GLOBAL SENSITIVITY AND UNCERTAINTY ANALYSES OF THE WATER QUALITY MODEL VFSMOD-W

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ABSTRACT. *This study presents the statistical evaluation of the vegetative filter strip modeling system VFSMOD-W as a tool to design vegetative filter strips to use in the mitigation plans required as a part of phosphate mining permitting process by the State of Florida. A two-step statistical evaluation framework using global techniques is presented based on: (1) a screening method (Morris) for qualitative ranking of parameters, and (2) a variance-based method (extended Fourier Analysis Sensitivity Test--extended FAST) for quantitative sensitivity and uncertainty analyses. Measured characteristics of the central Florida phosphate-mining region are used to construct the 16 probability distributions of input factors. Two design filter lengths (3 and 6 m) and two model structures (VFSM--the filter module alone, and UH/VFSM--combined filter and source area components) are considered and compared to previous local "one-parameter-at-a-time" (OAT) analyses. It was found that for this application the filter's saturated hydraulic conductivity (VKS) was the most important factor controlling the filter runoff response, explaining over 90% of total output variance irrespective of model structure. In the case of the VFSM structure, sediment-related outputs were mainly influenced by three parameters: sediment particle size diameter (DP), effective flow width of the strip (FWIDTH), and VKS. For UH/VFSM, there were six important parameters: DP, the source area erosion and runoff parameters (slope of the source area Y, USLE soil erodibility index K, and runoff curve number CN), FWIDTH, and VKS. The results show the model's additive nature for this specific application, i.e., there are no significant parameter interactions for all model outputs except sediment outflow concentration and sediment wedge geometry. The uncertainty analysis indicates that regardless of the model structure, the probability of meeting a minimum required 75% sediment reduction was acceptable at the 90% confidence level for the 6 m long filter, but not for the 3 m filter. In general the UH/VFSM model structure exhibited larger output uncertainty. Comparison with previous OAT analyses of the model indicates the importance of performing the global evaluation for each specific model application. The results illustrate four main products of the global analysis: ranking of importance of the VFSMOD-W parameters for different outputs, effect of changing modeling structure, type of influence of the important parameters, and assurance of the model's behavior.*

Keywords. *Computer modeling, Grass buffers, Hydrological modeling, Model evaluation, Probability of exceedance, Sensitivity analysis, Uncertainty analysis, Vegetative filter strips, Water quality.*

Historic and ongoing phosphate mining in the Peace River watershed (Polk County, Florida) has disturbed the land and affected water quality in the Peace River. Surface runoff from mining lands can be a potential source of sediment, particulate, and dissolved phosphorus into surface water bodies. Vegetative filter strips (areas of grass or other dense vegetation) can effectively reduce surface runoff phosphorus and sediment transport from reclaimed mining areas (Kuo, 2007). Performance of these filters depends on characteristics of the incoming pollutants and of the filter design (length, slope, and densities of vegetation cover). Water quality models, when properly field calibrated and tested, can minimize the need for field-testing of management alternatives and provide significant time and cost savings. The vegetative filter strip (VFS) modeling design system VFSMOD-W (Muñoz-Carpena et al., 1999; Muñoz-Carpena and Parsons, 2004, 2005) is a field-scale, mechanistic, storm-based model developed to route the incoming hydrograph and sedigraph from an adjacent field through a VFS and to calculate the resulting outflow, infiltration, and sediment trapping efficiency. The Florida Department of Environmental Protection, Bureau of Mine Reclamation, is considering the model as a tool to design optimal vegetative filters in mining reclamation plans.

Mathematical models are built in the presence of uncertainties of various types (parameter input variability, model algorithms or structure, model calibration data, scale, model boundary conditions, etc.) (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

Submitted for review in March 2006 as manuscript number SW 6941; approved for publication by the Soil & Water Division of ASABE in September 2007 as a contribution to the ASABE 100th Anniversary Soil and Water Invited Review Series.

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sensitivity and uncertainty analyses allows the modeler to: (1) examine model behavior, (2) simplify the model, (3) identify important input factors and interactions to guide the calibration of the model, (4) identify input data or parameters that should be measured or estimated more accurately to reduce the uncertainty of the model outputs, (5) identify optimal locations where additional data should be measured to reduce the uncertainty of the model, and (6) quantify the uncertainty of the modeling results (Saltelli et al., 2005). When modeling a complex environmental problem like surface runoff pollution from reclaimed mining areas, the uncertainty of the model results is often a major concern, since it has policy, regulatory, and management implications (Shirmohammadi et al., 2006). However, in spite of their strengths, formal sensitivity and uncertainty analyses are frequently ignored in water quality modeling efforts (Haan et al., 1995; Muñoz-Carpena et al., 2006; Shirmohammadi et al., 2006), usually due to the considerable effort these involve as the complexity and size of the models increase and also due to the limited data available specific to the model application (Reckhow, 1994). Beven (2006) has recently proposed that not doing formal sensitivity and uncertainty analyses when applying a model ultimately results in undermining the science and value of models.

The sensitivity of a model output to a given input factor has been traditionally expressed mathematically as the derivative of the model output with respect to the input variation, sometimes normalized by either the central values where the derivative is calculated or by the standard deviations of the input and output values (Haan et al., 1995). These sensitivity measurements are "local" because they are fixed to a point (base value) or narrow range where the derivative is taken. These local sensitivity indexes are classified as "one-parameter-at-a-time" (OAT) methods, i.e., they quantify the effect of a single parameter by assuming all others are fixed (Saltelli et al., 2005). Local OAT sensitivity indices are only efficient if all factors in a model produce linear output responses, or if some type of average can be used over the parametric space. Often, the model outputs' responses to changes in the input factors are non-linear, and an alternative "global" sensitivity approach, where the entire parametric space of the model is explored simultaneously for all input factors, is needed. The advantage of the global approach over a local OAT method is that it results in the ranking of parameter importance and provides information not only about the direct (first order) effect of the individual factors over the output, but also about their interaction (higher order) effects. Different types of global sensitivity methods can be selected based of the objective of the analysis, the number of uncertain input factors, the degree of regularity of the model, and the computing time for single model simulation (Cukier et al., 1973, 1978; Koda et al., 1979; Morris, 1991; Saltelli et al., 2000a, 2004, 2005; Sobol, 1990; Wallach et al., 2006).

An extensive review of uncertainty analysis methods applied to environmental models can be found in Morgan and Henrion (1992), Haan (2002), and Shirmohammadi et al. (2006). The best method to quantify model uncertainty is based on probability distribution functions (PDFs) of the model outputs (Haan, 1989, 2002; Haan et al., 1995; Shirmohammadi et al., 2006). Haan et al. (1995) presented two methods for generating the general probability distri–butions of the output variables of interest. The first method was the First-Order-Approximation (FOA) (Morgan and Henrion, 1992). In this method, the mean or expected value of the output is estimated based on the variance and covariance of the input parameters and their local absolute sensitivity indices. If the input parameters are independent, then the covariance is zero and the variance of the output becomes a function of the variance of the inputs and their absolute sensitivities. This type of analysis produces good estimates of the mean and variance of the model output when the coefficient of variation (mean/standard deviation) of the input parameter is small and the relationship between the output and input is linear. An alternative and more general approach is the technique of Monte Carlo simulations (MCS), which is performed by randomly sampling the multivariate input distribution, running model simulations with the sampled values to produce estimates of model output values, and combining these to produce a PDF. The procedure is typically computationally expensive since the process must be repeated many times to obtain a smooth PDF. More efficient sampling methods have been proposed and widely used based on stratified sampling of the input PDF, such as replicated Latin hypercube sampling (r-LHS) (McKay et al., 1979; McKay, 1995). An advantage of the MCS method over FOA is that it does not require *a priori* knowledge on the linearity of the model, and it does not introduce assumptions about the form of the output PDF distribution, although it relies on the correct determination of the input parameter distributions. The output PDFs can be used for decision-making by placing confidence levels on the outputs, usually in the form of a margin of safety (MOS) component, or by calculating a probability of exceedance of a threshold value (Morgan and Henrion, 1992). However, MOS is often arbitrarily selected as a fixed percent range around the model output (Sexton et al., 2005) rather than based on the output PDF.

Haan et al. (1995) outlined a statistical procedure for evaluating hydrology and water quality models. Their procedure included: conducting local OAT sensitivity analysis, generating probability distributions for model inputs, generating probability distributions for the model outputs, and using the probability distributions of the model outputs to assess uncertainty. Recently, Saltelli et al. (2004, 2005) proposed that a desirable statistical framework for model evaluation should be based on a set of global analyses techniques that meet the following requirements: (1) are model-independent so they can be used with any model without modification; (2) contain a screening method to efficiently identify the subset of important inputs controlling the output variability; (3) contain a method that, based on the reduced set of sensitive inputs, can provide a quantitative decomposition of the output variance in terms of first and higher order effects of the input factors; and (4) allow for uncertainty analysis of the model based on the construction of PDFs using outputs derived simultaneously from the variance-based method. The modified method of Morris (Morris, 1991; Campolongo et al., 2005) can be an effective screening method since it provides, with a relatively small number of simulations, a qualitative ranking of input factors in terms of their relative effect over the model output, and a measure of possible interactions for that output. A variance-based technique, like the extended Fourier Amplitude Sensitivity Test (FAST) (Saltelli, 1999) can be applied over the subset of important input parameters to complete the analysis with quantitative sensitivity information. A statistical model evaluation procedure based on these techniques can be applied to a wide spectrum of models and applications. However, it is especially efficient for computationally expensive models, or if a large number of parameters need to be evaluated simultaneously.

Although analyses of sensitivity (Muñoz-Carpena et al., 1999; Abu-Zreig, 2001) and uncertainty (Parsons and Muñoz-Carpena, 2001; Shirmohammadi et al., 2006) of the VFSMOD-W model have been previously reported for other applications, only classical local OAT and Monte Carlo approaches were used. The main objective of this study is the application of a modern global sensitivity and uncertainty analysis framework to modeling vegetative filter strips using VFSMOD-W, for the conditions of the reclaimed phosphate-mining region of central Florida. This approach represents an unique combination of powerful features, including: (1) identification of input probability distributions based on field data, (2) consideration of the effect of model structural error, (3) quantification of the effect of each input on the overall output variance, and (4) separation of first-order versus higher-order effects (interactions).

Materials and Methods

Application Case and Analysis Procedure

The specific conditions selected for the evaluation of the model are those of the phosphate-mining region of central Florida along the Peace River basin (fig. 1). Continued mining of phosphorus ore has degraded water quality in the Peace River watershed and has left behind large mounds of refuse material (tailings) that now shape the landscape surrounding the river. The tailings are essentially homogenous clean sand (>94% in weight) with a high concentration of apatite, the phosphorus mineral ore, mixed with small pockets of clay in some areas. Currently, there is interest in studying the potential of vegetative filter strips as a best management practice (BMP) to use in the mitigation plans that are required as part of the mining permitting process by the State of Florida. Field experiments have been conducted to quantify runoff quantity and quality from the refuse mining mounds and the effectiveness of VFS in the area (Kuo et al., 2005; Kuo, 2007). Eight fully instrumented runoff plots were constructed at two different locations to represent the range of conditions found in the region (landscape slope and lengths, soil variability, locally recommended grasses, climate characteristics, etc.) (Kuo, 2007).

Values from these experiments are used as the basis for the global evaluation of VFSMOD-W. The model contains two components, the main program (VFSM) and a front-end

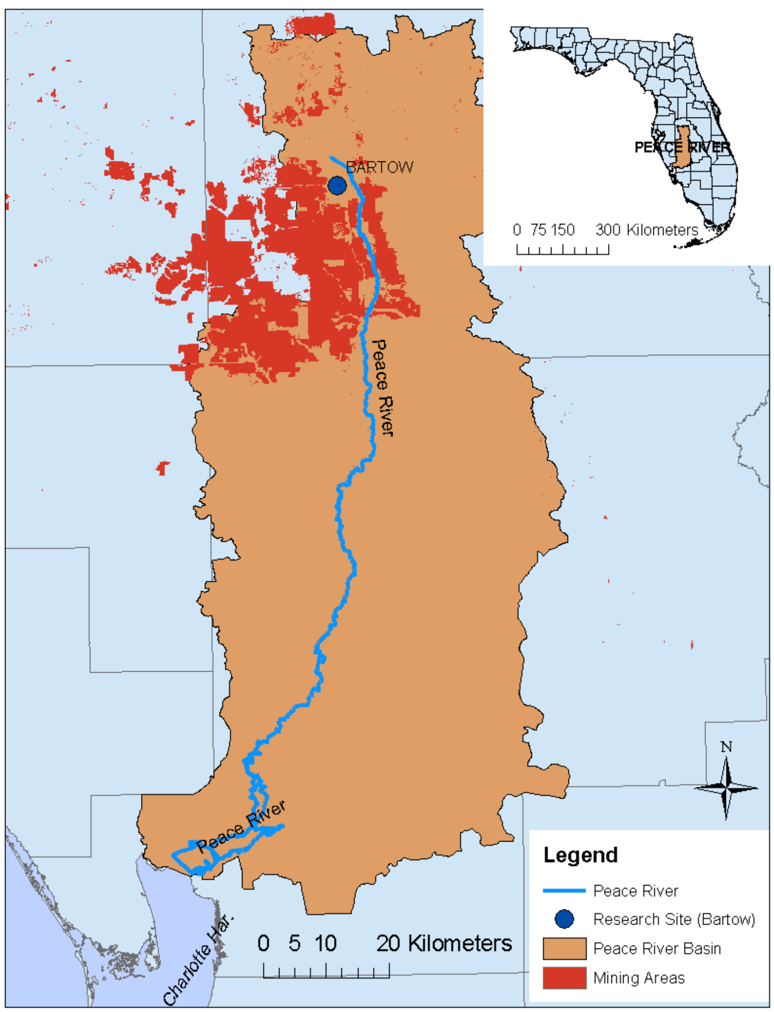

Figure 1. Location of the model application area, phosphate mining region in the Peace River basin, Florida (data from FGDL, 2003).

Table 1. Simulation parameters for the combined VFSMOD-W model (source area UH and grass buffer VFSM components).

No.	Parameter	Units	Description
UH (source area) simulation parameters			
1	P	mm	Design storm precipitation
2	CN	--	NRCS curve number for source area
3	A	ha	Area of upstream portion
4	Storm type	--	NRCS storm type (1 = I, 2 = II, 3 = III, and 4 = Ia)
5	D	h	Storm duration
6	L	m	Length of the source area along the slope
7	Y	m/m	Slope of the source area
8	Soil type	--	USDA texture for source area top soil (label)
9	K	(kg*h)/(m^2*N)	USLE soil erodibility index
10	C	--	USLE cover and management factor
11	Pfact	--	USLE conservation practice factor
VFSM (vegetative filter strip) simulation parameters			
12	FWIDTH	m	Effective flow width of the strip
13	VL	m	Length of the filter (flow direction)
14	RNA	s /m$^{1/3}$	Filter Manning's *n* for each segment
15	SOA	m/m	Filter slope for each segment
16	VKS	m/s	Soil vertical saturated hydraulic conductivity in the VFS
17	SAV	m	Green-Ampt's average suction at wetting front
18	OS	m^3/m^3	Saturated soil water content, θ_s
19	OI	m^3/m^3	Initial soil water content, θ_i
20	SM	m	Maximum surface storage
21	SCHK	--	Relative distance from the upper filter edge where check for ponding conditions is made (i.e., 1 = end, 0.5 = midpoint, and 0 = beginning)
22	SS	cm	Average spacing of grass stems
23	VN	s /cm$^{1/3}$	Filter media (grass) modified Manning's n_m (0.012 for cylindrical media)
24	H	cm	Filter grass height
25	VN2	s /m$^{1/3}$	Bare surface Manning's *n* for sediment inundated area in grass filter
26	DP	cm	Sediment particle size diameter (d_{50})
27	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)

program (UH), that are selectable by the user through the Microsoft Windows graphical user interface (GUI) (Muñoz-Carpena and Parsons, 2005). When no measured VFS input data are available, the UH front-end component can be selected to generate source area inputs for each design storm, including a rainfall hyetograph, a runoff hydrograph, and sediment loss from the source area using a combination of the NRCS curve number, the unit hydrograph, and the modified Universal Soil Loss Equation methods. With these inputs (table 1), a set of response curves, i.e., sediment and runoff reduction vs. filter design/construction characteristics (filter length, width, grass type, slope), can be developed from VFSMOD-W outputs for a given design scenario (Muñoz-Carpena and Parsons, 2004).

In general, the proposed analysis procedure follows six main steps (fig. 2): (1) PDFs are constructed for uncertain input factors; (2) input sets are 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 are executed for each input set; (4) global sensitivity analysis is performed according to the selected method; (5) if the Morris screening method is selected, it results in a subset of important parameters and steps 2 through 4 are repeated only for those important parameters using the extended FAST method; and (6) uncertainty is assessed based on the outputs from the extended FAST simulations by constructing PDFs/CDFs and statistics of calculated errors. Details on the Morris and extended FAST methods are provided in the Appendix.

The software package SimLab v2.2 (Saltelli et al., 2004) was coupled with VFSMOD-W to perform the procedure outlined in figure 2. SimLab's statistical pre-processor module executes step 1 (fig. 2) based on the PDF types and statistics provided (described in the next section) and the analysis method selected (Morris or extended FAST). With this information, the pre-processor produces a matrix of sample inputs to run the model (step 2, fig. 2). An interface program was written in C# (C-sharp language) and added to the VFSMOD-W 4.x GUI to automatically run the model for each new set of sample inputs generated by SimLab. The program automatically substitutes the new parameter set into the VFSMOD-W input files, runs the model, and performs the necessary post-processing tasks to obtain the selected model outputs for the analysis, which are stored in a matrix (step 3, fig. 2). The statistical post-processor module of SimLab uses the input and output matrices to calculate the sensitivity indexes of the Morris and the extended FAST methods (step 4, fig. 2). The Data Analysis Toolpack of Excel (Microsoft Corp., Redmond, Wash.), was used to construct the output probability distributions and to quantify the uncertainty based on the set of extended FAST simulation outputs (step 6, fig. 2).

Selection of Input PDFs and Model Outputs

Input factors of interest in the sensitivity analysis are those that are uncertain, that is, their value lies within a finite interval of non-zero width. Values of common environmental parameters usually depend on the general variability of the application area selected and the scale (size) for which the

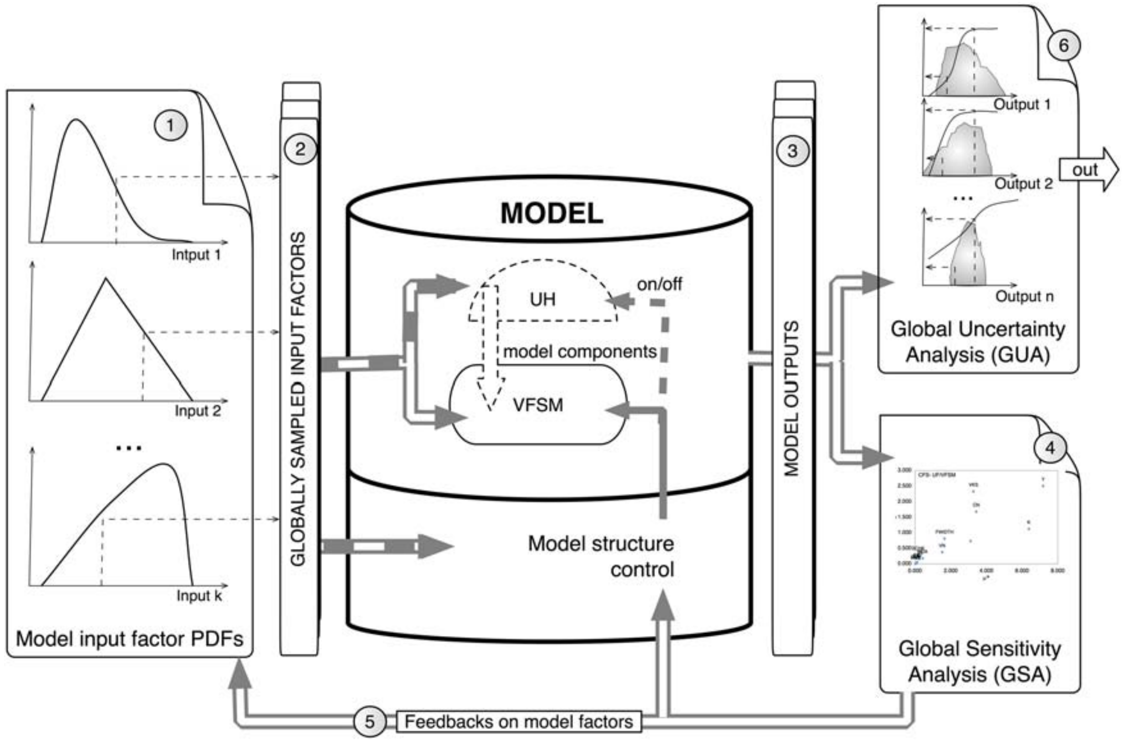

Figure 2. General schematic of the global sensitivity and uncertainty analysis. Numbers in circles represent the steps in the global evaluation procedure explained in the text.

Table 2. Input probability density functions (PDF) for the model inputs used in the global sensitivity and uncertainty analyses of VFSMOD-W.

Parameter	Base Value	PDF	Statistics	Source
P	106.7 (T = 10 years)	Fixed	--	Florida Department of Transportation
CN	87	Triangular	Peak = 87; min. = 75; max. = 94	Calculated on-site
A	0.1	Fixed	--	From field site
Storm type	III	Fixed	--	NRCS for Florida
D	6	Fixed	--	Recommended in area
L	21.1	--	--	NRCS standard runoff plot
Y	0.042	Normal	μ_X = 0.042; σ_X = 0.0104	Measured, n = 86
Soil type	Sand	Fixed	--	Measured on-site
K	0.0326	Triangular	Peak = 0.0326; min. = 0.019; max. = 0.0327	Measured, n = 16
C	1	Fixed	--	Bare surface
Pfact	1	Fixed	--	No conservation
FWIDTH	39	Beta	α = 21.199; β = 5.474; min. = 10; max. = 46	Measured, n = 20
VL	3 and 6	Fixed	--	--
RNA	0.12	Triangular	Peak = 0.12; min. = 0.06; max. = 0.4	--
SOA	0.041	Normal	μ_X = 0.041; σ_X = 0.018	Measured, n = 48
VKS	1.69E-05	Lognormal	μ_Y = -11.14; σ_Y = 0.8	Measured, n = 28
SAV	0.08-0.28	Uniform	Min. = 0.08; max. = 0.28	Measured, n = 28
OS	0.478	Triangular	Peak = 0.477; min. = 0.4; max. = 0.478	Measured, n = 28
OI	0.260	Beta	α = 9.77; β = 4.34; min. = 0.04; max. =0.31	Measured, n = 28
SM	0	Fixed	--	No storage assumed
SCHK	0-1	Uniform	Min. = 0; max. = 1	VFSMOD manual
SS	3.6	Triangular	Peak = 3.6; min. = 3.45; max. = 4.84	Measured, n = 30
VN	0.012	Triangular	Peak = 0.012; min. = 0.0084; max. = 0.016	Haan et al. (1994)
H	18.5	Normal	μ_X = 18.5; σ_X = 2.88	Measured, n = 56
VN2	0.021	Triangular	Peak = 0.021; min. = 0.011; max.= 0.04	Maidment (1992)
DP	0.0012	Triangular	Peak = 0.0012; min. = 0.0009; max. = 0.003	Measured, n = 29
COARSE	0.154	Lognormal	μ_Y = -1.9; σ_Y = 0.78	Measured, n = 29

measurement is expressed (Hillel, 1998). Marginal PDFs can be derived from scientific literature, physical bounds, opinion polls, surveys, expert judgment, and experiments (Saltelli et al, 2005). In general, the means, variances, and ranges of the input parameters have more influence on the output uncertainty than the form of the distribution (Haan at al., 1998), although characteristics like symmetry and skewness may also play a role (Wallach et al., 2006). The field-scale ambient variability of many inputs has been reported to be modeled adequately using log-normal

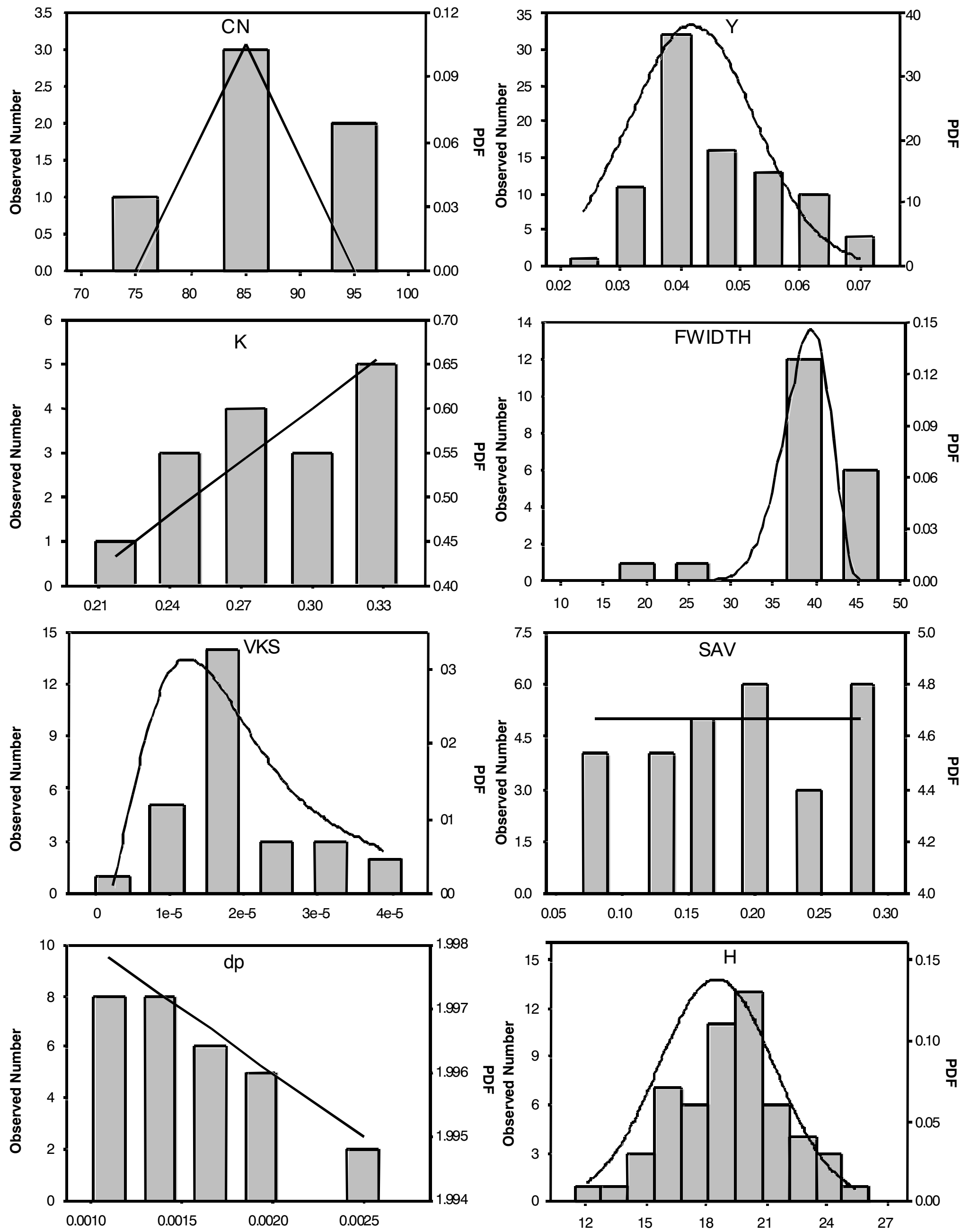

Figure 3. Selected input probability distributions used in the global analyses of VFSMOD-W.

distributions (Haan et al., 1998; Jury et al., 1991; Loáiciga et al., 2006). When there is a lack of data to estimate means and standard deviations for PDFs thought to be Gaussian, the β (beta) distribution can be used (Wyss and Jørgensen, 1998). Finally, when only the range and a base (effective) value are known, a simple triangular distribution can be used, while in the case when values seemed distributed equally along the parametric range, a uniform distribution is recommended.

The input factors of the model (table 1) were assigned ranges and PDFs representative of the application area in Bartow, Florida (table 2). Normal distributions were fitted to parameters with centrally distributed frequencies and a sufficient amount of data available ($n > 30$), such as slope of the source area and filter slope (Y and SOA) and grass height (H) (fig. 3). A log-normal PDF was selected for soil saturated hydraulic conductivity of the filter (VKS) since this distribution is commonly used for this factor (Loáiciga et al., 2006), and it fit the measured data well (fig. 3). The same distribution was also used for the fraction of coarse sediment (COARSE) to match the narrow range of particle size distribution of the soil and sediment from the area (sand > 94%). The beta distribution was used for FWIDTH (effective flow width of the strip) and OI (initial soil water content) to match their smooth but biased (to the right of the mean) distributions (fig. 3). Factors with reduced numbers of measurements, such as parameters related to vegetation [i.e., spacing of grass stems (SS) and grass modified Manning's coefficient (VN)] and soil [i.e., NRCS curve number for source area (CN), USLE soil erodibility index (K), filter Manning's roughness coefficient (RNA), saturated

Table 3. Selected model outputs used in the global sensitivity and uncertainty analyses of VFSMOD-W.

Component	Output	Units	Description
Hydrology			
UH	TRS	mm (depth over source area)	Total runoff from source into filter
VFSM	TRF	mm (depth over source + filter)	Total runoff output from filter
VFSM	TIF	mm (over filter)	Total infiltration in filter
VFSM	RDR	--	Runoff delivery ratio (flow out from filter / flow in)
Sediment transport			
UH	MSS	kg	Mass sediment input from source area
UH	CSS	g/L	Concentration sediment in runoff from source area
VFSM	MSF	kg	Mass sediment output from filter
VFSM	CSF	g/L	Concentration sediment in runoff exiting the filter
VFSM	MSR	kg	Mass sediment retained in filter
VFSM	SDR	--	Sediment delivery ratio (mass out from filter / mass in)
VFSM	EFL	m	Effective filter length
VFSM	WD	m	Sediment wedge distance

soil water content (OS), and sediment particle diameter (DP)], were given triangular PDFs, based on the limited data available. Finally, the user-selectable parameter SCHK (node to check ponding during infiltration calculations) and Green-Ampt suction at the wetting front (SAV) were assigned uniform distributions since no known frequency pattern was identified through their ranges (fig. 3). Parameters such as the filter design lengths (VL), soil textural class (sand), and design storm characteristics (i.e., design storm precipitation-P, NRCS storm type) were fixed for the application. Finally, the remaining factors (C, Pfact, and SM) were fixed to represent the source area worst-case conditions (i.e., bare, non-terraced, and sloping smooth surface).

All input factors were assumed to be independent of each other. In this study, the assumption of orthogonality (parameter independence) is based on the conceptual model characteristics (numerical and mechanistic) and supported by the parameter estimation methods selected, i.e., the parameters were measured directly or estimated independently from applicable literature values. If parameter correlation was identified, it would require generating the samples from joint multivariate probability distributions (Wallach et al., 2006; Iman and Conover, 1982), which is not amenable to simple Monte Carlo evaluation and is computationally expensive (Saltelli et al., 2000b). Finally, in addition to the VFSMOD-W model parameters, the effect of the model structure (VFSM with or without the UH component) on the output uncertainty was also considered in the analysis. In many model applications, the change in user-selectable model structure typically results in a conceptual modification of the model that can have profound impacts on the sensitivity and uncertainty of the model and must be evaluated.

Table 4. Comparison of the number of simulations run for each of the global analyses methods in the application.

Model Structure	VL (m)	Morris NP[a]	Morris Runs	FAST NP[a]	FAST Runs	Total Runs
VFSM	3	14	150	3	4995	5145
UH/VFSM	3	16	170	6	7974	8144
VFSM	6	14	150	3	4995	5145
UH/VFSM	6	16	170	6	7974	8144
Total simulations			640		25938	

[a] NP = number of parameters considered in each analysis.

Several model outputs were selected in the analysis to represent the potential variability of the hydrology and sediment transport components of the model (Muñoz-Carpena et al., 1999) (table 3). Two of these outputs, runoff delivery ratio (RDR) and sediment delivery ratio (SDR), have been proposed as the objective functions for the design of the VFS (Muñoz-Carpena and Parsons, 2004). Although all the selected outputs are presented in the tables and figures below, detailed results are presented only for these two representative outputs (RDR and SDR) in an effort to simplify the discussion.

In summary, four input sample sets were generated for the Morris and FAST methods. Each sample set represented a combination of the two model structures (VFSM or UH/VFSM) and the two design filter lengths studied in the area (VL = 3 m or 6 m). The number of model runs for each method was selected according to the number of uncertain parameters in each model structure based on equations 1 and 4 in the Appendix. The number of simulations needed for each method (table 4) illustrates one of the potential advantages of the Morris method over FAST, i.e., the significantly shorter computation time needed.

Results and Discussion

Global Sensitivity Analysis

Screening Method: The Method of Morris

The ranking of the relative importance of VFSMOD-W input factors, based on the value of Morris' measure μ^*, is presented in table 5 for filter length VL = 6 m. As suggested by Morris, only parameters separated from the origin of the μ^*-σ plane are considered important. Figure 4 shows the graphical representation of the Morris results for a selected subset of model outputs. The number of parameters identified as important was effectively smaller than the full set of the model inputs, i.e., it was reduced from 14 to 3 and from 16 to 6 for the VFSM and UH/VFSM model structures, respectively.

The Morris analysis of VFSM shows a strong influence of the filter's Green-Ampt infiltration parameter (VKS) on the hydrological component of the model. This is illustrated in figure 4 for the RDR output (top of the figure), where only VKS is shown away from the origin on the μ^*-σ plane. Since VKS is not far away from the σ axis, its influence is mostly through first-order effects with a small interaction com-

Table 5. Ranking of sensitive parameters obtained by the method of Morris for a filter length of VL = 6 m.[a]

Model Structure	Output	CN	Y	K	FWIDTH	RNA	SOA	VKS	SAV	OS	OI	SS	VN	VN2	SCHK	COARSE	DP	H
VFSM	TRS				--	--	--	--	--	--	--	--	--	--	--	--	--	--
	TRF				--	--	--	1	--	--	--	--	--	--	--	--	--	--
	TIF				--	--	--	1	--	--	--	--	--	--	--	--	--	--
	RDR				--	--	--	1	--	--	--	--	--	--	--	--	--	--
	MSS				--	--	--	--	--	--	--	--	--	--	--	--	--	--
	CSS				--	--	--	--	--	--	--	--	--	--	--	--	--	--
	MSF				2	--	--	3	--	--	--	--	--	--	--	--	1	--
	CSF				3	--	--	2	--	--	--	--	--	--	--	--	1	--
	MSR				2	--	--	3	--	--	--	--	--	--	--	--	1	--
	SDR				2	--	--	3	--	--	--	--	--	--	--	--	1	--
	EFL				--	--	--	--	--	--	--	--	--	--	--	--	--	--
	WD				--	--	--	--	--	--	--	--	--	--	--	--	--	--
UH/VFSM	TRS	1	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--
	TRF	2	--	--	--	--	--	1	--	--	--	--	--	--	--	--	--	--
	TIF	2	--	--	3	--	--	1	--	--	--	--	--	--	--	--	--	--
	RDR	--	--	--	--	--	--	1	--	--	--	--	--	--	--	--	--	--
	MSS	2	1	3	--	--	--	--	--	--	--	--	--	--	--	--	--	--
	CSS	3	1	2	--	--	--	--	--	--	--	--	--	--	--	--	--	--
	MSF	2	1	3	5	--	--	6	--	--	--	--	--	--	--	--	4	--
	CSF	4	1	3	6	--	--	2	--	--	--	--	--	--	--	--	5	--
	MSR	3	1	2	5	--	--	6	--	--	--	--	--	--	--	--	4	--
	SDR	2	3	4	5	--	--	6	--	--	--	--	--	--	--	--	1	--
	EFL	2	--	--	--	--	1	--	--	--	--	--	4	--	--	--	3	--
	WD	2	--	--	--	--	1	--	--	--	--	--	4	--	--	--	3	--

[a] Numbers for each parameter represent the parameter ranking in decreasing order of importance for each output (1 = most important for that level, and -- = no significant influence). Missing values or symbols indicate that they are not part of the simulation.

ponent. As expected, VKS controls the infiltration (TIF) in the VFS and thus the runoff outputs (RDR and TRF) (table 5). These results are not altered when changing to the UH/VFSM model structure (fig. 4), although the source area CN and the filter effective width (FWIDTH) gain small importance.

In the case of the sediment component, for the VFSM model structure, the main sediment outputs (MSF and SDR) are controlled mainly by DP and, to a smaller extent, by FWIDTH and VKS. In case of the filter outflow sediment concentration (CSF), DP and VKS appear to be the most important of the three. This can be explained by the fact that the sediment concentration is calculated directly from both mass of sediment and water outflow (thus the importance of VKS), where MSF and SDR represent the dry mass of sediment alone. For the UH/VFSM structure, the erosion (Y, K) and runoff (CN) parameters in UH (source area submodel) are the most important for MSF and CFS, followed by the parameters identified for VFSM alone. This ranking changes for SDR, where DP is ranked in the same order of importance as CN and Y (fig. 4 and table 5). The interactions among the important parameters controlling the sediment outputs seem limited (σ values are low in fig. 4). It is interesting to note that when parameters are lumped together in the μ^*-σ plane, but separated form the origin, an element of subjectivity may be introduced into the Morris parameter ranking. This issue is illustrated in figure 4 for CSF-UH/VFSM (parameters VKS, CN, K, and DP) or for SDR-UH/VFSM (parameters DP and CN).

The previously performed local OAT sensitivity analysis of VFSM (Muñoz-Carpena et al., 1999) did not allow for a relative and objective ranking of all model input parameters like that obtained with the Morris method (table 5) because the parameters were varied independently and their ranges and magnitudes of variation were grossly different. In spite of these limitations, the local OAT results showed that among the parameters studied, the main parameters controlling the runoff from the filter were saturated hydraulic conductivity and initial soil water content (VKS and OI). The importance of VKS is corroborated in the Morris results. However, OI was not found important by Morris since the present model application is different from the previously performed local OAT study. The local OAT analysis was intended to be general by varying the input factors within a wide range of conditions (i.e., soils, sediment, and filter characteristics) encountered in the literature and not specific to any particular application area. For the sandy soil conditions of this study, soil infiltration is dominated by the relatively large hydraulic conductivity that outweighs the moisture deficit in the Green-Ampt equation. The local OAT showed that the main parameters controlling sediment outflow were particle class (DP) and the media spacing (SS) (Muñoz-Carpena et al., 1999). The high ranking of DP in current studies is also in agreement with findings of Abu-Zreig (2001) that sediment class is influential for SDR. The lack of influence by SS observed in the Morris results can be explained by the relatively narrow range of this factor measured in the experimental conditions (uniform vegetation types). Abu-Zreig (2001) also identified FWIDTH as an important factor for sediment trapping in VFS. This is confirmed by the Morris analysis that identifies FWIDTH as either the second or third most important parameter for VFSM filter sediment outputs.

Four products of the global sensitivity analysis are illustrated by the initial screening results. First, the ranking of parameters' importance for different model outputs is obtained. Secondly, the effect of the change in model

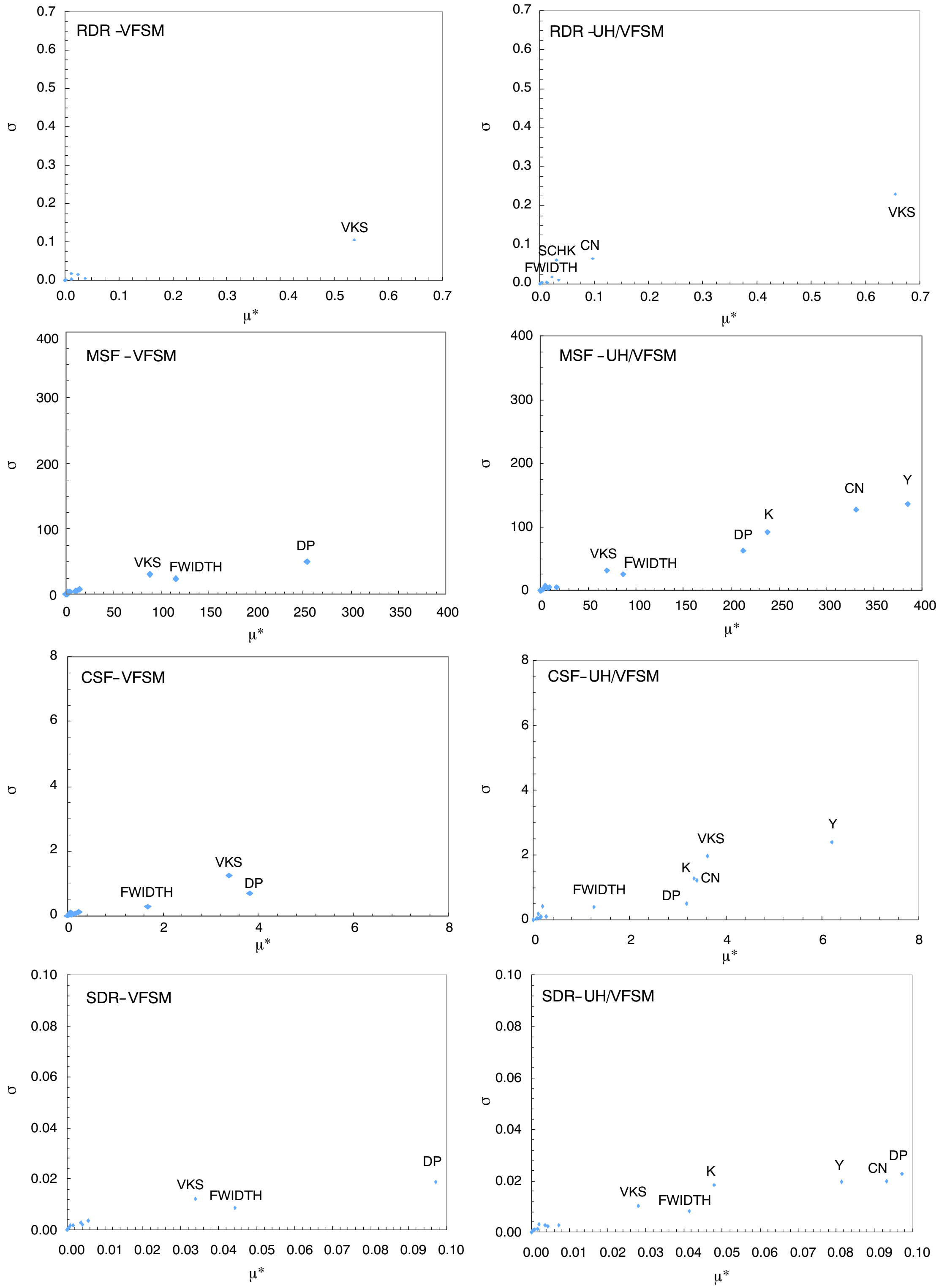

Figure 4. Global sensitivity analysis results for selected VFSMOD-W outputs, obtained from the Morris screening method of VFSMOD-W (VL = 6 m). Labels of input factors close to the origin have been removed for clarity.

structure is identified. It is found to be limited for the hydrology component but strong in the case of the sediment component, where the source area parameters associated with UH take priority over those of the filter. Furthermore, as for most of the parameters, σ is relatively small, and the first-order effects dominate the model response (there are small interactions between factors). Finally, since the relations between factors and model outputs can be explained by the model assumptions, assurance of the model behavior is positively evaluated. When compared to local OAT methods, the results show that the specific conditions of the application typically dominate the importance of some parameters (i.e., OI and SS).

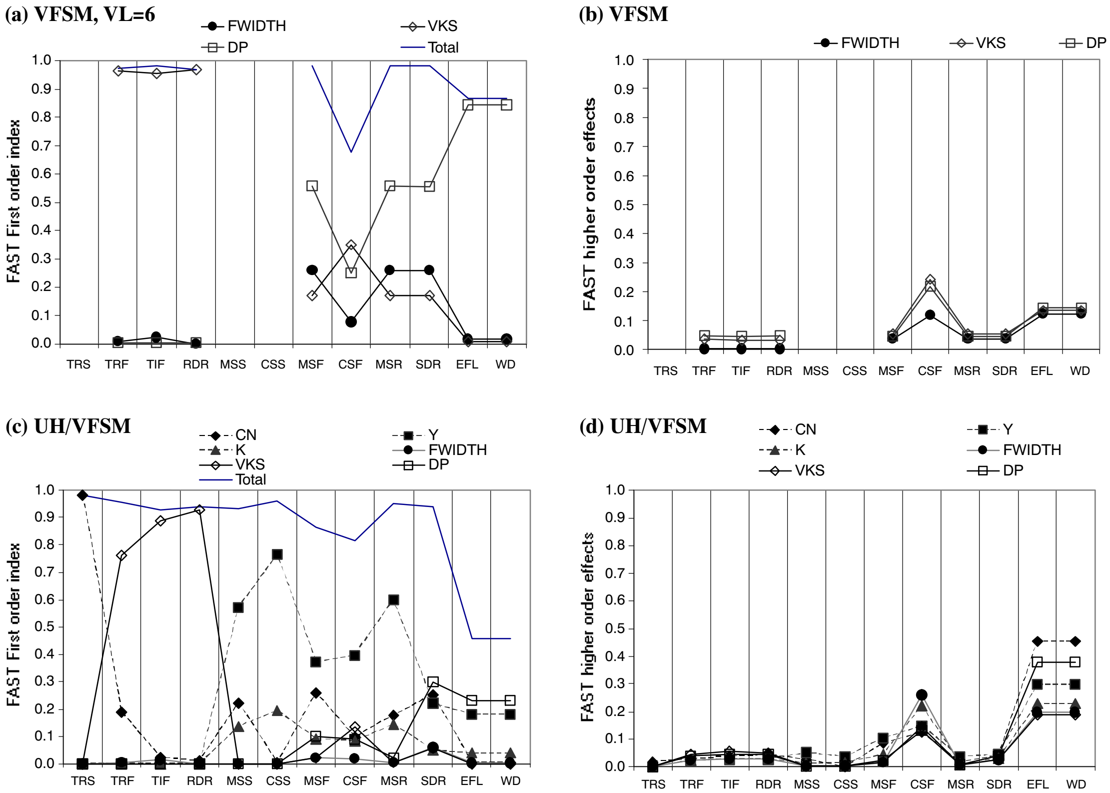

Figure 5. Global sensitivity analysis of VFSMOD-W obtained from the extended FAST method (VL = 6 m): (a and c) first-order effects; (b and d) higher-order effects. Units on the vertical axis are fraction of total output variance.

Variance-Based Method: Extended FAST

The subset of important parameters selected by the screening method for each model combination was used for further analysis with the extended FAST method. These parameters were: VKS, DP, and FWIDTH for the VFSM model structure and, additionally, Y, K, and CN for the UH/VFSM model structure.

Figure 5 presents the results for all the outputs and the filter length of VL = 6 m. This figure depicts the fraction of the total output variance explained by each parameter (vertical axis) for each of the outputs (horizontal axis). The first-order effects (S_i) are presented first for each model structure (fig. 5a,c), followed by the higher-order effects (interactions) (S_i - S_{Ti}) (fig. 5b,d). The extended FAST results obtained reinforce and quantify those from Morris. As an example, the results show that VKS is responsible for 97% and 93% of the RDR variance for VFSM and UH/VFSM, respectively (compare fig. 4, top, and fig. 5a,c). In some cases, FAST eliminates the subjectivity introduced in the qualitative approach of Morris (fig. 4). For the CSF-UH/VFSM output, it is now easy to separate VKS, CN, K, and DP (with 13%, 10%, 8%, and 9% of the variance explained) (fig. 5c). Similarly, FAST results for SDR-UH/VFSM closely match the ranking obtained with the Morris method (compare fig. 4, bottom, and fig. 5c), and allow the quantification of the output variance attributed to DP (30%), CN (25%), Y (23%), FWIDTH (6%), VKS (6%) and K (5%) (fig. 5c). It should be recognized that the extended FAST results are considered more reliable than Morris results, since they are based on a much larger number of simulations (table 4) and a less structured sampling scheme (Saltelli et al., 2004).

The sum of the total effects (ΣS_i) is graphically presented for both model structures by a solid line in figures 5a and 5c. In general, the sum of first-order effects is greater than 80% of the total variance for most outputs for both model structures, with the exception of the sediment concentration from the filter and the sediment wedge dimensions EFL and WD (fig. 5a,c). The interaction found for CSF can be explained by the fact that the value is the ratio between mass of sediment and water outflow, i.e. closely depends on the important parameters behind these quantities (fig. 5b,d). Since in general the sum of the total effects is close to 100%, the model behaves as additive. This indicates that VFSMOD-W could be efficiently calibrated if reliable data are provided.

Global Uncertainty Analysis from Extended FAST Results

Uncertainty analysis statistics for the selected output probability distributions obtained from extended FAST results are presented in table 6. Following Morgan and Henrion (1992), to communicate uncertainty graphically to end users, the density and cumulative probability distributions (CDFs) are constructed for the selected outputs and both model structures (fig. 6). Another method recommended by these authors, the 95% confidence interval (i.e., range of output values between 2.5% and 97.5% cumulative distribution percentiles), can also be calculated on the basis of these distributions (table 6). Example uncertainty analysis statistics for the sediment delivery ratio obtained from FAST results are presented in figure 6. The difference between CDFs for VFSM and UH/VFSM illustrates the relative effects of model structure on output uncertainties. Generally, larger output variances are observed

Table 6. Uncertainty analysis statistics for selected output probability distributions obtained from FAST results.[a]

Output[b]	Length	Components	Range	Mean	Median	95% CI	SD	SE	Min.	Q1	Q2	Q3	Max.	Skew	Kurtosis
RDR	3	VFSM	0.762	0.916	0.943	0.635-1.065	0.114	0.002	0.337	0.863	0.943	0.998	1.099	-1.213	1.722
		UH/VFSM	0.917	0.924	0.954	0.610-1.083	0.123	0.001	0.220	0.867	0.954	1.009	1.137	-1.380	2.515
	6	VFSM	1.173	0.858	0.903	0.388-1.130	0.197	0.003	0.025	0.759	0.903	0.999	1.198	-0.991	0.847
		UH/VFSM	1.276	0.873	0.922	0.346-1.167	0.214	0.002	0.000	0.763	0.922	1.022	1.276	-1.064	1.071
MSF	3	VFSM	876.6	1025.5	1014.9	834.1-1283.4	117.4	1.7	713.6	940.6	1014.9	1096.8	1590.2	0.6	0.5
		UH/VFSM	2682.6	740.0	675.2	176.6-1678.2	397.4	4.5	48.8	442.1	675.2	962.0	2731.4	1.0	1.2
	6	VFSM	928.3	486.7	474.4	306.7-734.9	109.5	1.5	118.3	408.8	474.4	552.5	1046.6	0.6	0.8
		UH/VFSM	1729.3	346.0	295.7	66.59-904.9	223.3	2.5	0.0	180.7	295.7	451.8	1729.3	1.4	2.8
CSF	3	VFSM	26.520	15.729	15.376	12.13-21.47	2.460	0.035	10.755	14.008	15.376	16.972	37.275	1.362	4.436
		UH/VFSM	42.628	11.646	10.803	3.07-25.47	5.756	0.064	0.836	7.439	10.803	14.786	43.464	0.915	1.110
	6	VFSM	62.061	8.290	7.789	5.02-14.32	2.881	0.041	4.153	6.579	7.789	9.310	66.214	5.504	75.212
		UH/VFSM	83.340	6.007	5.136	1.21-16.07	4.072	0.046	0.000	3.359	5.136	7.624	83.340	3.259	32.137
SDR	3	VFSM	0.335	0.392	0.388	0.319-0.492	0.045	0.001	0.273	0.360	0.388	0.420	0.608	0.576	0.458
		UH/VFSM	0.547	0.324	0.324	0.158-0.495	0.088	0.001	0.069	0.261	0.324	0.385	0.616	0.057	-0.387
	6	VFSM	0.355	0.186	0.182	0.117-0.281	0.042	0.001	0.045	0.156	0.182	0.211	0.400	0.600	0.761
		UH/VFSM	0.401	0.149	0.143	0.055-0.276	0.058	0.001	0.000	0.106	0.143	0.185	0.401	0.523	0.106

[a] 95% CI = 95% confidence interval (i.e., range of output values between 2.5% and 97.5% cumulative distribution percentiles); SD = standard deviation; SE = standard error of the mean; Q1, Q2, Q3 = 1st, 2nd, and 3rd quartiles of the output probability distribution.

[b] See table 3 for output descriptions.

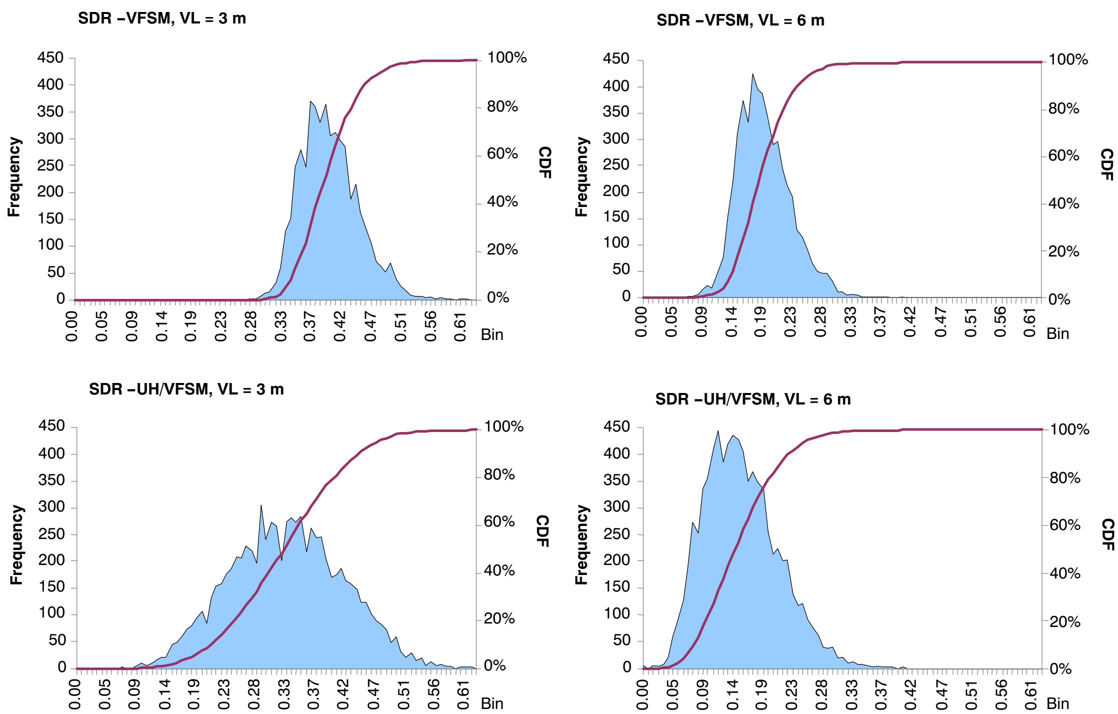

Figure 6. Global uncertainty results for selected VFSMOD-W outputs obtained by extended FAST (VL = 6 m). Left vertical axis units indicate the output probability density distribution (frequency) and the right vertical axis the cumulative probability distribution (CDF).

for UH/VFSM, which is expected, since additional variance is introduced by the larger number of uncertain parameters. The filter length does not systematically affect the ranges of the output PDFs.

The uncertainty of the results can also be communicated as probability of exceedance of a desired regulatory or design value. For example, if a 75% reduction of runoff sediment (SDR $\leq$ 0.25) is desired for the 10-year design storm in the area, then the results in table 6 and figure 6 indicate that, for the 6 m filter, the probability of SDR > 0.25 will be approximately 5% for the combined model (UH/VFSM) and 7% for simpler model structure (VFSM). Therefore, it may be concluded that, depending on model structure, the 6 m filter will perform as desired in, respectively, 95% and 93% of the time (acceptable at the 90% level). In the case of the 3 m filter, the filter will only performs as expected less than 25% of the time for both model structures, which indicates that this filter does not meet the design criteria in the area of application.

The uncertainty analysis performed with the extended FAST outputs proved to be very efficient when compared to a classical MCS approach. Previously, Shirmohammadi et al. (2006) showed that the number of VFSMOD simulations needed to obtain smooth output PDFs for each parameter was around 2000. In this study, around 5000 to 8000 simulations were sufficient to obtain a global assessment of the model for all sensitive parameters (3 to 6 parameters). The reduced number of simulations is due to the efficiencies built into the Extended FAST evaluation procedure. Firstly, sampling of PDFs of input factors is based on the more efficient r-LHS, so a reduced number of simulations are required compared to the fully randomized-sampling of MCS. Secondly, because in the proposed framework, the extended FAST focuses on the subset of important parameters identified by the Morris method, the number of simulations to obtain a global uncertainty assessment is reduced. . The uncertainty analysis based on the extended FAST results also proved to be superior when compared to the local First-Order-Approximation method, since FAST does not require previous knowledge about the additivity of the model or the form of the model output probability distributions.

Summary and Conclusions

An advanced model evaluation framework is applied to VFSMOD-W that combines two types of global sensitivity (screening method of Morris and variance-based extended FAST) and one uncertainty (based on extended FAST results) analysis techniques. The Morris method allows for qualitative ranking of the important model parameters and their potential interactions at a relatively small computational cost. The extended FAST uses the subset of important input factors identified by Morris to provide the quantitative measures of sensitivity in terms of each parameter's contribution to the output variance and higher-order effects (interactions) for specific outputs. Since the extended FAST is based on randomized sampling of the multivariate input distribution, the outputs from the analysis can be used to construct output probability distribution functions suitable for uncertainty analysis. The main outputs of interest in the analysis were runoff and sediment delivery ratios (RDR and SDR), which are commonly used as objective functions in filter design. Consideration to the change in model structure changes was given in the analyses by simultaneously evaluating two user-defined model structures: the filter module alone (VFSM) and the source area and filter components combined (UH/VFSM).

In contrast to previously performed local OAT sensitivity analysis, the method of Morris was able to provide a ranking of the significant parameters for a variety of outputs and to identify interactions between parameters. For the simpler model structure (VFSM), VKS was identified as the important parameter controlling RDR, whereas the order of importance with respect to SDR was DP > FWIDTH > VKS. For the combined UH/VFSM model structure, the ranking of importance remained the same for runoff outputs but changed for sediment, where the order of importance was Y > CN > K. In contrast with previously performed local OAT analyses, SS (average spacing of grass stems) and initial soil water content (OI) were not found to be important, probably due to the narrow range of values measured in the region of application (sand and homogeneous filter vegetation). The extended FAST results reinforced and quantified those of Morris and indicated the additive nature of the model (sum of first-order effects, $S_i > 0.8$ for RDR and SDR). This model characteristic can lead to its effective calibration if reliable input data are available.

As expected, the predicted model uncertainty was higher for UH/VFSM than for VFSM, since more uncertain inputs were used in the combined model. Performance of global uncertainty techniques (for filters of 3 and 6 m in length) enabled evaluation of filter length (VL) as a VFS design criteria. Under the conditions of the study, the 6 m filter would trap at least 75% of incoming sediment approximately 93% and 95% of the time for UH/VFSM and VFSM model structures, respectively. For the alternative 3 m filter, the required sediment trapping efficiency would be achieved less than 25% of the time (unacceptable at the 90% level). Given the prior information on the characteristics of the VFSMOD-W input factors in the application region, it is advised to construct 6 m filters if these design criteria are to be met. These results also indicate that the uncertainty of the model outputs could be reduced due to more accurate measurements or estimates of input factors identified as important (i.e., VKS in the case of RDR). The uncertainty analysis performed with the extended FAST outputs proved to be very efficient when compared to a classical Monte Carlo Simulation approach, with a 33% reduction in the number of simulations needed. The uncertainty analysis based on the extended FAST results also proved to be superior when compared to the local First-Order-Approximation method since no previous knowledge of the additivity of the model or the form of the model output probability distributions is needed.

The results obtained are particular to the specific application (reclaimed phosphate-mining areas of the Peace River basin). Since different input parameter ranges can significantly affect the sensitivity and uncertainty results, it is recommended that these analyses are performed for each particular model application. Although no evaluation method can be considered objective, since it relies on the interpretation by the modeler of the input variation, the model evaluation framework applied here is found reproducible and robust, since it considers concurrent variation of all the input factors without *a priori* judgment of their relative importance over the output.

Acknowledgements

The authors wish to thank Lukasz Ziemba, Stuart Muller, Jayantha Obeysekera, Rich Sands, and Wendy Graham for their support of this project, and Jesus Carrera (CSIC-Barcelona) and David Kaplan for the attentive review of the manuscript. Funding for this project was obtained from South Florida Water Management (PO No. 4500005607) and Florida Water Resources Center. Partial support was received from the University of Florida IFAS, Dean of Research, Graduate Assistantship Matching Program.

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Appendix: Global Sensitivity Methods

The Method of Morris

The screening method proposed by Morris (1991) (herein "Morris method" or "Morris") and later modified by Campolongo et al. (2005) 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., 2005). 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. (2005) 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 results as:

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

where r is the sampling size for 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., 2005). 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(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

A variance-based method like the Fourier Amplitude Sensitivity Test (FAST) can be used to obtain a quantitative measure of sensitivity (Cukier et al., 1973, 1978; Koda et al., 1979). FAST decomposes the total variance ($V = \sigma_Y^2$) of the model output $Y = f(\overline{X}_1, \overline{X}_2, ..., \overline{X}_k)$ in terms of the individual factors X_i, using spectral analysis so that:

$$V = \sigma_Y^2 = V_1 + V_2 + V_3 + ... + V_k + R \tag{2}$$

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, i.e.:

$$S_i = V_i \,/\, V \tag{3}$$

To calculate S_i, the FAST technique randomly samples the k-dimensional space of the input parameters using the replicated Latin hypercube sampling (r-LHS) design (McKay et al., 1979; McKay 1995). The number of evaluations required in the analysis can be expressed as:

$$N = M(k + 2) \tag{4}$$

where M is a number between 500 and 1000.

For a perfectly additive model, $\Sigma S_i = 1$, i.e., no interactions are present and total output variance is explained as a summation of the individual variances introduced by varying each parameter alone. In general, models are not perfectly additive, and $\Sigma S_i < 1$. FAST was extended by Saltelli et al. (1999) to incorporate the calculation of 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. For example, for $\overline{X}_1$:

$$S_{T1} = S_1 + S_{1i} + S_{1jk}, + ... + S_{1...n}$$

and then

$$S_{T1} - S_1 = S_{1i} + S_{1jk}, + ... + S_{1...n} \tag{5}$$

For a given parameter X_i, interactions can be isolated by calculating $S_{Ti} - S_i$, which makes the extended FAST 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.