Chapter 17

Comparison of Models for Estimating the Removal of Pesticides by Vegetated Filter Strips

Michael F. Winchell,*,[1] Russell L. Jones,[2] and Tammara L. Estes[1]

[1]Stone Environmental, 535 Stone Cutters Way, Montpelier, VT 05602, USA
[2]Bayer CropScience, 17745 South Metcalf, Stilwell, KS 66085, USA
***mwinchell@stone-env.com**

Vegetated filter strips (VFSs) established at the downslope edge of agricultural fields have long been recommended as a management practice to reduce sediment, nutrients, and pesticides in surface runoff before it enters water bodies. Recently VFSs have been mandated as label requirements for plant protection products in Europe and North America. Several simulation models have been developed to predict the amount of pesticide active ingredients and their metabolites removed from runoff flowing through these strips. Removal efficiency is a function of several parameters and must be predicted on an event basis. The predictions of four simulation models (APEX, PRZM-BUFF, REMM, and VFSMOD) were compared using three data sets. Conditions simulated included a range of soil properties, slopes, rainfall events, and pesticide characteristics. All four models predicted reductions of pesticides in the VSFs consistent with the observed reductions, with VFSMOD simulations in closest agreement with the measured data across the three data sets.

Introduction

Use of VFSs as agricultural best management practices (BMPs) has gained in popularity over the past 15 years, in part due to the National Conservation Buffer Initiative of the US Department of Agriculture, Natural Resources Conservation Service (NRCS) (*1*). Increasingly, of VFSs use is recommended or required on pesticide labels as a mitigation measure to reduce pesticide runoff. In order to

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estimate the effectiveness of VFSs, one of two approaches is generally employed. The first involves designing and conducting field experiments to assess VFS effectiveness in reducing pesticide mass transport at the field edge. The second approach involves use of simulation models to evaluate buffer system efficacy in removing pesticides from runoff. Recent reviews of field studies have shown that a wide range in VFS effectiveness has been observed in the field (*2–4*), making it difficult to generalize their effectiveness. Furthermore, the characteristics of a VSF that affect pesticide removal efficiency have been shown to be more complex than simply buffer width (*5*), as has been the current approach until recently.

An unpublished report (*6*) reviewed five currently available simulation models for evaluating VFS effectiveness in reducing pesticide runoff from treated agricultural fields. This chapter reports on a follow-up study designed to compare the performance of four of these models using three different datasets (additional details of the study are provided in an unpublished report available upon request (*7*)).

Materials and Methods

Models Evaluated

APEX (*8*) is a farm/small watershed scale model for simulating the effects of agricultural management practices on water quality and agricultural productivity. It is a physically-based, continuous, distributed parameter model which can be used to model up to 4,000 distinct and hydrologically connected "subareas." The APEX model can be obtained from http://www.brc.tamus.edu/simulation-models/epic-and-apex.aspx.

PRZM-BUFF is a modified version of the field scale model PRZM used to evaluate the effectiveness of VFSs and unmanaged buffers in reducing pesticide runoff, erosion, and spray drift to downstream areas. PRZM-BUFF, is configured as a run-off / run-on model with main field water and chemical mass from runoff and erosion input as boundary condition inflows into adjacent untreated areas. Multiple PRZM simulations are performed to simulate various portions of the field and surrounding areas. Requests for the model can be made at http://www.waterborne-env.com/.

REMM (*9*) is a field scale model for evaluating the movement of water, sediment, and nutrients in riparian zones adjacent to agricultural fields and includes subsurface lateral flow and ground water in addition to overland runoff. REMM was modified in 2008 to include simulation of pesticide behavior. A preliminary version was used in this study. Inquiries about the model and its current status can be made by contacting Randy Williams (randy.williams@ars.usda.gov) or R. Richard Lowrance (Richard.lowrance@ars.usda.gov).

VSFMOD links a field-scale, storm-based numerical simulation model (*10*) with a pesticide trapping equation (*4*). The model is capable of simulating runoff and infiltration of water, sediment transport, and pesticide trapping through VFSs. The software, users manual, and associated publications can be obtained from the author R. Munoz-Carpena at http://carpena.ifas.ufl.edu/VFSMOD.

Study Site Descriptions

Three data sets, one from Europe and the other two from North America, were used for the comparison of model predictions. The study sites differed in soil, topographic, and climatic characteristics. Environmental fate properties of the four pesticides investigated also varied widely (see Table I). The study sites and buffer characteristics are described in the following sections and in Table II.

Table I. Pesticide Properties at Each Study Site

Study Site	*Pesticide*	*Koc (mL g^{-1})*	*Half-Life (days)*
Gibbs Farm	Alachlor[a]	54	30
Velbert- Neviges	Pendimethalin[b]	12,500	97
Sioux County	Atrazine[c]	171	61
Sioux County	Chlorpyrifos[a]	9,930	30.5

[a] Source: (*11*). [b] Source: (*12*). [c] Source: (*13*).

The Gibbs Farm data set was obtained during field studies near Tifton, Georgia (*14*, *15*). A grassed VFS located at the endge of the farm field was 8 m wide (field to buffer area ratio of 11.5). Inputs and outputs to the VFS were monitored continuously for three years from 1992 through 1994. For model comparison described in this chapter, the model PRZM was used to simulate the loadings of runoff, sediment, and pesticide coming from the adjacent field into the VFS. PRZM was parameterized using the known field characteristics and pesticide application dates and rates for each year. Reductions in runoff, sediment and pesticide (alachlor, a compound weakly to moderately sorbed to soil) through the buffer were measured over the period from 1992 through 1994. The annual averages of these reductions (as a percent of the fluxes entering the buffer) were compared with the results each each of the VFS models.

Velbert-Neviges is a data set generated in North Rhine-Westphalia, Germany (*12*). The VFS was a three meter wide grass buffer strip (field to buffer area ratio of 2.3) on a silty loam soil with a 10% slope. The plot draining to the VFS received simulated rainfall representing six events spread over two years (1998 and 1999). The size of the rainfall events ranges from 60 mm to 71 mm, and occurred between 3 and 23 days after pesticide application. In each of these events, the buffer also received simulated rainfall. The reduction in runoff, sediment, and pendimethalin, a compound highly sorbed to soil, was simulated by each of the models and compared with the reductions observed in the field for each event.

Table II. Buffer Characteristics at Each Study Site

			Sioux County, Iowa[e]			
Parameter	*Gibbs Farm*	*Velbert- Neviges*	*Treatment 1*	*Treatment 2*	*Treatment 3*	*Treatment 4*
Treated Area (m^2)	11,000	10.5 (15)[c]	N/A	N/A	N/A	N/A
Buffer Width[a] (m)	8	3	4.6	4.6	4.6	4.6
Buffer Length[b] (m)	120	1.5	4.6	4.6	0.46	0.46
Buffer Slope (%)	2.5	10	5.25	5.25	5.25	5.25
Effective Field to Buffer Area Ratio	11.46	2.33[d]	15	30	150	300
Buffer Vegetation Type	Bermuda grass	Pasture grass mix	Brome grass / bluegrass	Brome grass / bluegrass	Brome grass / bluegrass	Brome grass / bluegrass
Soil	Loamy sand	Silty loam	Silty clay loam	Silty clay loam	Silty clay loam	Silty clay loam

[a] Distance parallel to slope. [b] Distance perpendicular to slope. [c] Area was 15 m^2 for 1 event. [d] Ratio was 3.33 for 1 event [e] No treated area; synthetic run-on matrix was applied directly to buffer)

Sioux County is a data set from a study conducted in the northwest corner of Iowa (*16*). The 12 VFSs were 4.6 m in length (simulated field to buffer ratios of 15 and 30 were tested) and were on a silty clay loam soil with a 5% slope. Flow uniformity was investigated by applying a simulated runoff matrix (water, sediment, and pesticide) to 100% of the plot area (uniform) or to only 10% of the plot area (concentrated). In each of these events, the VFS itself received simulated rainfall. The pesticides evaluated at the Sioux County site were atrazine (a compound with moderate sorption to soil) and chlorpyrifos (a compound fairly strongly sorbed to soil but less so than pendimethalin).

Parameterization and Conduct of Simulations

Uncalibrated simulations using best estimates of model parameters were conducted. Models were parameterized, using as consistent values as possible, while considering that each model has somewhat different requirements and recommendations for implementation. The inputs and outputs from the VFSs at each of the study sites used for comparison between observed and simulated represented the total runoff, sediment, and pesticide loads.

For the Sioux County site, sensitivity of predicted reductions in runoff, sediment, and pesticide to changes in a few key input parameters was evaluated. Included in this analysis were saturated hydraulic conductivity (the curve number was substituted for PRZM), Manning's N, and the antecedent soil moisture.

Results and Discussion

Gibbs Farm

Simulations were continuous from 1992 through 1994. Total runoff reductions and sediment were evaluated for 1993 and 1994 only. Of the four models, VFSMOD provided the closest agreement to the observed values in both years (runoff reduction differences of +2% and -31% in 1994 and 1994 respectively), followed by APEX, PRZM-BUFF, and REMM. Observed reductions in sediment were low in 1993 compared to all model predictions and the observed reductions in 1994. In the later year, all four models predicted a reduction of sediment within 10% of the observed value. The comparisons of simulated versus observed reductions in alachlor are shown in Figure 1. The "percent reduction" was calculated as shown in equation 1.

$$PctRed = 100 * [1 - (PestOut / PestIn)] \qquad \text{Eqn. 1}$$

where, PctRed = percent reduction in buffer (%)
PestOut = pesticide leaving buffer (mass)
PestIn = pesticide entering buffer (mass)

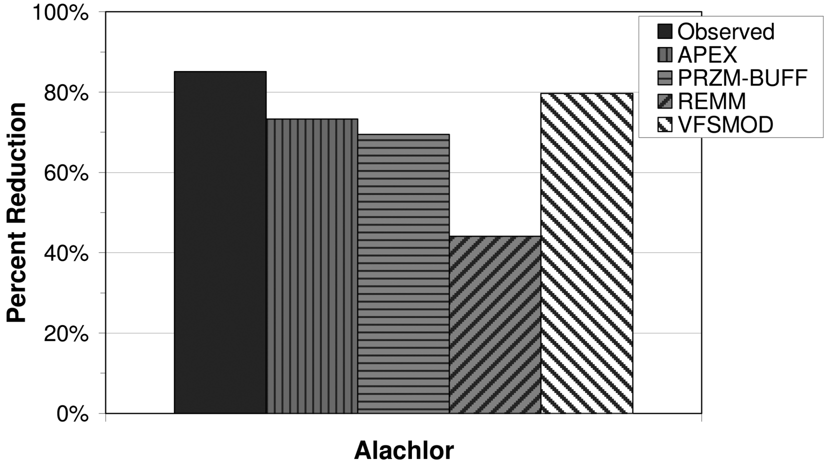

Figure 1. Total Alachlor Mass Reduction, 1992-1994, at Gibbs Farm.

The observed total reduction in alachlor mass over the three-year period was approximately 85%. The model simulations of alachlor reductions with VFSMOD were closer to the observed data than the other three models (5% less than observed). APEX and PRZM-BUFF showed greater deviations from the observed reductions, predicting reductions of 12% and 16% less than the observed value respectively. REMM prediction of alachlor reduction was 41% lower than the observed value.

Velbert-Neviges

The model simulations evaluated six events during the two year period with simulated reductions in runoff, sediment, and pesticide (pendimethalin) compared to the observed results (*12*). Simulated versus observed reductions for pendimethalin are shown in Figure 2. A comparison of predicted versus observed expressed as mean absolute error (absolute value of predicted minus observed) in runoff, sediment, and pendimethalin is shown in Figure 3. The calculation of mean absolute error is shown in equation 2.

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|obs_i - sim_i| \qquad \text{Eqn. 2}$$

where, MAE = mean absolute error
obs_i= ith observed buffer reduction (%)
sim_i = ith simulated buffer reduction (%)

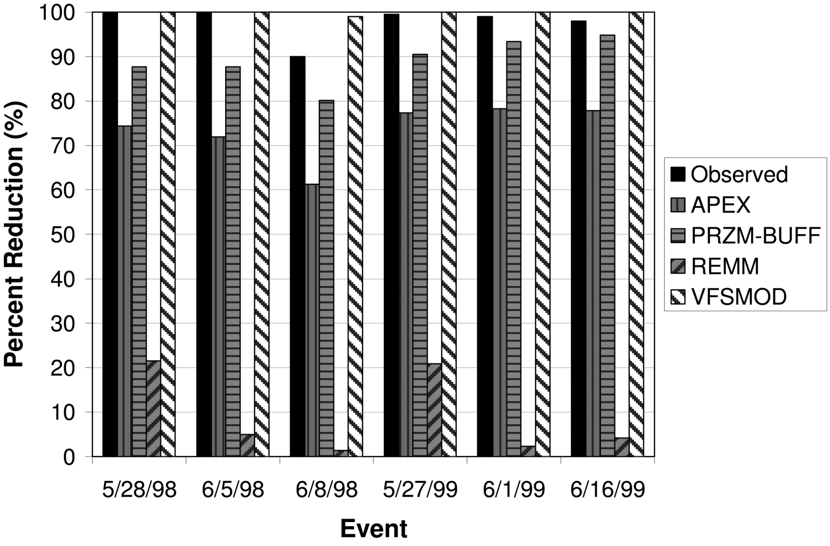

Figure 2. Total Pendimethalin Mass Reduction over the six Velbert-Nevige Events.

The observed runoff reduction at Velbert-Neviges was high, greater than 95% for all but one of the six events. For all six events, VFSMOD was closest to the observed runoff reduction, often within 5% (Figure 3). APEX, PRZM-BUFF, and REMM under-predicted the runoff reduction, by 40% or more. Observed sediment reductions in the buffer were greater than 90% for all six events. All four models performed well in predicting the sediment reduction, generally within 15% of the observed reductions (Figure 3). The observed pendimethalin reductions (Figure 2) were all greater than 90%, showing strong similarity to sediment behavior. This is not surprising given pendimethalin's high sorption coefficient and tendency for sediment-sorbed transport. The VFSMOD simulations were generally closest to the observed pendimethalin reductions, followed by PRZM-BUFF, APEX, and then REMM (Figure 3). The low percent differences (between observed and simulated) in runoff, sediment, and pendimethalin reductions obtained using VFSMOD can be in part attributed to VFSMOD's method for calculating pesticide reduction as a function of infiltration and sediment trapping within the buffer (along with several other factors). The reductions predicted by REMM were lower than the other three models, and did not follow the high sediment reductions that REMM predicted. This behavior was not expected and the reason for it could not be determined.

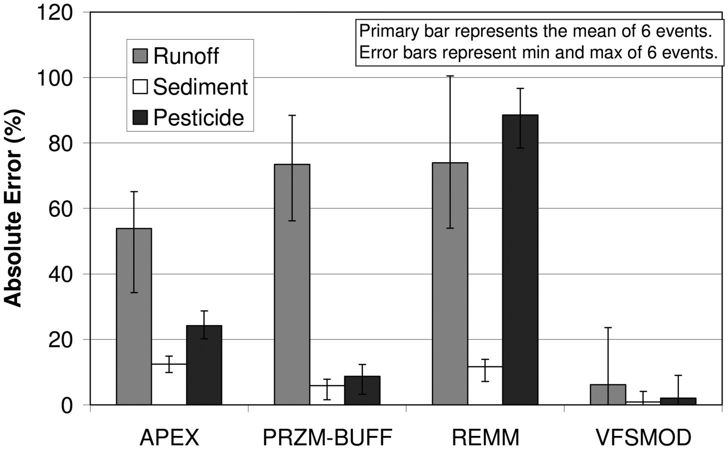

Figure 3. Mean Absolute Error in Buffer Reductions over the six Velbert-Neviges Events.

Sioux County, Iowa

Simulations evaluated four different scenarios, three replicates each, totaling 12 runoff events. The models were run in an event-based mode for each of the 12 events with assumed antecedent soil moisture equal to half the soil field capacity. Simulated reductions in runoff, sediment, and two pesticides, atrazine and chlorpyrifos (with contrasting soil adsorption behavior), were compared with the observed results (*16*). The comparisons of simulated versus observed reductions in atrazine, and chlorpyrifos are shown in Figures 4 and 5, respectively. A comparison of predicted versus observed expressed as mean absolute error in runoff, sediment, atrazine, and chlorpyrifos is shown in Figure 6.

In these simulations, APEX consistently over-predicted the amount of runoff reduction in the buffer, while the other three models tended to under-predict runoff reduction. Reductions in runoff were higher for sheet flow conditions than for concentrated flow conditions. Sheet flow was characterized by uniform shallow flow across a VFS, while concentrated flow was characterized by uneven flow depth across a VFS buffer, some sections with deeper and faster flow and some sections with shallower slower flow.

Trends for sediment reduction were not as clear as for runoff. VFSMOD results were closest to the observations for the sheet flow conditions, while APEX was closest to the observations for the concentrated flow conditions. REMM generally under-predicted the sediment reduction by the VFS. PRZM-BUFF always predicted 100% reduction in sediment. This behavior was attributed to its simplified treatment of sediment processes.

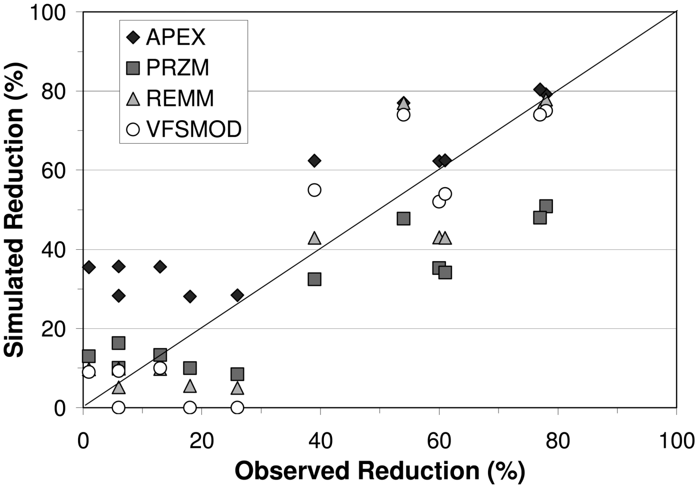

Figure 4. Total Atrazine Reduction in the 12 Sioux County Plots. (Sheet flow conditions area represented by the data points for each model with higher observed reductions (> 40%) while the concentrated flow conditions are represented by the data points for each model with lower observed reductions (< 30%).)

Atrazine simulations followed a similar pattern to the runoff simulations. This was expected since the compound is weakly sorbed by sediment and tends to dissolve in runoff. Three of the four models did well at predicting atrazine reductions for the sheet flow conditions (data points further from the origin in Figure 4), with PRZM-BUFF tending to under-predict the amount of reduction. Under concentrated flow conditions (data points nearer the origin), APEX indicated higher atrazine reduction under concentrated flow conditions compared to the predictions of other models as well as the experimental data. Overall, REMM performed slightly better than all the other models for total atrazine reduction.

For chlorpyrifos reduction (Figure 5) VFSMOD had the closest agreement with the observations (slightly better than APEX), with a tendency to under-predict the amount of pesticide reduction (summary statistics of model performance are presented in Table IV). APEX provided the closest estimate to measured values of the four models for concentrated flow conditions, but under-predicted the reductions under sheet flow conditions. REMM consistently under-predicted the reduction for both flow regimes, while PRZM-BUFF had a tendency to over-predict the reductions for the concentrated flow and under-predict the reductions for the sheet flow conditions.

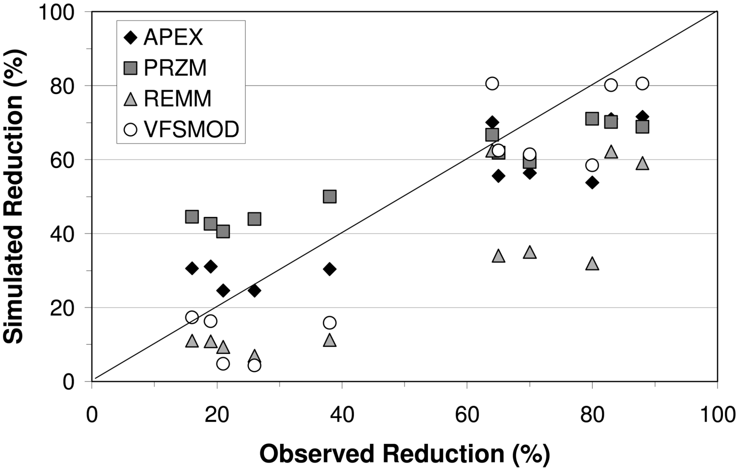

Figure 5. Total Chlorpyrifos Reduction in the 12 Sioux County Plots.)Sheet flow conditions area represented by the data points for each model with higher observed reductions (> 60%) while the concentrated flow conditions are represented by the data points for each model with lower observed reductions (< 40%).)

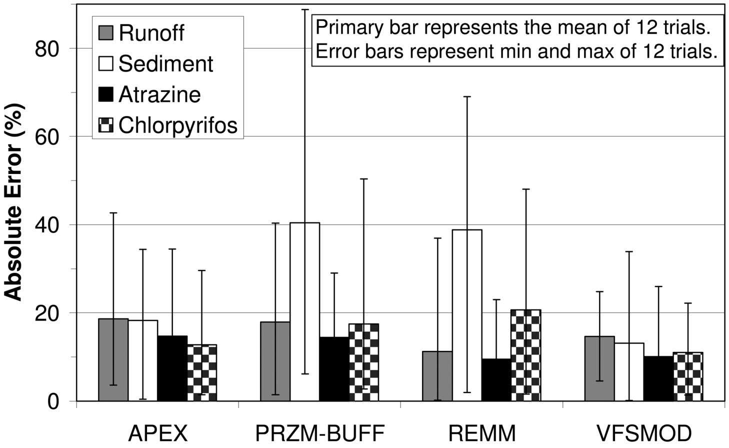

Figure 6. Mean Absolute Error in Buffer Reductions in the 12 Sioux County Plots.

Parameter distributions sampled for the limited sensitivity analysis are shown in Table III. Results showed that VFS reductions in runoff, sediment, atrazine, and chlorpyrifos were sensitive to changes in saturated hydraulic conductivity (or curve number with PRZM), with APEX being the most sensitive. All models showed little sensitivity to changes in Manning's N value, with only APEX showing any sensitivity to Manning's N. Sensitivity to initial soil moisture was negligible for APEX and low for the other models. Likely, this was due to the fact that by the time surface runoff enters a VFS the VFS surface soil will be close to saturation as a result of the rainfall, minimizing the importance of the soil moisture prior to the start of the rainfall event. However, antecedent soil moisture will still be important in determining the magnitude of a runoff event, and hence, the potential for pesticide mass to move off-field and into the VFS. These results highlight the importance of appropriately parameterizing the infiltration components of these models, as infiltration not only affects soluble pesticide reductions in the buffer, but also sediment deposition processes and sorbed pesticide reductions.

Table III. Model Sensitivity Analysis Parameter Distributions

Distribution Percentile	*Ksat Layer 1 (cm/hr)*	*Ksat Layer 2 (cm/hr)*	*Ksat Layer 3 (cm/hr)*	*CN*	*Manning's N Value*	*Initial Soil Moisture (% Field Capacity)*
1	0.82	0.28	0.48	82.3	0.40	1.0
10	1.97	0.66	1.15	73.9	0.43	10.0
50	5.73	1.93	3.36	60.7	0.47	50.0
90	16.71	5.61	9.78	45.7	0.56	90.0
99	39.88	13.40	23.35	33.9	0.61	99.0

Comparison of Model Predictions

Simulations using the three datasets (covering a wide range of buffers, storms, and pesticide properties) provided 73 data points to compare the models against each other and observed data. From these data points, the error (including the sign) and the absolute error (the absolute value of the simulated reduction minus the observed reduction) were calculated for each of the data points. The models were ranked for each data point according to the magnitude of the absolute error in the prediction. The mean and standard deviations of the rank and the arithmetic average of the absolute error, and the arithmetic average of the error (which indicates the positive or negative bias in the model, and results are summarized in Table IV. Also this analysis was performed with relative error in addition to absolute error, but the results are not included here for simplicity since the overall conclusions do not change, although there are changes in comparisons involving individual data points.

Table IV. Comparison of Model Performance

Statistic	*Parameter*	*APEX*[a]	*PRZM-BUFF*[a]	*REMM*[a]	*VFSMOD*[a]
Rank	Pesticide	2.6 (1.0)	2.6 (1.0)	3.0 (1.1)	1.9 (1.1)
	Runoff	2.5 (1.1)	3.2 (0.9)	2.6 (1.2)	1.8 (0.9)
	Sediment	2.7 (0.9)	2.8 (1.1)	3.0 (1.2)	1.6 (0.8)
Mean Absolute Error (%)	Pesticide	16 (10)	16 (14)	31 (31)	9 (8)
	Runoff	30 (20)	37 (28)	35 (32)	12 (9)
	Sediment	19 (17)	31 (31)	30 (24)	12 (17)
Mean Error (%)	Pesticide	-0.9 (18.7)	-5.3 (21.2)	-28.1 (33.9)	-3.0 (11.1)
	Runoff	-8.0 (35.9)	-36.5 (28.8)	-30.1 (36.7)	-6.2 (14.4)
	Sediment	-6.6 (25.4)	27.4 (34.7)	-23.8 (30.5)	-1.8 (20.7)

[a] Numbers in parentheses represent the standard deviation of the individual values.

Results show that the mean error statistics are almost entirely negative (PZRM-BUFF sediment is the only positive mean error value), indicating that the models were conservative, and, on average under-predicted VFS effectiveness. In addition, based on mean absolute error and the rank, VFSMOD simulations are consistently closer to the observations than the other three models. The order of the other three models depended on whether pesticide, runoff, or sediment is being considered. As might be expected, the standard deviations in the absolute error were smaller for the models with the lower mean absolute errors. Furthermore, all of the models will, on average, simulate the buffer effectiveness at reducing runoff, sediment, and pesticides within approximately 30% of field observations (based on absolute error).

This study has made numerous comparisons of model simulations with field observations. Implicit in these comparisons has been that the "observations" are accurately reflecting field conditions over the entire buffer. However, conducting field experiments to measure runoff, sediment, and pesticide loadings into and out of vegetative buffers is difficult, and field observations have various levels of uncertainty associated with them. While it is beyond the scope of this study to quantify these uncertainties, it is important to consider this when assessing model performance and comparing specific simulations to the observed data.

Conclusions

In our comparison of the performance of the four models, VFSMOD provided the best overall performance based on differences between predicted and observed pesticide, runoff, and sediment retention by the VFS. The other models evaluated in this study (APEX,PRZM-BUFF, and REMM) were found to make predictions of VFS effectiveness for pesticide removal that deviated from the effectiveness observed in the field studies by less than 31% on average (based on the absolute error). These results should provide risk assessment scientists and regulators with increased confidence for the evaluation of VFS performance as a mitigation strategy.

Acknowledgments

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References

1. USDA Natural Resources Conservation Service. *Conservation Buffers to Reduce Pesticide Losses*; 2000; p 21. http://www.in.nrcs.usda.gov/technical/agronomy/newconbuf.pdf.
2. Arora, K.; Mickelson, S. K.; Helmers, M. J.; Baker, J. L. *J. Am. Water Resour. Assoc.* **2010**, *46* (3), 618–647.
3. Reichenberger, S.; Bach, M.; Skitschak, A.; Frede, H.-G. *Sci. Total Environ.* **2007**, *384*, 1–35.
4. Sabbagh, G. J.; Fox, G. A.; Kamanzi, A.; Roepke, B.; Tang, J. Z. *J. Environ. Qual.* **2009**, *38* (2), 762–771.
5. Lacas, J. G.; Voltz, M.; Gouy, V.; Carluer, N.; Gril, J. J. *Agron. Sustainable Dev.* **2005**, *25*, 253–266.
6. Winchell, M.; Estes, T. *A Review of Simulation Models for Evaluating the Effectiveness of Buffers in Reducing Pesticide Exposure*; US EPA MRID #47773401; unpublished report, 2009.
7. Winchell, M. *A Comparison of Four Models for Simulating the Effectiveness of Vegetative Filter Strips at Reducing Off-Target Movement of Pesticides*. US EPA MRID #48451401, Unpublished report, 2010.
8. Williams, J. R.; Izaurralde, R. C.; Steglich, E. M. *Agricultural policy/environmental extender model theoretical documentation*; BREC Report #2008-17; Blackland Research and Extension Center: Blackland, TX, 2008; p 130.
9. Lowrance, R. R.; Altier, L. S.; Williams, R. G.; Inamdar, S. P.; Bosch, D. D.; Sheridan, J. M.; Thomas, D. L.; Hubbard, R. K. *The Riparian Ecosystem Management Model: simulator for ecological processes in riparian zones*; USDA-ARS Conservation Research Report 46; 2002.
10. Muñoz-Carpena, R.; Parsons, J. E.; Wendell, G. J. *J. Hydrol.* **1999**, *214*, 111–129.
11. Wauchope, R. D.; Buttler, T. M.; Hornsby, A. G.; Augustijn-Beckers, P. W.; Burt, J. P. *Rev. Environ. Contam. Toxicol.* **1992**, *123*, 1–155.

12. Pätzold, S.; Klein, C.; Brümmer, G. W. *Soil Use Manage.* **2007**, *23*, 294–305.
13. Giddings, J. M.; Anderson, T. A.; Hall, L. W., Jr.; Hosmer, A. J.; Kendall, R. J.; Richards, R. P.; Solomon, K. R.; Williams, W. M. *A Probabilistic Aquatic Ecological Risk Assessment of Atrazine in North American Surface Waters*; Society of Environmental Toxicology and Chemistry (SETAC): Pensacola, FL, 2005; p 432.
14. Lowrance, R. R.; Vellidis, G.; Wauchope, R. D.; Gay, P.; Bosch, D. D. *Trans. ASAE* **1997**, *40* (4), 1047–1057.
15. Sheridan, J. M.; Lowrance, R.; Bosch, D. D. *Trans. ASAE* **1999**, *42* (1), 55–64.
16. Poletika, N. N.; Coody, P. N.; Fox, G. A.; Sabbagh, G. J.; Dolder, S. C.; White, J. *J. Environ. Qual.* **2009**, *38*, 1042–1052.