended for reducing sediment and diffuse contaminant loads to receiving water bodies. Sediment and pesticide trapping efficiency of a VFS is predicted with limited success when using empirical equations based solely on field characteristics of vegetated filter strips such as the length of the filter in the direction of flow, slope, area ratios, and vegetation type (Neitsch et al., 2005; Lui et al., 2008). When properly field calibrated and tested, numerical water quality models can minimize the need for field-testing of management alternatives and provide significant time and cost savings. The Vegetative Filter Strip Modeling System, VFSMOD-W, is a field-scale, mechanistic, storm-based numerical model developed to route the incoming hydrograph and sediment from an adjacent field through a VFS and to calculate the resulting outflow, infiltration, and sediment trapping efficiency (Muñoz-Carpena et al., 1993a,b, 1999; Muñoz-Carpena and Parsons, 2004, 2008). 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).

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Abbreviations: ΔE, sedimentation; ΔP, pesticide reduction or trapping efficiency; ΔQ, infiltration or runoff reduction; CDF, cumulative distribution function; COARSE, particle diameters >0.0037 cm; DP, particle size diameter; FAST, Fourier Amplitude Sensitivity Test; FWIDTH, effective flow width; H, filter grass height; KOC, organic carbon sorption coefficient; OI, initial water content; OS, saturated water content; PCTC, percentage clay in the soil; PCTOC, percentage organic carbon in the soil; PDF, probability distribution function; RNA, Manning's roughness *n*; SOA, soil slope; SS, average spacing of grass stems; STDD, standard deviation of differences; SWAT, Soil and Water Assessment Tool; VFS, vegetative filter strip; VFSMOD-W, Vegetative Filter Strip Modeling System; VKS, saturated hydraulic conductivity; VL, length in the direction of the flow; VN, microscale modified Manning's *n* for cylindrical media.

Recent work has extended the model to successfully calculate pesticide trapping efficiency (Fox and Sabbagh, 2009; Sabbagh et al., 2009; Poletika et al., 2009). These authors identified 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). They proposed an empirical pesticide trapping equation with a foundation of hydrological, sedimentological, and chemical specific input factors:

$$\Delta P = a + b\left(\Delta Q\right) + c\left(\Delta E\right) + d\ln\left(F_{\mathrm{ph}} + 1\right) + e\left(\%C\right) \qquad [1]$$

where ΔP is the pesticide removal efficiency (%), ΔQ is the percent infiltration (%) defined as the ratio between the runoff from the VFS and the total water input to the VFS (inflow runon plus precipitation), ΔE is the sediment reduction (%), $\%C$ is the clay content of the sediment entering the VFS, and F_{ph} is a phase distribution factor (ratio between the mass of pesticide in the dissolved phase relative to the mass of the pesticide sorbed to sediment):

$$F_{\mathrm{ph}} = Q_i / \left(K_{\mathrm{d}} E_i\right) \qquad [2]$$

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 (mL g^{-1}), defined as the product of the organic carbon sorption coefficient (KOC in mL g^{-1}) and the percentage organic carbon in the soil (PCTOC, %) divided by 100. For five model development studies, Sabbagh et al. (2009) reported regression parameters: a = 24.8, b = 0.5, c = 0.5, d = −2.4, and e = −0.9. They also proposed a procedure linking VFSMOD-W with the proposed empirical trapping efficiency equation. For data sets with sufficient information, the linked numerical and empirical models significantly improved predictions of pesticide trapping over conventional equations, such as the one in the Soil and Water Assessment Tool (SWAT), which is based solely on field characteristics of the vegetated filter strip (Fox and Sabbagh, 2009; Poletika et al., 2009; Sabbagh et al., 2009). The linked numerical and empirical models had a R^2 = 0.74 with a slope not significantly different than 1.0, intercept not significantly different than 0.0, and standard deviation of differences, STDD, of 14.5%. In comparison, the SWAT equation based on buffer width had a R^2 = 0.05 with negative slope and STDD = 38.7%. In fact, a realization of limitations within the SWAT buffer width equation has led to the development of a simplified field-scale VFS submodel for SWAT based on a runoff retention model developed from VFSMOD-W simulations (White and Arnold, 2009).

Mathematical models are built in the presence of uncertainties of various types (e.g., parameter input variability, model algorithms or structure, model calibration data, scale, model boundary conditions; Haan, 1989; Beven, 1989; Luis and McLaughlin, 1992). In a broad sense, all sources of uncertainty that can affect the variability of the model output have been referred to as *input factors*. The role of the sensitivity analysis is to determine the strength of the relation between a given uncertain input factor and the model outputs. The role of the uncertainty analysis is to propagate uncertainties in input factors onto the model outputs of interest (Saltelli et al., 2004). The formal application of sensitivity and uncertainty analyses allows the modeler to examine model behavior, simplify the model, identify important input factors and interactions to guide the calibration of the model, identify input data or parameters that should be measured or estimated more accurately to reduce the uncertainty of the model outputs, identify optimal locations where additional data should be measured to reduce the uncertainty of the model, and quantify the uncertainty of the modeling results (Saltelli et al., 2005).

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. Thus, global methods are independent of model assumptions and provide not only a ranking of input factor importance and the direct (first order) effect of the individual factors over the output but also information about their interactions (higher order).

The objective of this research was to identify input factors of greatest importance and quantify uncertainty ranges of potential runoff, sediment and pesticide reduction (ΔQ, ΔE, and ΔP) at three unique VFS experimental field sites encompassing a wide range of conditions. Although the objective of this work was to evaluate model sensitivity and uncertainty with regard to input factors, we note that uncertainty does exist within the regression parameters for the empirical pesticide trapping equation. Future research should evaluate model uncertainty and sensitivity relative to the regression parameters of this equation and other empirical equations within the modeling package. Methods included the application of a modern global sensitivity and uncertainty analysis framework for modeling ΔP using VFSMOD-W. Although analyses of sensitivity (Muñoz-Carpena et al., 1999; Abu-Zreig, 2001; Muñoz-Carpena et al., 2007) and uncertainty (Parsons and Muñoz-Carpena, 2001; Shirmohammadi et al., 2006; Muñoz-Carpena et al., 2007) of the VFSMOD-W model have been previously reported for other applications, no study has focused on processes related to pesticide trapping in VFS. Statistical evaluation of the simulation tool will help us understand the overall effectiveness of VFS, and in particular, environmental conditions under which these may not be effective.

Materials and Methods

Vegetative Filter Strip Field Studies

The analyses were applied to three VFS field studies: Arora et al. (1996), Patzold et al. (2007), and Poletika et al. (2009), abbreviated hereafter by the primary authors' names. Overviews of the hydraulic loading rates (i.e., total inflow volume, precipitation, and runoff inflow), soil and VFS characteristics, and pesticides evaluated are provided in Table 1. The first two studies were discussed by Fox and Sabbagh (2009) and utilized by Sabbagh et al. (2009) in development of the empirical pesticide trapping efficiency equation embedded within VFSMOD-W (version 5; Muñoz-Carpena and Parsons, 2008). The Poletika

Table 1. Field studies utilized for sensitivity–uncertainty analyses with VFSMOD-W.

Study	Authors	Poletika et al., 2009	Arora et al., 1996	Patzold et al., 2007
	Location	Iowa, USA	Iowa, USA	North Rhine, Westphalia, Germany
	Years	1994–1995	1993–1994	1997–1999
Event description	Inflow vol. (mm)	282	100	148
	Rainfall (mm)	Simulated (7)	Natural (24)	Natural (71)
	Runoff (mm)	Simulated (275)	Natural (76)	Natural (77)
Soil description	Soil name	Galva	Canisteo	Eutric, Stagnic, Cambisol
	Type	Silty clay loam	Silty clay loam	Silt loam
	Hydrologic soil group	B	C	B
VFS description†	Type	90% smooth brome and 10% bluegrass	Smooth brome	Grass for pasture
	Length in direction of flow × width (m) and slope	4.6 × 4.6 5%	20.1 × 1.5 2.5%	3.0 × 3.0 10%
	Field-to-filter area ratio	15.0	30.0	2.3
Pesticides evaluated (% reduction)		Atrazine (70%) Chlorpyrifos (78%)	Atrazine (55%) Cyanazine (73%) Metolachlor (68%)	Metolachlor (73%) Pendimethalin (90%) Terbuthylazine (77%)

† VFS, vegetative filter strip.

study was used to evaluate the proposed VFSMOD-W and pesticide trapping efficiency equation modeling system.

Arora conducted a 2-yr natural rainfall study in Iowa of herbicide (i.e., atrazine [2-chloro-4-(ethylamino)-6-(isopropylamino)-s-triazine], metolachlor [2-chloro-6′-ethyl-N-(2-methoxy-1-methylethyl)acet-o-toluidide], and cyanazine [2-(4-chloro-6-ethylamino-1,3,5-triazin-2-ylamino)-2-methylpropionitrile]) retention by a 20.1-m-long by 1.5-m-wide VFS, consisting of 81% smooth brome grass (*Bromus inermis* Leyss.), 12% Kentucky bluegrass (*Poa pratensis* L.), 5% tall fescue [*Lolium arundinaceum* (Schreb.) Darbysh], and 2% other vegetation. Arora concluded that herbicide reduction was primarily a function of infiltration by the buffer strips, with antecedent moisture content being a key driver of the infiltration response. This research utilized data specifically for the 13 July 1994 event with 30:1 field-to-buffer area ratio. This specific event was selected because hydrologic data were explicitly reported by Arora for inflow and rain, outflow, and infiltration. For this event, the average ΔQ of the inflow water was approximately 65% and the average ΔE was approximately 84%. Also, the buffer reduced the mass loading of atrazine, metolachlor, and cyanazine by 55, 73, and 68%, respectively.

Field experiments were conducted in western Germany by Patzold for metolachlor, pendimethalin [N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine], and terbuthylazine [6-chloro-*N*-(1,1-dimethylethyl)-*N*′-ethyl-1,3,5-triazine-2,4-diamine] reduction by 3-, 6-, and 12-m grass filter strips, consisting of maize (*Zea mays* L.) and pasture. The Patzold study included experiments with natural rainfall events and experiments with simulated rainfall. The data considered for the modeling were for the simulated rainfall events because rain, runoff water, and sediment inflow and outflow for each simulated rainfall event were reported. These experiments were conducted on 7-m-long by 3-m-wide plots with 3-m grass filter strips (referred to as 3G). There were six different simulated rainfall events ranging from 57 to 71 mm. In this study, the 71-mm event was simulated as the worst-case scenario. For this event, the ΔQ was 65%, ΔE was 87%, and ΔP for metolachor, terbuthylazine, and pendimethalin was 73, 77, and 90%, respectively.

Poletika conducted a field study in western Sioux County, Iowa, with 4.6-m-long by 4.6-m-wide smooth brome and bluegrass strips. Runoff volumes were used to simulate drainage area (VFS-to-field) ratios of 15:1 and 30:1. 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 [O,O-diethyl O-(3,5,6-tricholoro-2-pyridyl) phosphorothioate] and atrazine. For drainage area ratios of 15:1 and 30:1, VFS performed well when flow across the strips was uniform (ΔQ = 59%, ΔE = 88%, ΔP = 85% for chlorpyrifos and 62% for atrazine). Increased flow volume had a minor impact on removal efficiency. Data from Poletika considered for the uncertainty and sensitivity analyses included the average data from the three blocks of uniform, sheet flow conditions (100% of the plot width or 4.60-m-wide buffer with a 15:1 drainage area ratio). The ΔQ averaged 66% (range 46–77%), ΔE averaged 91% (range 84–94%), and ΔP for chlorpyrifos and atrazine averaged 78% and 70%, respectively.

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 variance-based 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 effect is calculated by varying one parameter at a time across a discrete number of levels selected in the probability distribution 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 nonlinear 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 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 an additive model in which the total output variance is explained as a summation of individual variances introduced by varying each parameter alone, $\Sigma S_i = 1$. In addition to the calculation of first-order indices, the extended FAST method (Saltelli, 1999) calculates the sum of the first- and all higher-order indices (interactions) for a given input factor in what is called a *total sensitivity index*, S_{Ti}:

$$S_{Ti} = S_1 + S_{1i} + S_{1jk} \ldots + S_{1\ldots n} \qquad [3]$$

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 distribution functions (CDFs), and percentile statistics can be derived for each output of interest.

The screening method of Morris (1991) and extended FAST variance-based method were applied to the three VFS studies to investigate input factor importance in regard to ΔQ, ΔE, and ΔP. In total, eight pesticide scenarios were considered (Table 1). 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) when the Morris (1991) screening method was selected, it resulted in a subset of important input factors, and steps 2 through 4 were repeated using the extended FAST method to quantify the results; and (6) uncertainty was assessed based on the outputs from the extended FAST simulations by constructing PDFs 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, 121,472 simulations (190 Morris and 14,977 FAST simulations for each pesticide 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 may 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 2) followed Muñoz-Carpena et al. (2007) and was based on a combination of reported values for the individual study, literature reviews, and parameter databases. A summary of the statistical distributions and their statistics for each input factor is given in Table 3 for the Poletika, Arora, and Patzold studies. The reported rainfall–runoff was included in the model as specified in each study. The model outputs selected in the analysis were those representing the hydrological (ΔQ, %), sedimentological (ΔE, %) and pesticide (ΔP, %) response.

In the absence of explicit knowledge on input factor variability, a uniform distribution was used to give equal probability to the occurrence of some input factor values within an expected range. The soil slope (SOA) was reported in each study with varying specificity. Surface slopes of 5.0 to 5.5% were reported for the Poletika study and 2 to 3% for the Arora study; therefore, a uniform distribution was assumed within the measured range of values. One specific slope of 10% was reported by Patzold; therefore, a uniform distribution with a range of ±20% of the base value (i.e., 8–12%) was assumed. Uniform distributions with a ±20% range of the reported values were also selected for Green-Ampt's average suction at the wetting

Table 2. Input factors for VFSMOD-W explored in the sensitivity and uncertainty analysis.

No.	Input factor	Units	Description
Hydrological inputs			
1	FWIDTH	m	Effective flow width of the strip
2	VL	m	Length in the direction of the flow
3	RNA(I)	s m$^{-1/3}$	Filter Manning's roughness *n* for each segment
4	SOA(I)	m m^{-1}	Filter slope for each segment
5	VKS	m s^{-1}	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	m^3 m^{-3}	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 = end, 0.5 = midpoint, 0 = beginning)
Sedimentation 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	H	cm	Filter grass height
13	VN2	s m$^{-1/3}$	Bare surface Manning's *n* 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])
Pesticide component inputs			
16	KOC	–	Organic carbon sorption coefficient
17	PCTOC	%	Percentage of organic carbon in the soil
18	PCTC	%	Percentage clay in the soil

Table 3. Base values and assumed statistical distributions for the input factors of the Poletika et al. (2009), Arora et al. (1996), and Patzold et al. (2007) studies.

Input factor†	Poletika et al. (2009)		Arora et al. (1996)		Patzold et al. (2007)	
	Base value	Distribution‡	Base value	Distribution‡	Base value	Distribution‡
FWIDTH (m)	4.60	*U* (4.14,4.60)	1.50	*U*(1.35,1.50)	3.00	*U*(2.70,3.00)
VL (m)	4.60	*U*(4.60,5.06)	20.1	*U*(20.1,22.1)	3.00	*U*(3.00,3.30)
RNA (s $m^{-1/3}$)	0.40	*T*(0.3,0.4,0.5)	0.24	*T*(0.192,0.24,0.288)	0.24	*T*(0.192,0.24,0.288)
SOA (–)	0.0525	*U*(0.050,0.055)	0.025	*U*(0.02,0.03)	0.10	*U*(0.08,0.012)
VKS (m s^{-1})	3.022e-05	*LN*(−12.3,1.59)	2.2778e-05	*LN*(−10.9,0.64)	1.878e-05	*LN*(−11.2,0.74)
SAV (m)	0.4	*U*(0.32,0.48)	0.13	*U*(0.104,0.156)	0.46	*U*(0.368,0.552)
OS (–)	0.43	*N*(0.43,0.0699)	0.43	*N*(0.43,0.0699)	0.45	*N*(0.45,0.08)
OI (–)	0.347	*N*(0.347,0.071)	0.347	*N*(0.347,0.071)	0.252	*N*(0.252,0.0776)
SS (cm)	1.5	*T*(1.35,1.5,2.2)	1.35	*T*(1.34,1.35,2.2)	2.15	*T*(1.35,2.15,2.2)
VN (s $cm^{-1/3}$)	0.012	*T*(0.0084,0.012,0.016)	0.016	*T*(0.0084,0.016,0.016)	0.012	*T*(0.0084,0.012,0.016)
VN2 (s $m^{-1/3}$)	0.05	*T*(0.04,0.05,0.06)	0.05	*T*(0.04,0.05,0.06)	0.05	*T*(0.04,0.05,0.06)
SCHK (–)	0.5	*U*(0,1)	0.5	*U*(0,1)	0.5	*U*(0,1)
COARSE (–)	0.171	*U*(0.121,0.221)	0.2	*U*(0.16,0.24)	0.10	*U*(0.08,0.12)
DP (cm)	0.0010	*U*(0.0008,0.0012)	0.00025	*U*(0.0002,0.0003)	0.0002	*U*(0.0016,0.0024)
H (cm)	10.0	*N*(10.0,1.55)	13.0	*N*(13.0,2.02)	18.0	*N*(18.0,2.78)
KOC (–)						
Atrazine	147	*T*(38,147,288)	147	*T*(38,147,288)	–	–
Chlorpyrifos	6070	*T*(5300,6070,14800)	–	–	–	–
Cyanazine	–	–	218	*T*(40,218,235)	–	–
Metolachlor	–	–	70	*T*(22,70,307)	70	*T*(22,70,307)
Pendimethalin	–	–		–	13,400	*T*(5000,13400,29000)
Terbuthylazine	–	–		–	220	*T*(162,220,514)
PCTOC (%)	2.58	*U*(2.37,2.78)	3.5	*U*(2.8,4.2)	1.7	*U*(1.36,2.04)
PCTC (%)	28.9	*U*(27,30.7)	31	*U*(24.8,37.2)	25	*U*(20.0,30.0)

† Refer to Table 2 for the definition of each input factor.

‡ Statistics of the assumed distributions; uniform: *U*(min,max); triangular: *T*(min,mean,max); log normal: *LN*(μ_y,σ_y); normal: *N*(μ_x,σ_x). *LN* and *N* distributions are truncated between (0.001,0.999) except for H with (0.025, 0.975).

front (SAV). A uniform distribution with range of 0 to 1 was selected for the ponding check point, SCHK. In a previous study (Muñoz-Carpena et al., 1993b), VFSMOD-W was found not sensitive to SCHK values except for sandy soils.

The effective flow width of the strip (FWIDTH) is theoretically the width of the filter perpendicular to the primary flow direction under uniform, sheet flow conditions. 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 used 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 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.

Many of the soil texture and organic fraction input factors required by VFSMOD-W were not explicitly reported for each study site. Following Sabbagh et al. (2009), the fraction of incoming sediment with particle diameters >0.0037 cm (COARSE) was approximated as the sand fraction for each study. Similarly, the average sediment particle size diameter (DP) was estimated based on the reported fraction of clay (PCTC), silt, and sand. The studies reported single values of percent organic carbon (PCTOC) but no measurements of within field variability for deriving a statistical distribution. Therefore, uniform distributions were assumed for COARSE, DP, PCTC, and PCTOC with a range of ±20% around the reported base values (Table 3).

Following Haan et al. (1994), vegetation input factors were quantified on the basis of the vegetation type explicitly documented for each study (Table 1). Triangular distributions with peak at the recommended values and range of ±20% around the peak were selected for these biology-related inputs (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 triangular distribution was also used for the KOC for the specific pesticides investigated in the studies. The triangular distribution was centered at the recommended KOC from the USDA's pesticide database (USDA, 2006) and range matching that reported in the database. For terbuthylazine, the range in KOC was derived from various published and unpublished sources (Chefetz et al., 2004).

In several cases, more theoretical distributions were used to define input factor variability. The distribution types for saturated hydraulic conductivity (VKS), saturated water content (OS), and initial water content (OI), which was assumed to be the field capacity in each study following Sabbagh et al. (2009), were adopted directly from recommended distributions by Meyer et al. (1997) and Carsel and Parrish (1988) based on soil texture (Table 3). Parameters of the distributions for OS and OI were taken directly from Meyer et al. (1997) and Carsel and Parrish (1988). For these studies, VKS distributions for each soil texture provided wide-ranging statistical distributions with values that varied by more than three to four orders of magnitude. More plausible site-specific statistics for the log-normal distributions were selected for the soil texture of each study. The mean of log-values was obtained from the simulation values used originally by Sabbagh et al. (2009) and the standard deviation was assumed equal to the mean (i.e., CV of 100%). These values were deemed valid for each study when considering the variability of VKS at the scale of the specific field studies (Table 1), which is expected to be smaller than for the whole USDA textural class reported by Meyer et al. (1997) and Carsel and Parrish (1988).

The filter grass height (H) variation is probably driven by genetics. Therefore, a normal distribution was used to describe H with the mean as the grass height maintained and reported at one study (10 cm for the Poletika) or as the maximum rigidity for that vegetation type based on data from Haan et al. (1994) provided in the model documentation (20 cm for the Arora study and 18 cm for the Patzold study). The standard deviations of the assumed normal distributions were derived using a 15.5% CV, based on data reported by Muñoz-Carpena et al. (2007), and the means reported previously.

Results and Discussion

Global Sensitivity Analysis: Screening Method of Morris

As suggested by Morris, only input factors separated from the origin of the μ^*–σ plane were considered important. Relative input factor importance for ΔQ based on Morris results was similar among the three studies (Fig. 1). The number of input factors identified as important was considerably smaller than the full set of 18 model inputs. The VKS ranked as the most important input factor for ΔQ, appropriately independent of study site or scenarios for different pesticides (Fig. 1). These results matched those of previous researchers with data from other VFSMOD-W applications (e.g., Abu-Zreig, 2001; Muñoz-Carpena et al., 1993b, 1999, 2007). The next most important input factors for predicting hydrologic response included OS and OI in the Poletika and Patzold studies. Unique to the Arora study, performed on SOAs of approximately 2.5% compared with SOA of near 10% for Patzold and 5% for Poletika, was the importance of RNA, SOA, and VL (Fig. 1). The importance of these three variables in only the Arora study can be explained by the SOA. Muñoz-Carpena et al. (1993b) demonstrated that SOA, and correspondingly RNA, was only appreciable for less-steep VFS conditions. For the less-steep (2.5%) VFS in these studies, SOA was an influential factor, and for the more steep (5–10%) VFS, the importance of SOA in predicting ΔQ diminished.

The ΔE for all study sites and scenarios was governed by both hydrologic (VKS) and sediment (DP, VN and SS) characteristics, as shown in Fig. 1. The number of important input factors was slightly greater for ΔE than for ΔQ. The importance of several of these input factors is in agreement with the global sensitivity analysis discussed by Muñoz-Carpena et al. (2007). A slight difference between the three field sites of this research was the apparent importance of two vegetation-related input factors, VN and SS, in the Arora study. In fact, for Arora, VN was the most important input in regard to ΔE across all three pesticide scenarios (Fig. 1). The differences are explained not only by the different VN ranges but possibly as a result of the smallest SOA in Arora, which in turn resulted in slower velocities through the VFS. Since transport capacity was linked to flow velocity, greater sedimentation occurred and thus input factors that controlled sedimentation, like VN, became more important.

The VKS was consistently the most important input factor for ΔP across all three study sites and pesticide scenarios (Fig. 2). Therefore, ΔQ largely controlled ΔP under the hydrologic conditions of these studies. Such findings further support the proposed techniques of Fox and Sabbagh (2009) and Sabbagh et al. (2009) in predicting ΔP based on ΔQ and ΔE. Input factors of secondary importance below VKS included OS, OI, and PCTC in the Poletika and Patzold studies and PCTC, RNA, SOA, and VL in the Arora study (Fig. 2). Similar to ΔQ, a greater number of secondary input factors were important for ΔP in the Arora study, again due to the less-steep slope and increased sediment-bonded pesticide reduction dynamics.

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 (Fig. 2). In other words, it was less important which value within the KOC range was used to simulate trapping of a specific pesticide; however, the pesticide being simulated and its KOC range was still important, as more quantitatively demonstrated below in the extended FAST results. A shift in the importance of KOC could be observed when comparing pesticide scenarios. For example, in the Poletika study, the importance of KOC was greater when comparing the more soluble pesticide atrazine with chlorpyrifos, most probably due to the fact that sediment input factors already accounted for transport of the mostly sediment-bound chlorpyrifos (Fig. 2). Another input from the pesticide component, the PCTC, was the second most important input factor in the Arora and Patzold studies but was not as important in the Poletika study due to the much larger flow volumes (i.e., runoff) experienced by the VFS in this study.

The Morris (1991) method indicated the presence of interactions between input factors in terms of predicted ΔQ, ΔE, and ΔP, especially in the Arora study, as demonstrated by the σ values (Fig. 1 and 2). The closer the point is to zero on the σ axis means that first-order effects are more important with a small interaction component. The σ values obtained suggested that simple regressions based on VFS physical characteristics (e.g., slope, width, and roughness) are insufficient without interaction effects between variables considered. These complex results again support the need for process-based pesticide

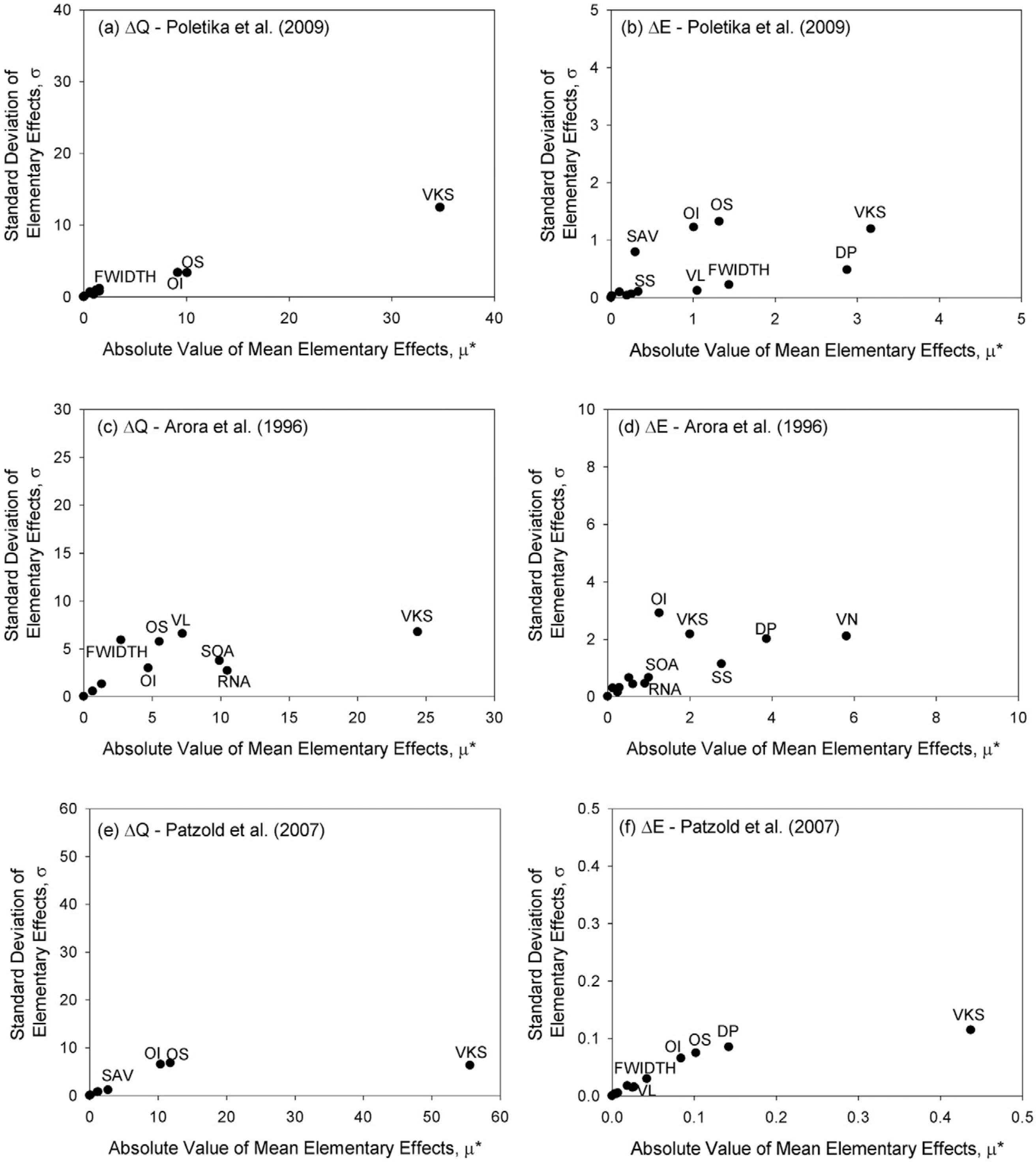

Fig. 1. Global sensitivity analysis results obtained from the Morris (1991) screening method for the vegetative filter strip hydrology (ΔQ, infiltration) and sedimentation (ΔE, sediment trapping) for the Poletika et al. (2009), Arora et al. (1996), and Patzold et al. (2007) studies. Input factors separated 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. Input factors are not comparable between the study sites. See Table 2 for the definition of each input factor.

runoff modeling, as suggested by Fox and Sabbagh (2009) and Sabbagh et al. (2009).

Global Sensitivity Analysis: Extended FAST

The extended FAST global sensitivity results confirmed and added insights to the Morris results. Table 4 outlines the global sensitivity analysis results in terms of the percentage of total output variance explained by each input factor, i.e., the first-order effects (S_i), and interactions, $S_{Ti} - S_1$. In general, filter removal efficiencies for the selected studies were not simple and were dominated by interactions and nonlinear responses, especially under cases of higher hydraulic loading rates (see $S_{Ti} - S_1$ results for Poletika in Table 4). For the Arora and Patzold studies, it appeared that infiltration dominated the filter hydrology in these two studies and the model behaved as strongly additive (ΣS_i was >84% for these

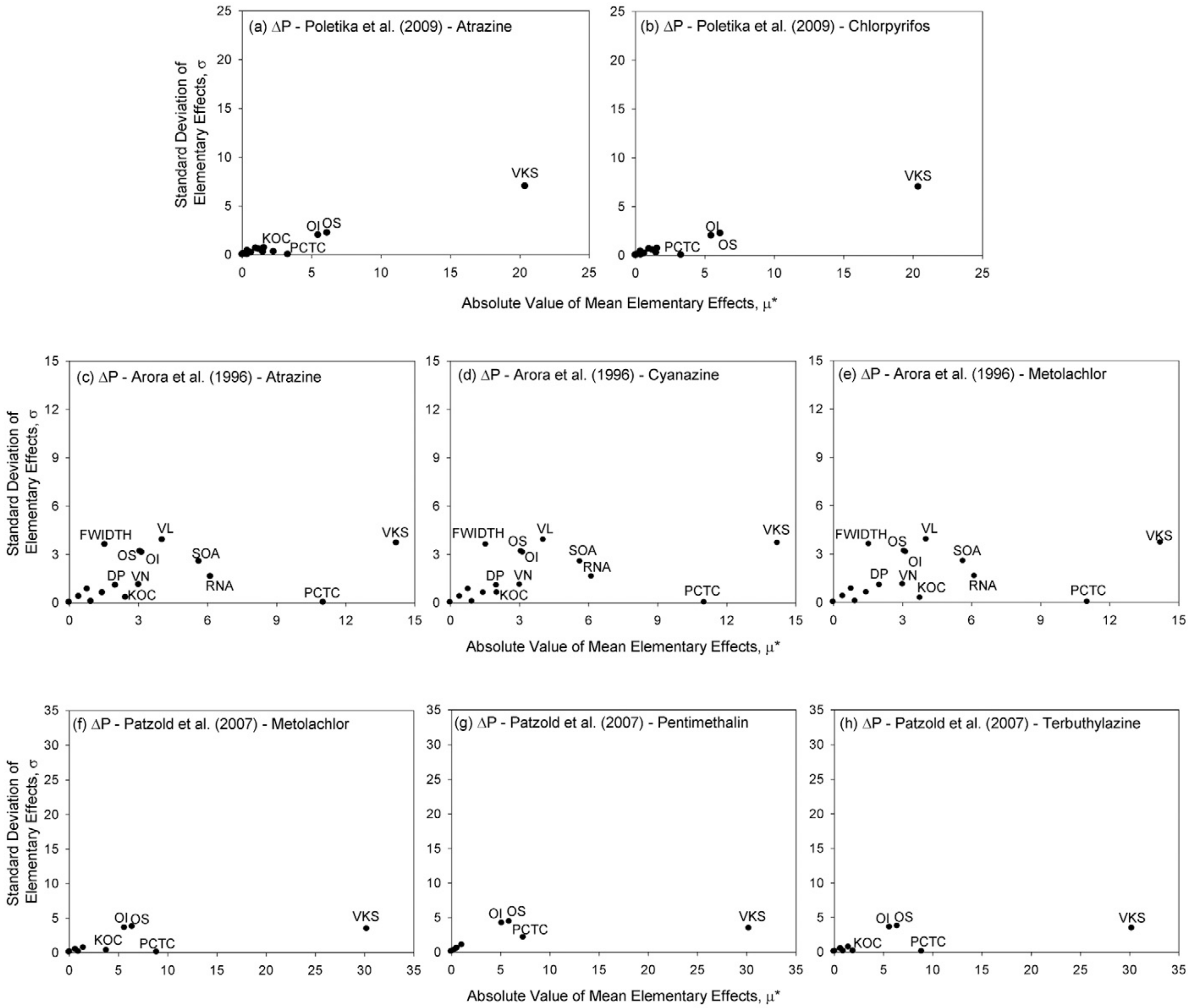

Fig. 2. Global sensitivity analysis results obtained from the Morris (1991) screening method for the vegetative filter strip pesticide reduction (Δ*P*, pesticide trapping) for (a) atrazine and (b) chlorpyrifos in the Poletika et al. (2009) study; (c) atrazine, (d) cyanazine, and (e) metolachlor in the Arora et al. (1996) study; and (f) metolachlor, (g) pendimethalin, and (h) terbuthylazine in the Patzold et al. (2007) study. Labels of unimportant input factors (close to the μ*–σ plane origin) have been removed for clarity. See Table 2 for the definition of each input factor.

studies, Table 4). Total first-order effects explained >95% of the output variability in the Patzold study, although as explained above, the smaller slope of the Arora study introduced some interactions for ΔE (ΣS_i = 84%).

Morris results indicated that VKS was the single most important input factor when considering all three study sites and the various outputs, especially for ΔQ and ΔP. Extended FAST results further supported that conclusion in terms of total output variance explained by VKS (Table 4): 49% for ΔQ and approximately 50% for atrazine and chlorpyrifos ΔP in the Poletika study; 75% for ΔQ and approximately 60% for atrazine, cyanazine, and metolachlor ΔP in the Arora study; and 85% for ΔQ and approximately 80% for metolachlor, pendimethalin, and terbuthylazine ΔP in the Patzold study. As before, PCTC also exhibited importance for the Arora study, second only to VKS in explaining the variance in ΔP.

Global Uncertainty Analysis: Extended FAST

The global uncertainty analysis results provided ranges in expected ΔQ, ΔE, and ΔP (Table 5, Fig. 3) along with some interesting comparisons between the three study sites. First, it was interesting to compare the differences in ΔQ PDFs/CDFs between the three study sites, with higher ΔQ for the Arora and Patzold studies (Fig. 3). The difference in ΔQ between the studies can be explained on the basis of the different flow amounts into the VFS in each study. For example, water input into the VFS for the Poletika study was higher (approximately 0.28 m^3 of inflow per m^2 of VFS area or an equivalent depth of 280 mm) than the Arora or Patzold studies (approximately 0.10–0.15 m^3 of inflow per m^2 of VFS area or equivalent depths of 100–150 mm), as shown in Table 1. As expected, for larger flow through the VFS, efficiencies of infiltration were smaller even though two of the studies were conducted on soils with the same textural class (i.e., silty clay loam). In terms of

Table 4. Fourier Amplitude Sensitivity Test (FAST) results for the vegetative filter strip studies.

	Outputs		Input factors†																	Total
		VL	FWIDTH	RNA	SOA	VKS	SAV	OS	OI	SS	VN	VN2	SCHK	COARSE	DP	H	KOC	PCTOC	PCTC	
		First-order sensitivity index, S_i (%)																		
Arora (1996)	ΔQ†	2	0	2	0	75	0	2	2	0	0	0	0	0	0	0	0	0	0	84
	ΔE†	1	0	0	0	11	0	0	1	4	50	0	0	0	8	0	0	0	0	77
	ΔP† (atrazine)	2	1	2	1	60	0	1	2	0	4	0	0	0	1	0	1	0	15	91
	ΔP (cyanazine)	3	1	2	1	61	0	1	2	0	4	0	0	0	1	0	1	0	15	92
	ΔP (metolachlor)	3	1	2	1	60	0	1	2	0	4	0	0	0	1	0	2	0	15	91
Patzold (2007)	ΔQ	0	0	0	0	85	0	6	5	0	0	0	0	0	0	0	0	0	0	96
	ΔE	0	1	0	0	67	0	4	4	0	0	0	0	0	14	0	0	0	0	91
	ΔP (metolachlor)	0	0	0	0	79	0	5	5	0	0	0	0	0	0	0	1	0	6	97
	ΔP (pendimethalin)	0	0	0	0	79	0	6	5	0	0	0	0	0	0	0	0	0	6	96
	ΔP (terbuthylazine)	0	0	0	0	80	0	5	5	0	0	0	0	0	0	0	0	0	6	97
Poletika (2009)	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
		Interactions, $S_{Ti} - S_i$ (%)‡																		
Arora (1996)	ΔQ	9	6	9	8	10	4	4	4	5	5	4	4	4	3	4	4	4	4	
	ΔE	17	16	14	17	23	18	17	19	17	21	20	17	20	16	27	16	16	21	
	ΔP (atrazine)	14	13	12	15	11	5	6	6	8	6	7	5	5	5	6	6	5	5	
	ΔP (cyanazine)	12	13	12	15	11	5	6	6	8	6	7	5	5	5	7	6	5	5	
	ΔP (metolachlor)	12	13	12	15	11	5	6	6	7	6	7	5	5	5	6	6	5	5	
Patzold (2007)	ΔQ	1	1	1	1	3	1	2	2	1	1	1	1	1	1	1	1	1	1	
	ΔE	1	1	1	1	5	1	1	2	1	1	1	1	1	4	1	1	1	1	
	ΔP (metolachlor)	0	0	1	1	3	1	2	2	1	1	1	1	1	1	1	1	1	1	
	ΔP (pendimethalin)	1	0	1	1	3	1	2	2	1	1	1	1	1	1	1	1	1	1	
	ΔP (terbuthylazine)	1	0	0	1	2	1	2	2	1	1	1	1	1	1	1	1	1	1	
Poletika (2009)	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	

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

‡ S_{Ti}, total sensitivity index.

Table 5. Uncertainty analysis statistics for selected output probability distributions obtained from the outputs of the extended Fourier Amplitude Sensitivity Test (FAST) simulations.

Study	Output	Mean	Median	95CI‡	SD	SE	Min.	Max.	Skew‡	Kurt‡
		%					%			
Poletika et al. (2009)	ΔQ†	29.2	22.0	6.9–61.0§	24.2	0.20	0.0	100.0	1.8	2.6
	ΔE†	92.0	91.7	89.0–93.7§	2.5	0.02	87.3	100.0	1.8	4.0
	ΔP† (atrazine)	56.1	51.9	42.7–73.5§	14.5	0.12	36.2	100.0	1.9	3.0
	ΔP† (chlorpyrifos)	61.9	58.0	49.0–78.3§	13.3	0.11	44.1	100.0	1.7	2.3
Arora et al. (1996)	ΔQ	57.3	56.1	39.9–78.3	11.6	0.10	26.4	100.0	0.8	1.3
	ΔE	92.8	94.0	84.3–97.3	4.8	0.04	32.3	100.0	–3.1	18.3
	ΔP (atrazine)	65.9	66.0	53.2–79.0	8.0	0.07	16.9	100.0	0.3	1.7
	ΔP (cyanazine)	66.0	66.1	53.3–79.1	7.9	0.06	17.2	100.0	0.3	1.7
	ΔP (metolachlor)	65.4	65.4	52.6–78.5	8.0	0.07	15.9	100.0	0.3	1.7
Patzold et al. (2007)	ΔQ	62.9	62.6	32.4–92.7	18.7	0.15	6.5	100.0	–0.1	–0.7
	ΔE	99.7	99.7	99.4–99.9	0.2	0.00	99.0	100.0	–0.1	–0.4
	ΔP (metolachlor)	78.4	78.4	60.7–96.1	10.7	0.09	47.7	100.0	0.0	–0.6
	ΔP (pendimethalin)	86.8	87.4	69.7–100.0	9.8	0.08	57.0	100.0	–0.4	–0.8
	ΔP (terbuthylazine)	80.4	80.5	62.8–97.9	10.6	0.09	50.0	100.0	–0.1	–0.7

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

‡ 95CI = 95% confidence interval; Skew = skewness; Kurt = kurtosis.

§ 95CI for Poletika et al. (2009) study calculated by neglecting accumulation of values at the upper limit of 100% (second peak in the bimodal distribution).

ΔE, the PDFs/CDFs between the Arora and Poletika studies were approximately equivalent (Table 5, Fig. 3). Slower flow rates should lead to higher removal efficiencies if the sediment particles of the two studies were the same. However, the particle sizes were different between the two studies with larger sediment for the Poletika study. It should be noted that sedimentation dynamics in VFSMOD-W shift between coarse particles that are transported primarily as bedload transport and retained more easily and fine sediment that is transported mainly as suspended load and retained less easily (Barfield et al., 1979; Hayes et al., 1984). The range in ΔE for the Patzold study was confined between 99 and 100% (Table 5, Fig. 3).

Also shown in Fig. 3, ΔP consistently fell between ΔQ and ΔE PDFs/CDFs. Depending on the range in KOC of the pesticide being simulated, ΔP would shift either to the left toward the ΔQ PDF/CDF or to the right toward the ΔE PDF/CDF. For example, in the Poletika study shown in Fig. 3, a shift to the left toward the ΔQ PDF/CDF occurred for the lower KOC (more soluble) pesticide (atrazine) and a shift to the right toward the ΔE PDF/CDF for the higher (more sediment-bound) KOC pesticide (chlorpyrifos). Fairly equivalent PDFs/CDFs were observed in terms of ΔP between the three pesticides in the Arora et al. (1996) study, most likely due to the approximately equivalent literature ranges for the pesticides' KOC values (Table 3, Fig. 3). For the Patzold study, ΔP PDFs/CDFs were approximately equivalent for metolachlor and terbuthylazine due to similar KOC input distributions but shifted to higher trapping efficiencies for pendimethalin (Fig. 3f).

The uncertainty of the results can also be communicated as a probability of exceedance of a desired ΔP regulatory or design value, derived from the CDFs in Fig. 3. Notice how these probabilities would change widely across the sites and pesticide scenarios. For example, if a 50% ΔP was sought, the probability of exceedance would vary between 0% for the Patzold study and 40 to 80% for the Poletika study. It should be noted that for regulatory or design purposes, a specific design storm is typically required, and that these CDFs are for the events simulated and included only for illustration purposes.

Summary and Conclusions

Vertical saturated hydraulic conductivity was the most important hydrological input factor for predicting infiltration or runoff reduction across all three VFS studies. The slope, filter strip length, and Manning's roughness were important input factors for less steep slopes (<5%). More input factors became important for predicting sedimentation, including the average particle size of the sediment and the initial and saturated water content of the VFS soil. Filter strip length was not consistently ranked as one of the most important input factors for the conditions simulated in these scenarios. Input factor importance for predicting pesticide reduction through surface runoff mechanisms appeared to mimic runoff reduction results, with saturated hydraulic conductivity consistently the most important input factor for predicting pesticide reduction across all study sites and pesticide scenarios. Hydrologic response in terms of infiltration processes largely controlled pesticide response under the hydrologic conditions of these studies. This research focused on pesticide reduction in surface runoff. In some hydrological settings, infiltrated water and contaminants can enter the shallow groundwater system and reach adjacent rivers and streams through perched groundwater flow (e.g., Fuchs et al., 2009). Future research should be devoted to better understanding both surface and subsurface processes of flow, sediment, and contaminant movement through VFS.

Pesticide reduction in surface runoff was nonlinearly related to slope, even though many regression-based empirical equations use linear regression relationships with slope as an input factor. Pesticide-specific input factors were of secondary importance to those representing infiltration and sediment reduction. Interactions were observed between input factors for predicted infiltration, sedimentation, and pesticide reduction. Simple linear or nonlinear regressions based on VFS physical

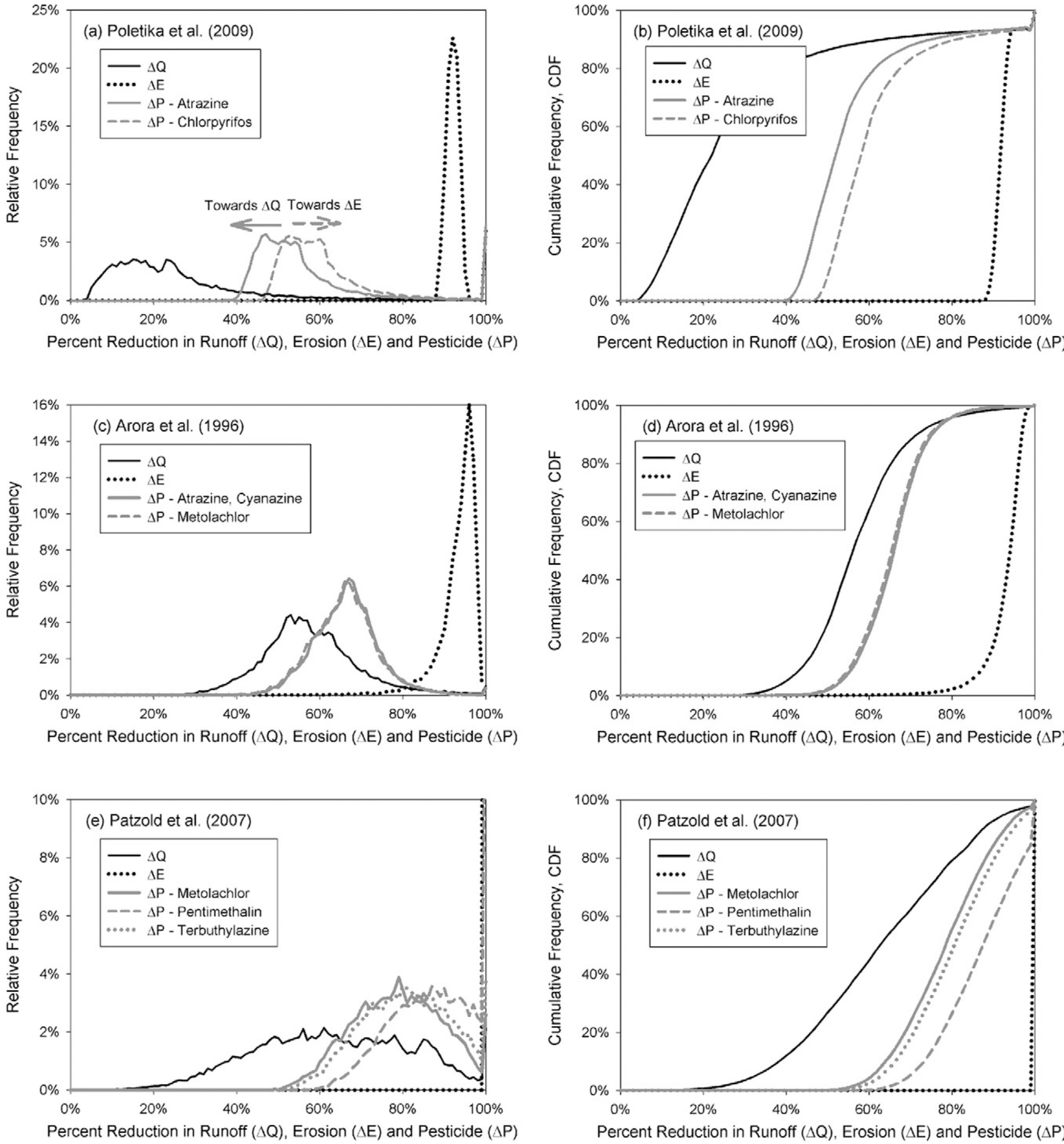

Fig. 3. Global uncertainty analysis results obtained from the extended FAST variance-based method: infiltration (ΔQ), sedimentation (ΔE), and pesticide reduction (ΔP) probability distribution function (PDF) and cumulative distribution function (CDF) distributions. (a) PDF and (b) CDF for the Poletika et al. (2009) study; (c) PDF and (d) CDF for the Arora et al. (1996) study; and (e) PDF and (f) CDF for the Patzold et al. (2007) study.

characteristics (e.g., slope, length, and roughness) are insufficient without considering the VFS hydrological and sedimentological conditions and the interaction between input factors. Distributions of predicted pesticide reduction consistently fell between infiltration and sedimentation probability and cumulative distribution functions, PDFs/CDFs. Depending on the pesticide scenario simulated, the pesticide reduction would shift either to the left toward the runoff reduction PDF/CDF or to the right toward the sedimentation PDF/CDF. Whether looking at an individual scenario or comparatively across all scenarios, it was clear that the potential range in runoff reduction, sedimentation, and pesticide trapping efficiency for a specific VFS was large. Therefore, filter removal efficiencies are not simple and are dominated by nonlinear responses, especially under cases of higher hydraulic loading rates. The present work clearly illustrates how an equivalent filter in terms of soil and vegetation characteristics may have unique runoff, sedimentation, and pesticide reduction characteristics depending on the hydraulic loading rate of the system (a function of the storm event and the hydrologic conditions of the VFS). Such results further support the use of process-based modeling for VFS hydrologic and sedimentological conditions to estimate pesticide-trapping efficiency.

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