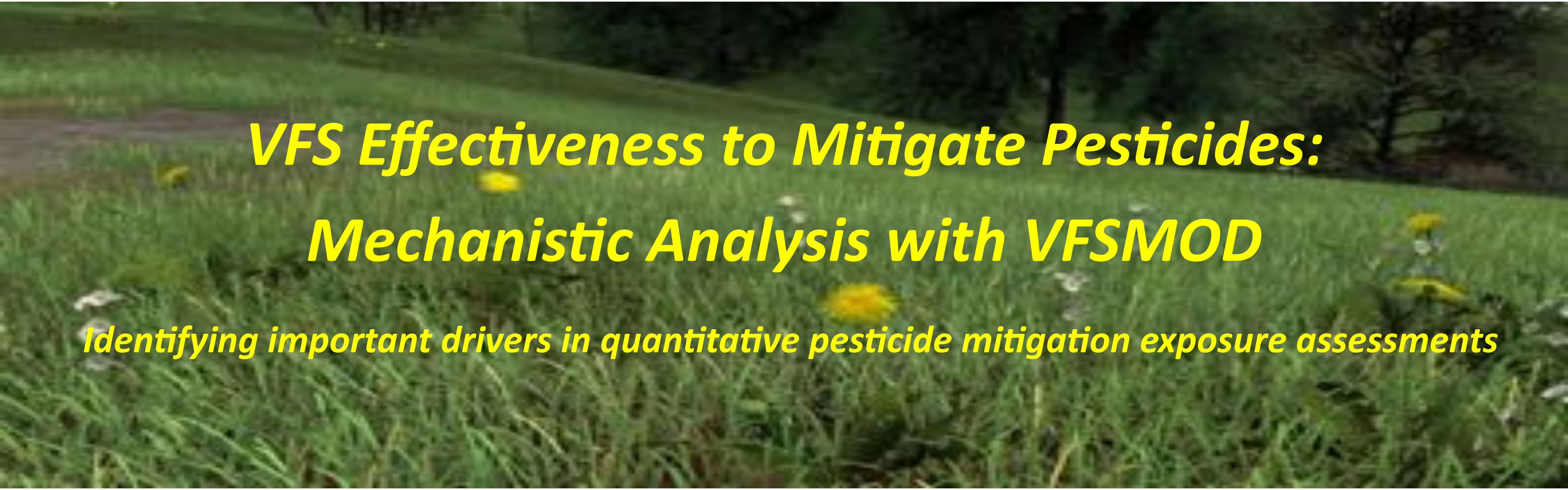


VFS Effectiveness to Mitigate Pesticides: Mechanistic Analysis with VFSMOD

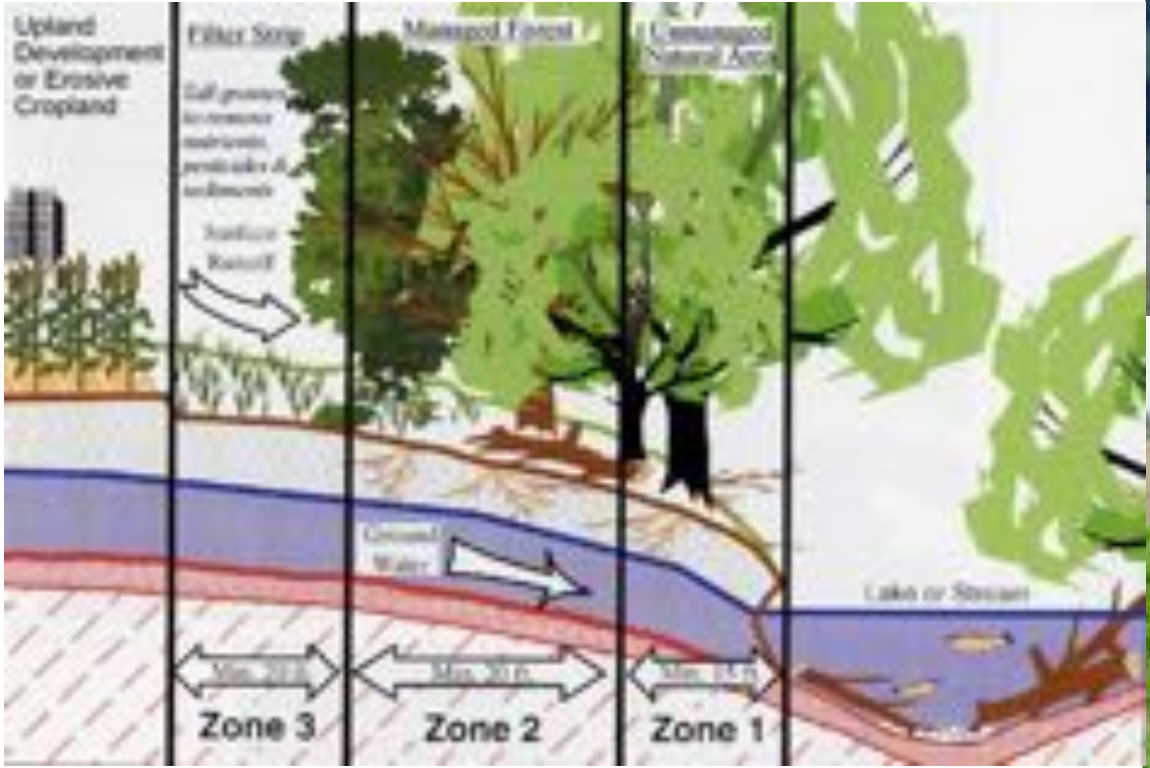
Identifying important drivers in quantitative pesticide mitigation exposure assessments

Rafael Muñoz-Carpena[1]

Garey Fox[2], Amy Ritter[3], Stefan Reichenberber[4], …

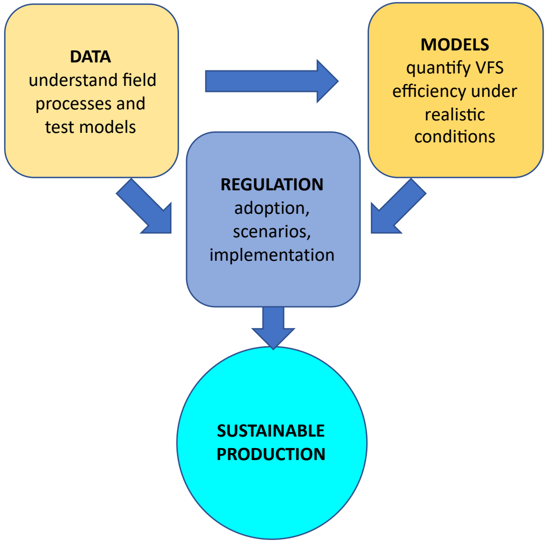
[1]Agricultural & Biological Engineering, University of Florida, USA; [2]NC State University, USA;
[3]Waterborne, USA; [4]knoell, Germany…

Runoff pollution mitigation: Vegetative Filter Strips (VFS)




[photo: NRCS-Ohio]


[photo: Mats Allmyr, Swedish Chemical Agency KEMI]



DATA
understand field processes and test models

MODELS
quantify VFS efficiency under realistic conditions

REGULATION
adoption, scenarios, implementation

SUSTAINABLE PRODUCTION

- Principles of runoff pesticide mitigation with VFS

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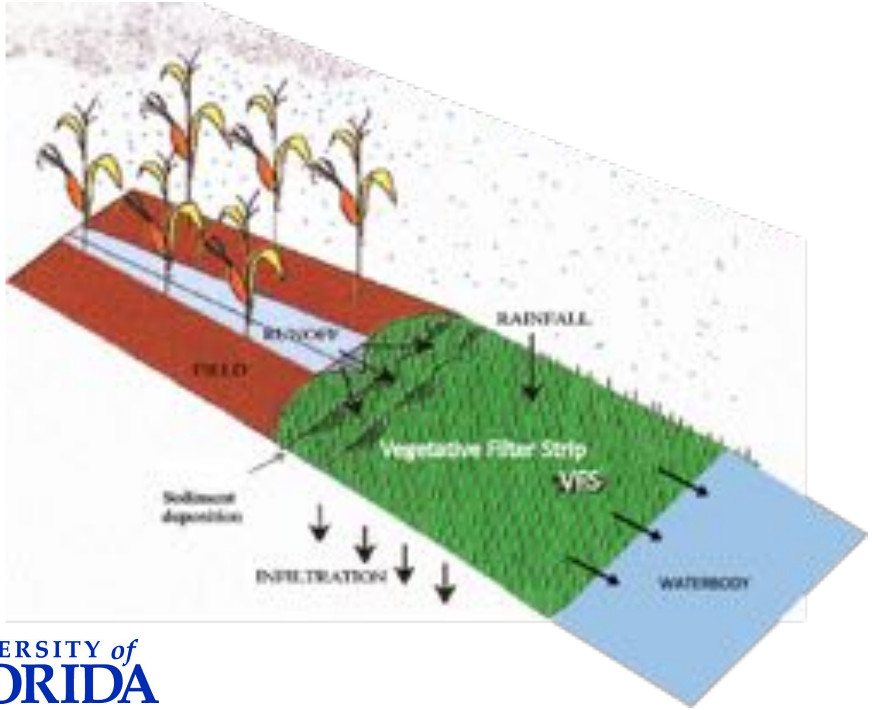
Pesticide runoff VFS mitigation - processes

VFS: Vegetative Filter Strip = Runoff Buffer



Vegetation increases hydraulic resistance to flow and soil infiltration

↓

VFS delays and reduces overland flow (and dissolved pollutants)

↓

Delay settles sediment/particles (and sorbed pollutants)

↓

Final reduction in runoff volume, sediment, and dissolved and sorbed pollutants

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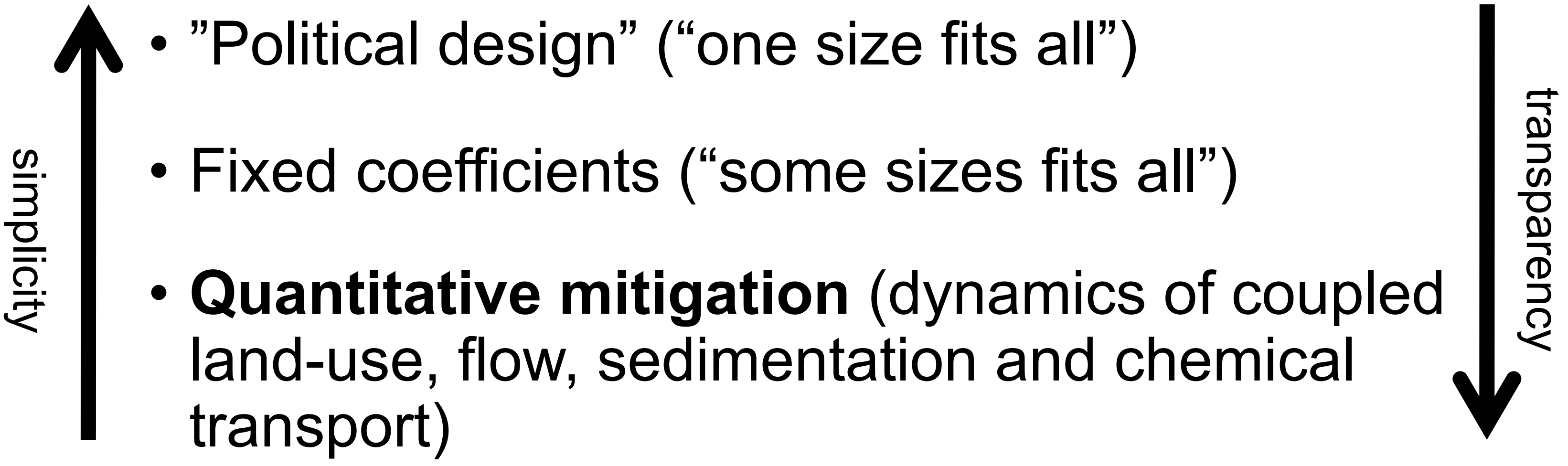
VFS Mitigation Efficiency: approaches

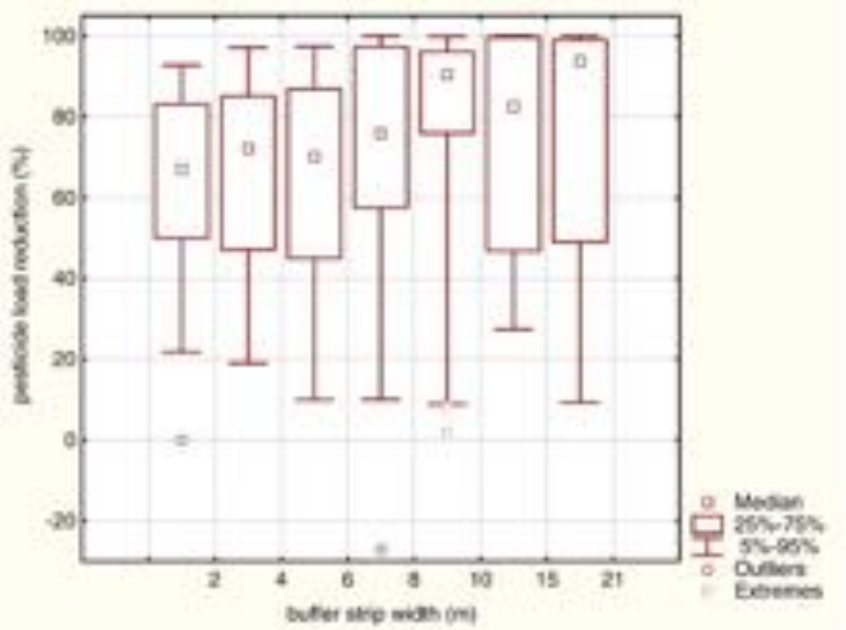


- ”Political design” (“one size fits all”)
- Fixed coefficients (“some sizes fits all”)
- **Quantitative mitigation** (dynamics of coupled land-use, flow, sedimentation and chemical transport)

Occam: simpler is better (but <u>only</u> if it works!)

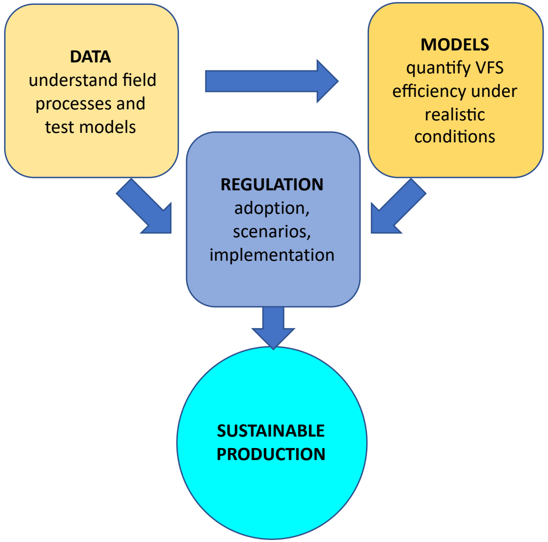
VFS Efficiency- Bigger is better?

International review (Reichenberger et al., 2007):



- Individual events trapping efficiency ΔP = 0-99 %.
- Long-term $\Delta P > 50\%$.
- Variability driven by site characteristics (hydrology, sedimentology and pesticide)
- Infiltration is the main process of this control (followed by sedimentation and surface adsorption)
- Aggregated data insensitive to filter size → Other processes!!

Reichenberger, S., M. Bach, A. Skitschak, H.-G. Frede. 2007. Mitigation strategies to reduce pesticide inputs into ground and surface water and their effectiveness; a review. Sci. Total Environ., 384 (2007), pp. 1-35, 10.1016/j.scitotenv.2007.04.046



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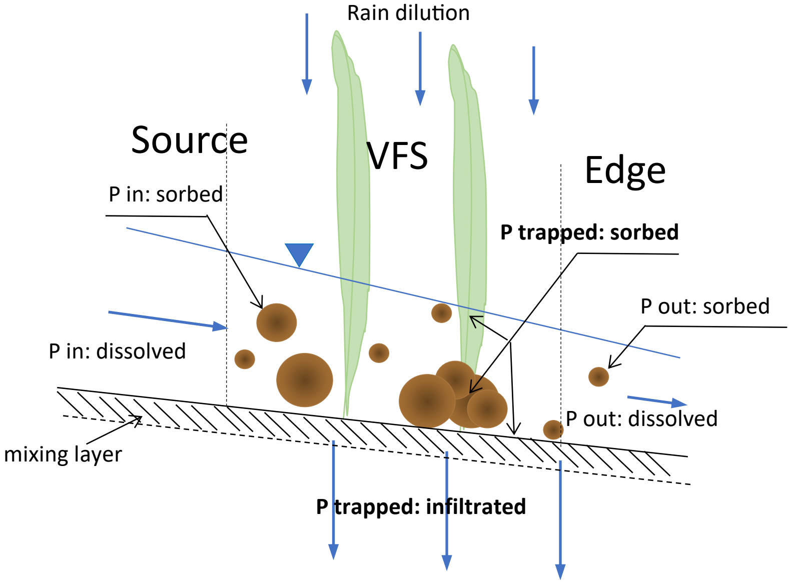
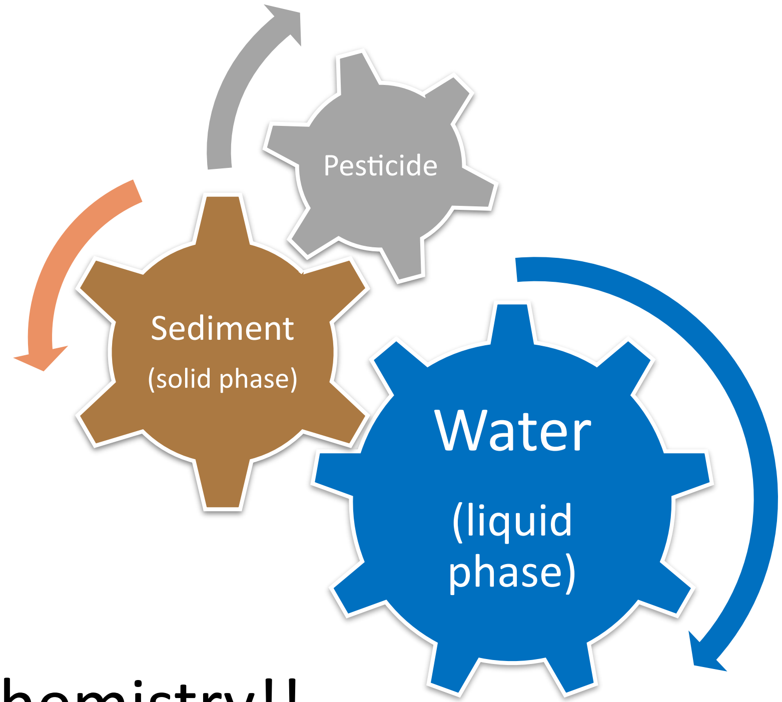
- VFSMOD: processes

Quantitative VFS Mitigation: Mechanistic View

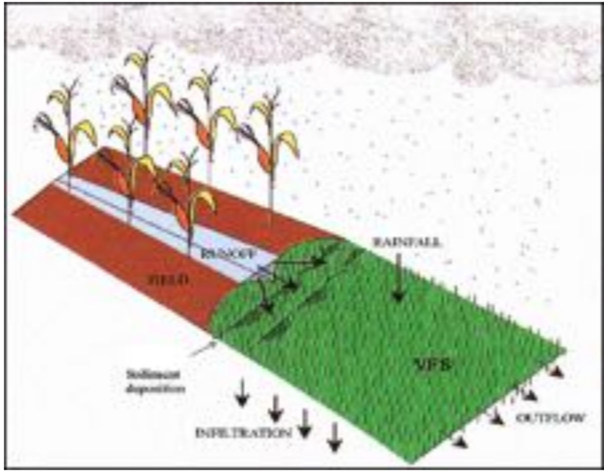




Is not about (just) chemistry!!

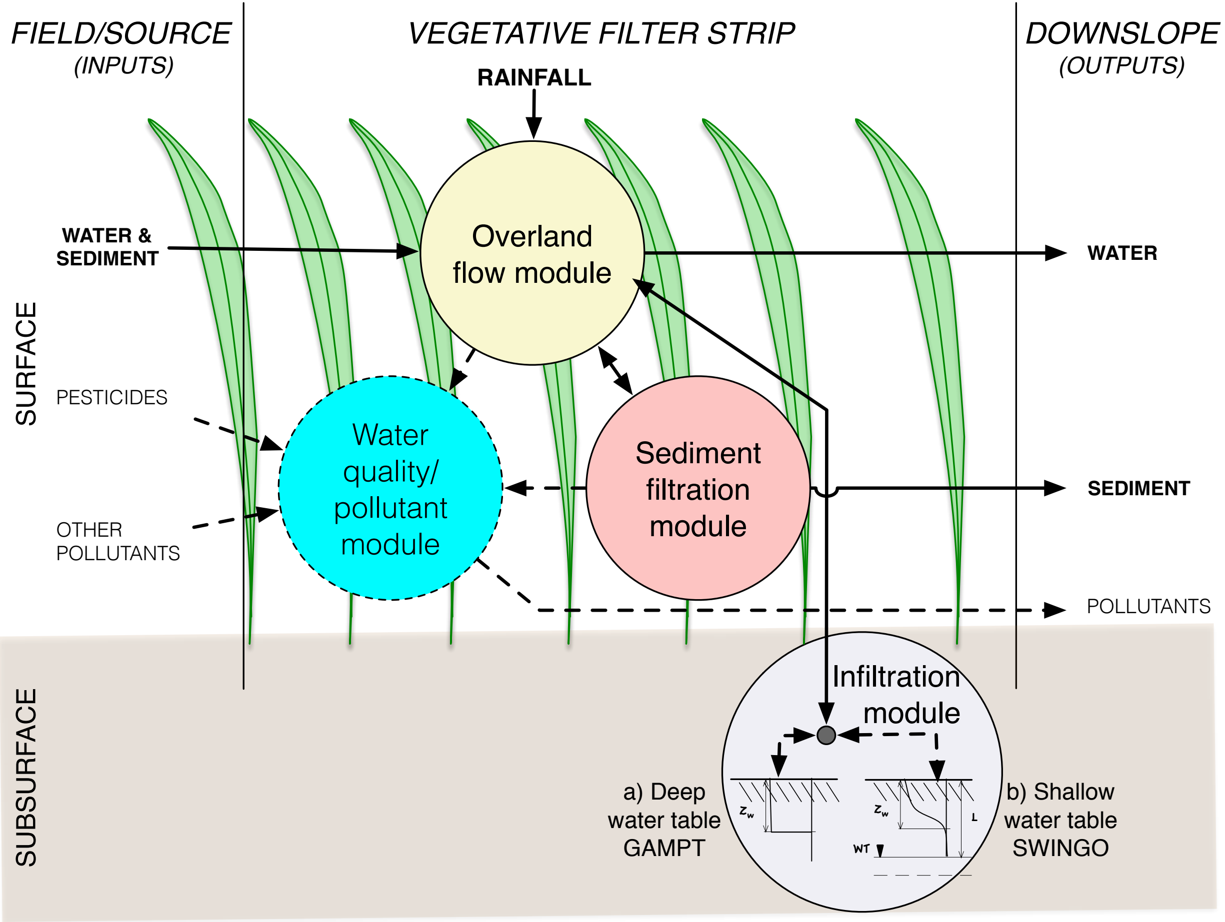
Pesticide VFS runoff mitigation - Modeling

VFSMOD: Vegetative filter strip model



- Public domain model
- Free distribution and documentation
- Actively maintained
- In continuous development and testing
- 100+ publications with testing, application, analysis, metamodeling, and conceptual framework used by others.
- Model distribution web site: https://abe.ufl.edu/vfsmod

  (Google: VFSMOD)



FIELD/SOURCE
(INPUTS)

VEGETATIVE FILTER STRIP

DOWNSLOPE
(OUTPUTS)

RAINFALL

SURFACE

WATER & SEDIMENT

PESTICIDES

OTHER POLLUTANTS

Overland flow module

Water quality/ pollutant module

Sediment filtration module

WATER

SEDIMENT

POLLUTANTS

SUBSURFACE

Infiltration module

a) Deep water table GAMPT

b) Shallow water table SWINGO

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Overland flow module

- Petrov-Galerkin finite element numerical solution of the overland flow kinematic wave for the 1-D case [*Lighthill and Whitham*, 1955; *Muñoz-Carpena, et al.*, 1993a,b]

$$\frac{\partial h}{\partial t}+\frac{\partial q}{\partial x}=i_e(t)\quad \textit{(Continuity equatio}$$

$$S_o = S_f \quad \textit{(Momentum equatio}$$

$$q = q(h) = \frac{\sqrt{S_o}}{n}h^{\frac{5}{3}}$$

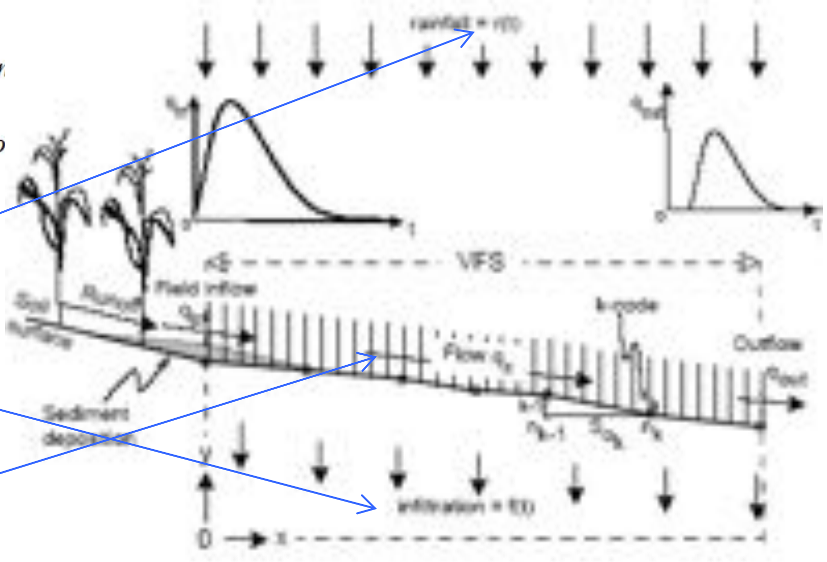
$$i_e(t) = r(t) - f(t)$$

The initial and boundary conditions

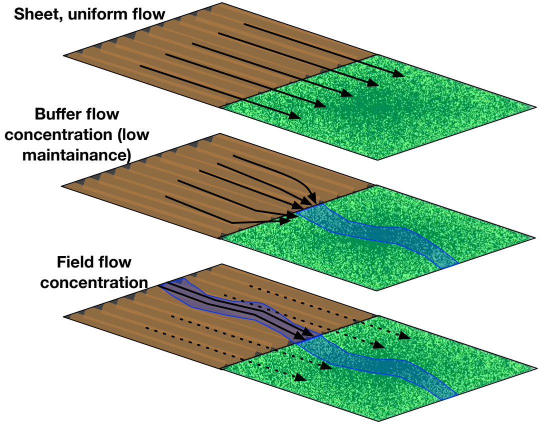
$$h = 0; 0 \le x \le L; t = 0$$

$$\boxed{h = h_o; x = 0;\ t > 0}$$

$$Fr = \frac{v}{\sqrt{gh}} < 1.5 \text{ and } k = \frac{LS_o g}{v^2} > 10$$

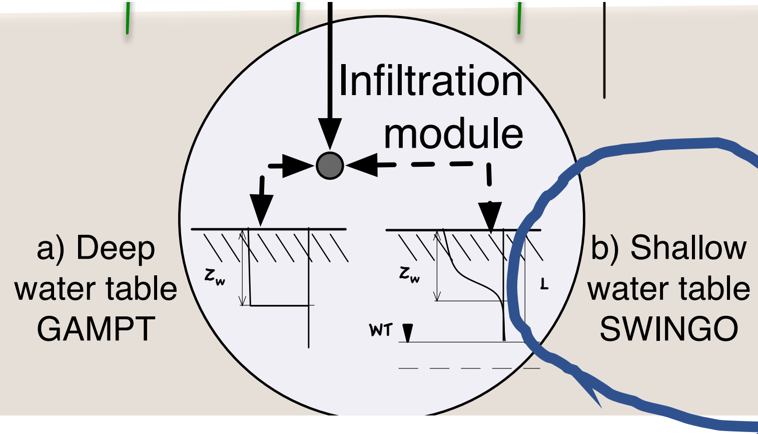


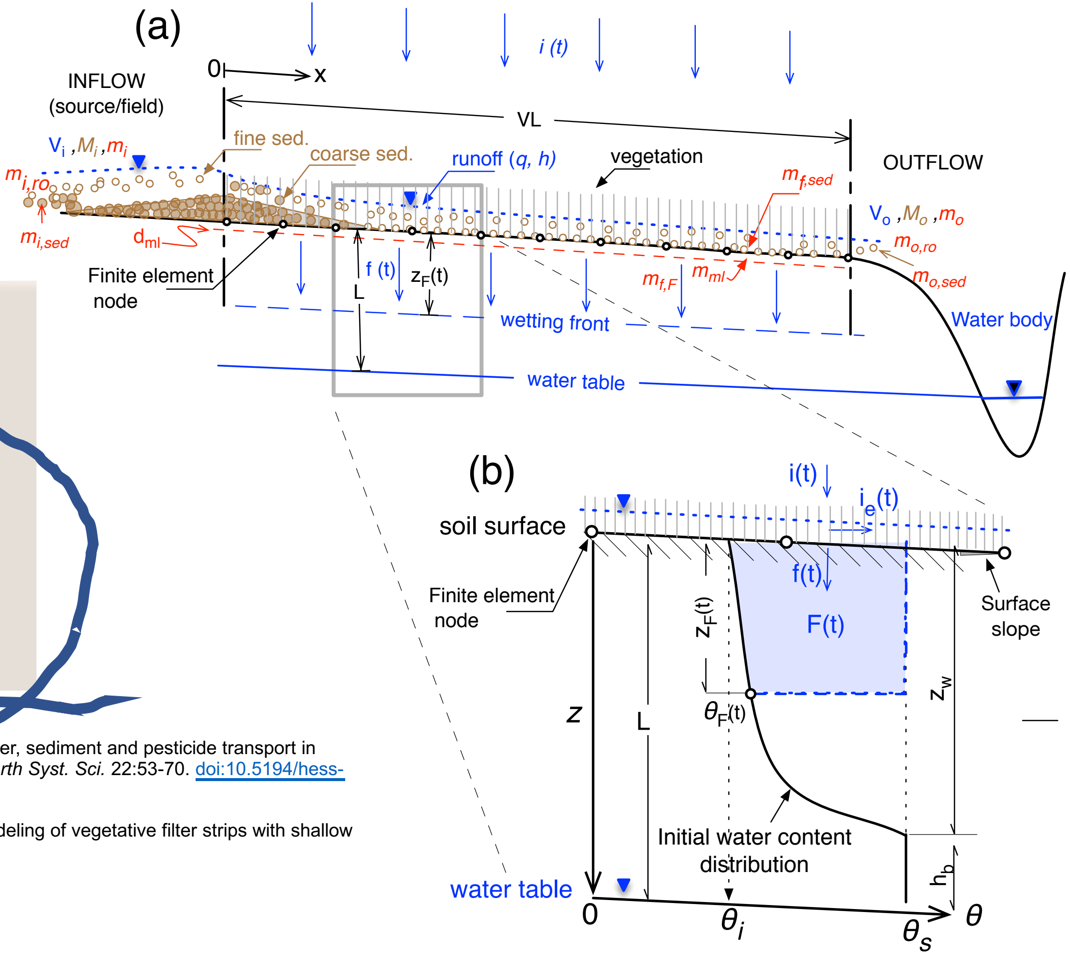
Domain Discretization (Muñoz-Carpena et al., 1999)



Muñoz-Carpena, R., C.T. Miller, and J.E. Parsons. 1993a. A Quadratic Petrov-Galerkin Solution for Kinematic Wave Overland Flow. *Water Resources Research* 29(8):2615-2627.
Muñoz-Carpena, R., J.E. Parsons, and J.W. Gilliam. 1993b. Numerical Approach to the Overland Flow Process in Vegetative Filter Strips. *Trans. of ASAE* 36(3):761-770.

Soil infiltration module





Muñoz-Carpena, R., Lauvernet, C., and Carluer, N. 2018. Shallow water table effects on water, sediment and pesticide transport in vegetative filter strips: Part A. non-uniform infiltration and soil water redistribution, *Hydrol. Earth Syst. Sci.* 22:53-70. doi:10.5194/hess-22-53-2018

Fox, G., R. Muñoz-Carpena and R. Purvis. 2018. Controlled laboratory experiments and modeling of vegetative filter strips with shallow water tables. *J. of Hydrology* 556(1):1–9, doi:10.1016/j.jhydrol.2017.10.069

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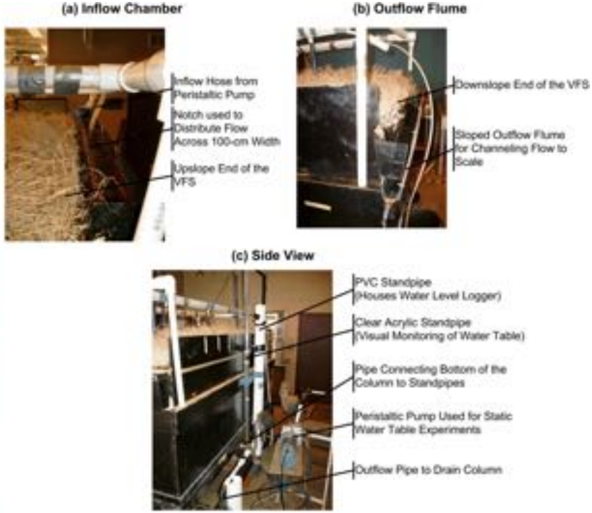
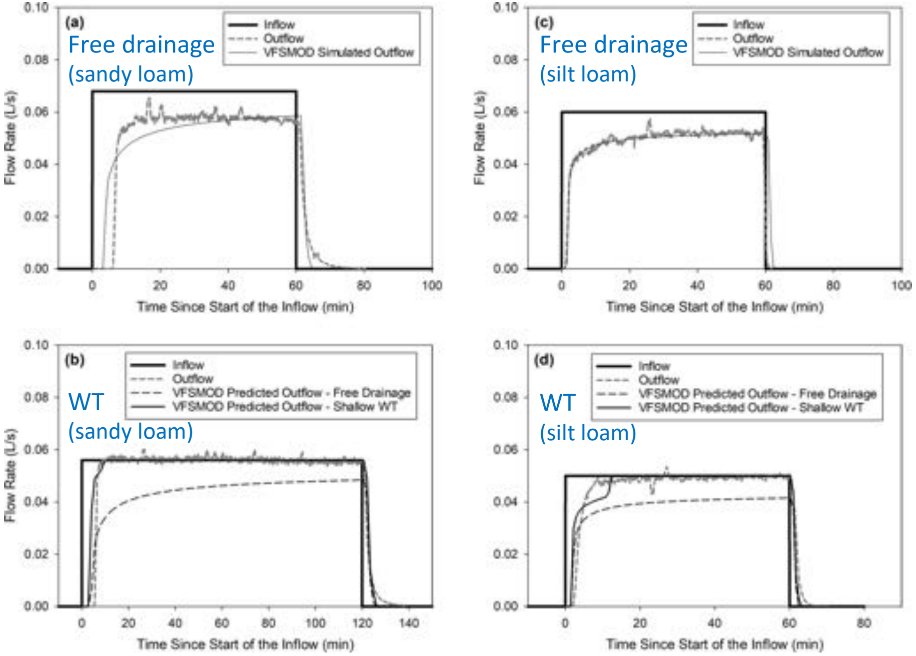
Shallow water table: laboratory testing





Observed versus VFSMOD-predicted runoff from the simulated vegetative filter strip for a silt loam (a and b) and sandy loam (c and d) soils with free drainage (a and c) and shallow water table WT (depths = 0.4 and 0.3 m below ground surface for the silt loam (b) and sandy loam (d) soils, respectively).

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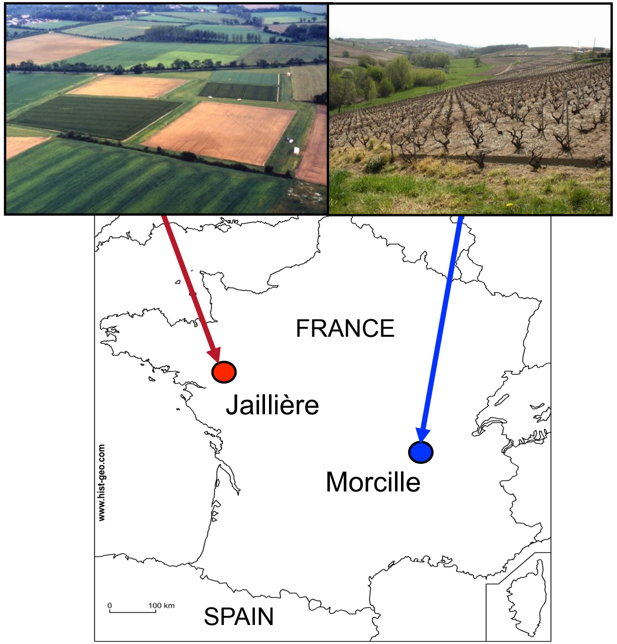
[Fox, G., R. Muñoz-Carpena and R. Purvis. 2018. Controlled laboratory experiments and modeling of vegetative filter strips with shallow water tables. J. of Hydrology 556(1):1–9, doi:10.1016/j.jhydrol.2017.10.069]

Soil infiltration: shallow water table

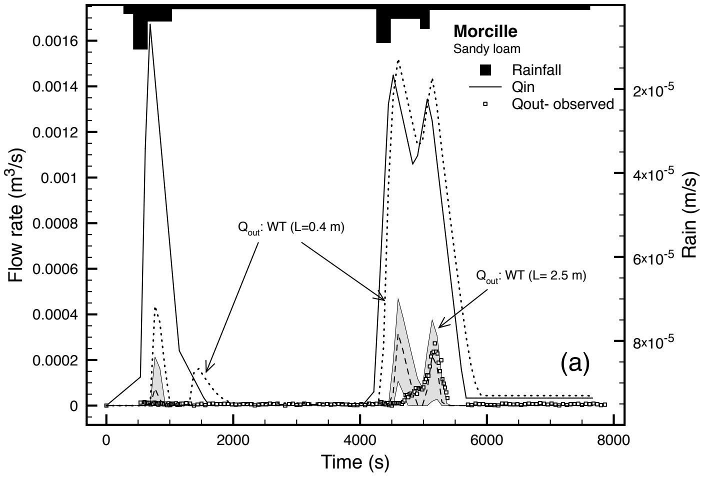
Testing and application – shallow water table

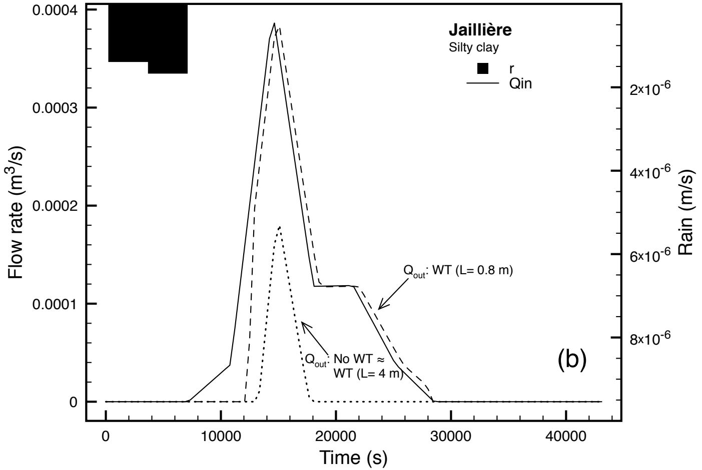


2 pesticides:

Isoproturon (M, J)

Diflufenican (J)





Lauvernet, C. and Muñoz-Carpena, R.. 2018. Shallow water table effects on water, sediment and pesticide transport in vegetative filter strips: Part B. model coupling, application, factor importance and uncertainty, *Hydrol. Earth Syst. Sci.* 22:71-87. doi:10.5194/hess-22-71-2018

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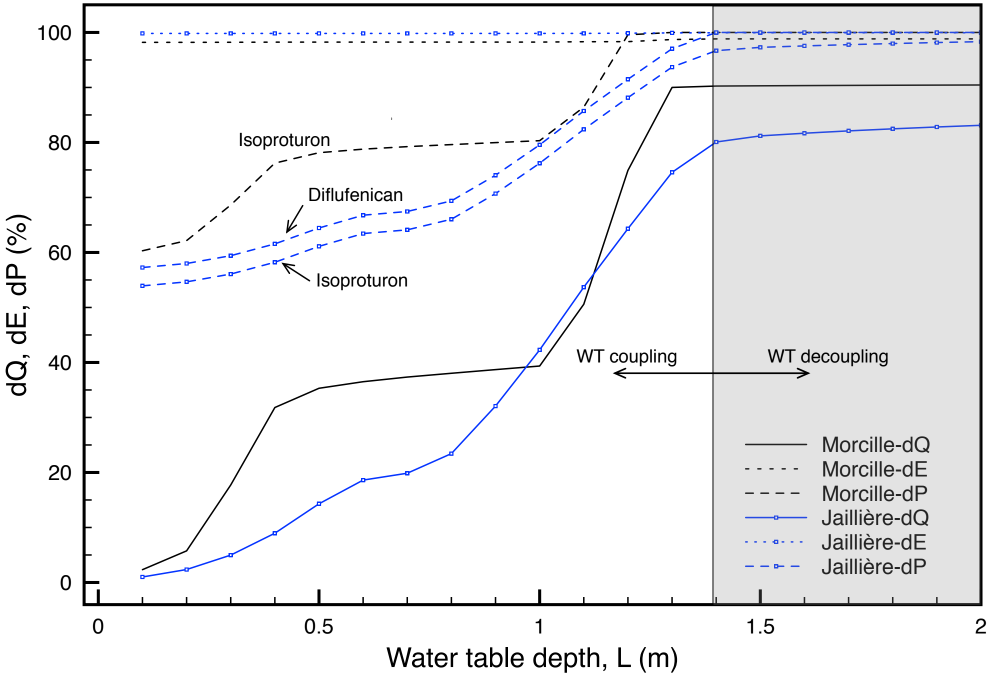
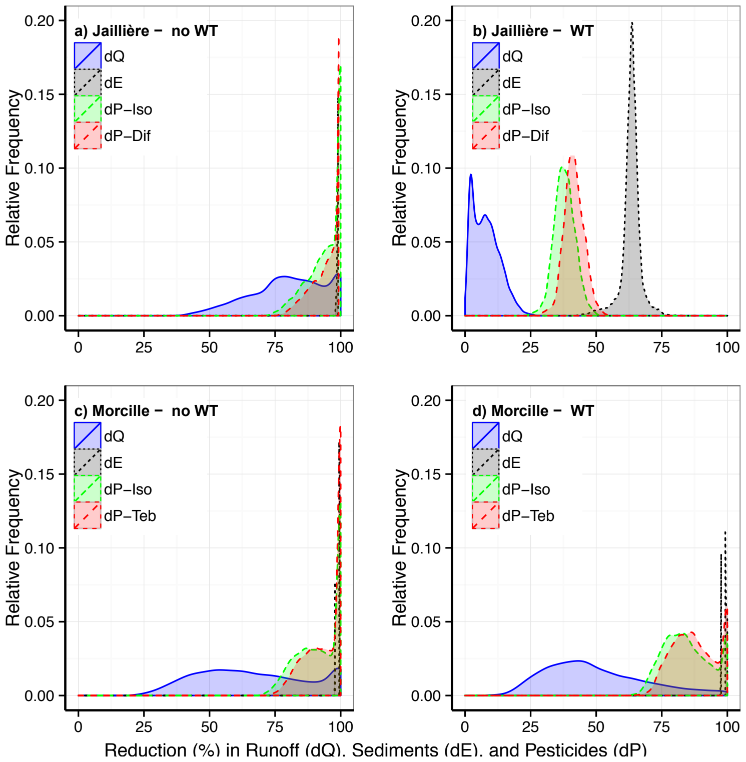
Soil infiltration: shallow water table

Sensitivity to water table of reduction of VFS runoff (dQ), sediment (dE), and pesticide (dP)



Uncertainty Analysis

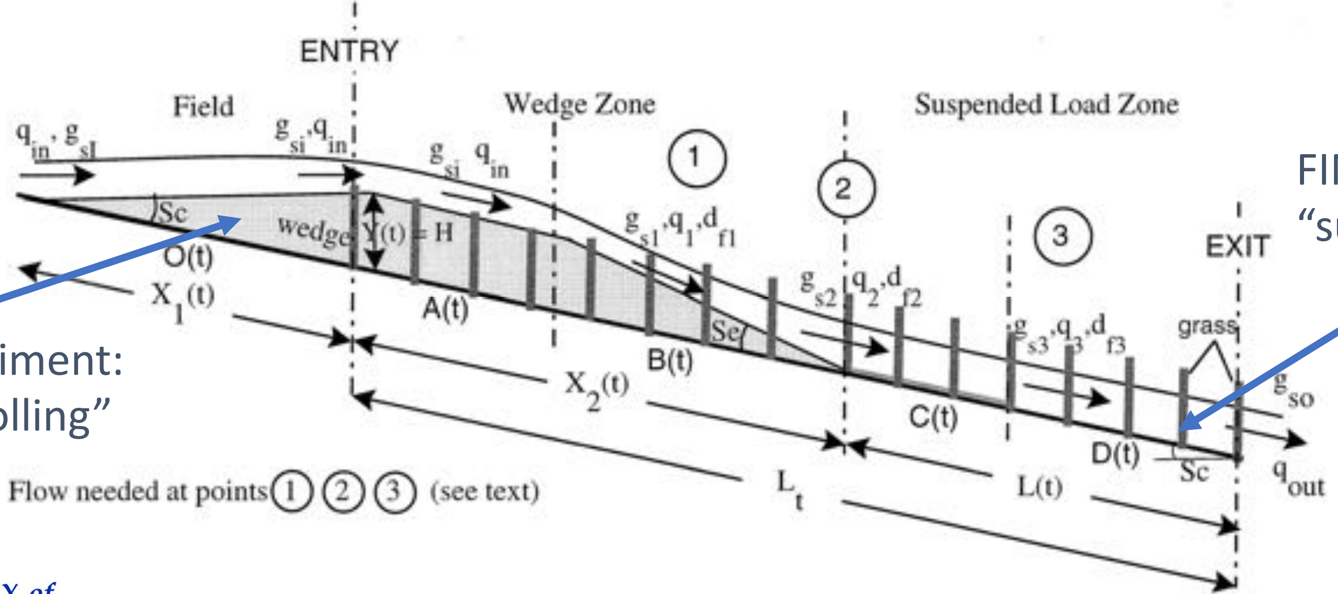


Lauvernet, C. and Muñoz-Carpena, R.. 2018. Shallow water table effects on water, sediment and pesticide transport in vegetative filter strips: Part B. model coupling, application, factor importance and uncertainty, *Hydrol. Earth Syst. Sci.* 22:71-87. doi:10.5194/hess-22-71-2018

Sediment: particle filtration module

[University of Kentucky- GRASSF]

- For <u>COARSE particles</u> (dp>37 µm), a form of Einstein bed-load transport equation successfully tested for dense vegetation at the U. of Kentucky is used.
- For <u>FINE particles</u> (dp<37 µm), suspended based on probabilistic approach of turbulent diffusion developed for non-submerged dense vegetation conditions (Tollner et al., 1976; Barfield et al., 1978; Wilson et al., 1981]
- The particle deposition pattern on the filter is predicted based on a conceptual sediment wedge model (fig. above).



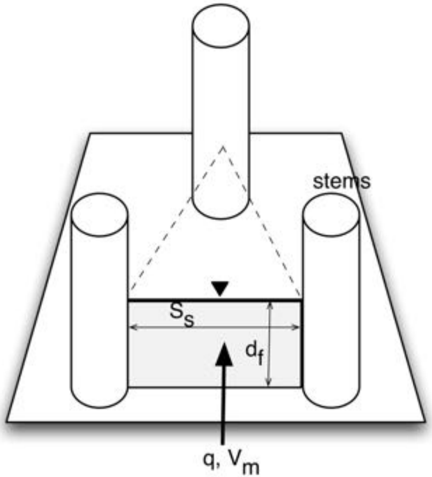
COARSE sediment: bed-load "rolling"

FINE sediment: "suspended"

Muñoz-Carpena, R., J.E. Parsons, and J.W. Gilliam. 1999. Modeling hydrology and sediment transport in vegetative filter strips. *Journal of Hydrology* 214(1-4):111-129.

***Bed-load sediment transport (d_p>37** µm)*

For coarse particles, a form of Einstein Jr. (the son!) bed load transport equation successfully tested for dense vegetation (Barfield et al., 1978) is used,



$$\frac{\gamma_s-\gamma}{\gamma}\frac{d_p}{R_s S_o}=1.08\left[\frac{g_s}{\gamma\sqrt{\frac{\gamma_s-\gamma}{\gamma}g d_p^3}}\right]^{-0.28}$$

$$q=V_m d_f$$

$$R_s=\frac{S_s d_f}{2d_f+S_s}$$

$$V_m=\frac{\sqrt{S_o}}{n_m}R_s^{2/3}$$

where R_s is the hydraulic radius (depends on **flow velocity**/stage and **grass spacing**), d_p median **sediment size**, g_s is the transport capacity of the flow [$ML^{-1}T^{-1}$], γ_s and γ are the particle and water specific densities [ML^{-3}]

***Suspended particle transport (d_p<37** µm)*

For suspended particles, a probabilistic approach of turbulent diffusion developed for non-submerged dense vegetation conditions (Tollner et al., 1976). Rate of settling is governed by Stokes settling velocity (V_f [LT^{-1}], a function of the **particle size** d_p and density γ_s, surface flow conditions described by the Reynolds number (R_e), flow characteristics (**velocity,** V [LT^{-1}], and depth, h[L]), and the distance along the flow path ($L(t)$, [L]) available for settling.

$$\frac{g_{si}-g_{so}}{g_{si}}=e^{\left[-1.05x10^{-3}R_e^{0.82}\left(\frac{V_f L(t)}{Vh}\right)^{-0.91}\right]}$$

where:

$$R_e=\frac{VR_s}{\nu}$$

with g_{si} and g_{so} the vegetation segment's incoming and outgoing particle load [$ML^{-1}T^{-1}$], and ν is the kinematic viscosity of water [L^2T^{-1}]

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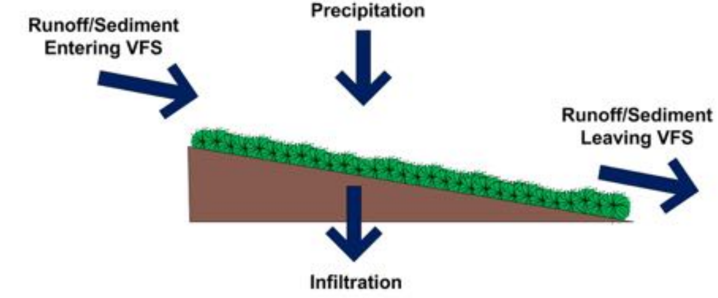
Muñoz-Carpena, R., J.E. Parsons, and J.W. Gilliam. 1999. Modeling hydrology and sediment transport in vegetative filter strips. *Journal of Hydrology* 214(1-4):111-129.

Pesticide Trapping Efficiency Calculation

Hydrology+Sediment



ΔQ = Infiltration = (Runoff Entering + Preciptation) – Runoff Leaving

ΔE = Sedimentation = Sediment Entering – Sediment Leaving

Pesticides

- Sorption Coefficient: Phase distribution factor
  K_{oc} = organic carbon sorption coefficient
  K_d = distribution coefficient
- Sediment: %OC and clay content of incoming sediment

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

$$K_d = \frac{K_{oc}(\%OC)}{100}$$

1. **Semi-empirical equation:** "original" using 47 data points (Sabbagh et al., 2009), and "recalibrated" using 244 data points (Reichenberger et al, 2018)

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

5 regression parameters (*a*-*d*) and 6 independent variables: ΔQ, ΔE, Q_i, E_i, K_d, %clay

2. **Mechanistic mass balance** (Reichenberger et al, 2018)

$$\boxed{\frac{\Delta P}{100\%} = \frac{\min\left[(V_i + K_d E_i);\left(\frac{\Delta Q}{100\%}V_i + \frac{\Delta E}{100\%}K_d E_i\right)\right]}{(V_i + K_d E_i)}}$$

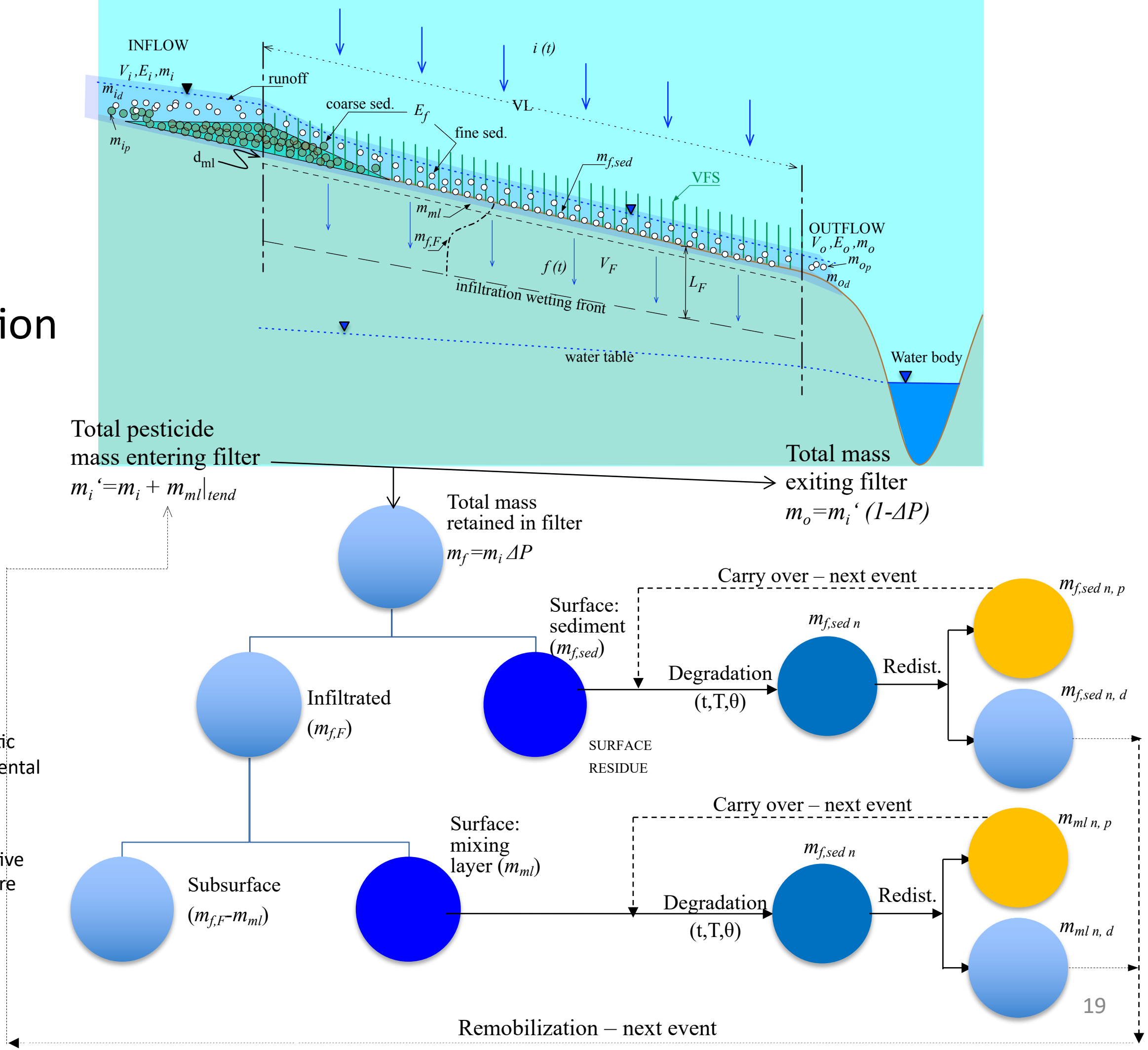
NO (0) regression parameters, 5 independent variables: Vi, K_d, E_i, ΔE and ΔQ (with V_i = incoming run-on volume (L))

Reichenberger, S., R. Sur, C. Kley, S. Sittig, S. Multsch. 2019. Recalibration and cross-validation of pesticide trapping equations for vegetative filter strips (VFS) using additional experimental data. *Science of the Total Environment* 647 (2019) 534–550 doi:10.1016/j.scitotenv.2018.07.429

Sabbagh, G.J.; Fox, G.A.; Kamanzi, A.; Roepke, B.; Tang, J.Z. Effectiveness of vegetative filter strips in reducing pesticide loading: Quantifying pesticide trapping efficiency. *J. Environ. Qual.* **2009**, 38 (2), 762-771.

Fate of VFS pesticide residues

- Dissolved & sorbed P redistribution in surface mixing layer and deposited sediment.
- Degradation
- Remobilization
- Carry over



Total pesticide mass entering filter
$m_i' = m_i + m_{ml}|_{tend}$

Total mass exiting filter
$m_o = m_i' (1-\Delta P)$

Total mass retained in filter
$m_f = m_i \Delta P$

Carry over – next event

$m_{f,sed\ n,\ p}$

Surface: sediment ($m_{f,sed}$)

$m_{f,sed\ n}$

Degradation (t,T,θ)

Redist.

$m_{f,sed\ n,\ d}$

Infiltrated ($m_{f,F}$)

SURFACE RESIDUE

Carry over – next event

$m_{ml\ n,\ p}$

Surface: mixing layer (m_{ml})

$m_{f,sed\ n}$

Degradation (t,T,θ)

Redist.

$m_{ml\ n,\ d}$

Subsurface ($m_{f,F}-m_{ml}$)

Remobilization – next event

Muñoz-Carpena, R. A. Ritter, G.A. Fox and O. Perez-Ovilla. 2015. Does mechanistic modeling of filter strip pesticide mass balance and degradation affect environmental exposure assessments? *Chemosphere* 139:410-421. doi:10.1016/j.chemosphere.2015.07.010

Muñoz-Carpena, R., G. Fox, A. Ritter, I. Rodea-Palomares. 2018 .Effect of vegetative filter strip pesticide residue degradation assumptions for environmental exposure assessments. *Science of the Total Environmen*t 619–620:977–987, doi:10.1016/j.scitotenv.2017.11.093

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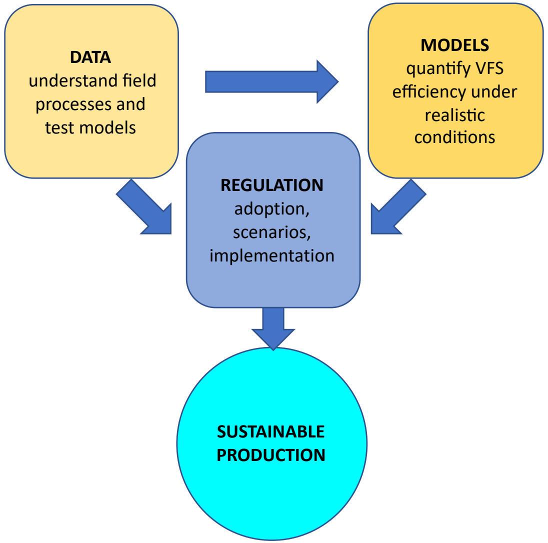

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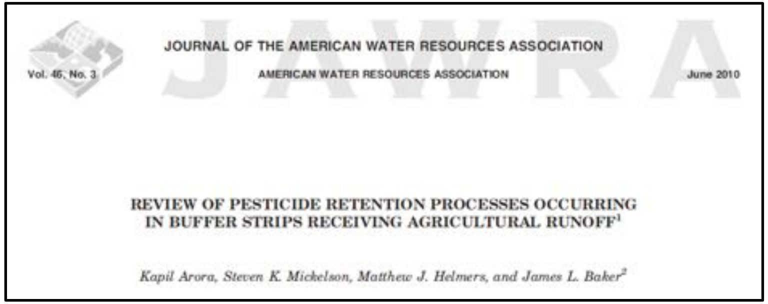
SUSTAINABLE PRODUCTION

- Field Data and Model Testing

Many Published Data on VFS Effectiveness for Pesticide Removal

- Industry funded the compilation and analysis of available published data on vegetative buffer strip efficiency compiled and analyzed at Iowa State (Arora et al, 2010)
  - 57 studies (35 with pesticides), 304 individual test results for 30 pesticides and metabolites
- Latest publication (Reichenberger et al, 2018) compiled published data for evaluations of pesticide trapping efficiency equations
  - 15 studies and 244 individual test results for 18 pesticides and metabolites

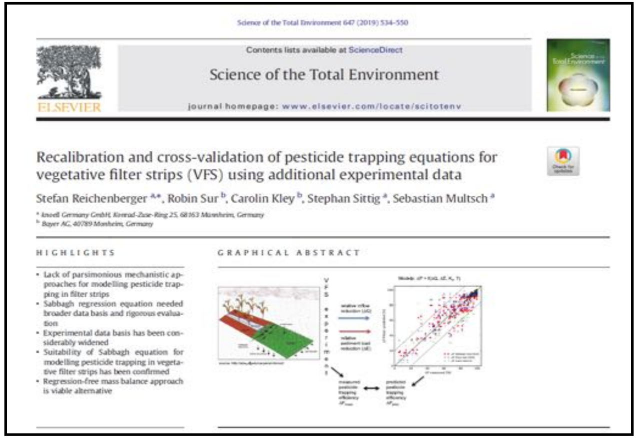


JOURNAL OF THE AMERICAN WATER RESOURCES ASSOCIATION

Vol. 46, No. 3 AMERICAN WATER RESOURCES ASSOCIATION June 2010

REVIEW OF PESTICIDE RETENTION PROCESSES OCCURRING IN BUFFER STRIPS RECEIVING AGRICULTURAL RUNOFF[1]

Kapil Arora, Steven K. Mickelson, Matthew J. Helmers, and James L. Baker[2]



Science of the Total Environment 647 (2019) 534–550

Contents lists available at ScienceDirect

Science of the Total Environment

journal homepage: www.elsevier.com/locate/scitotenv

Recalibration and cross-validation of pesticide trapping equations for vegetative filter strips (VFS) using additional experimental data

Stefan Reichenberger[a,*], Robin Sur[b], Carolin Kley[b], Stephan Sittig[a], Sebastian Multsch[a]

[a] *knoell Germany GmbH, Konrad-Zuse-Ring 25, 68163 Mannheim, Germany*
[b] *Bayer AG, 40789 Monheim, Germany*

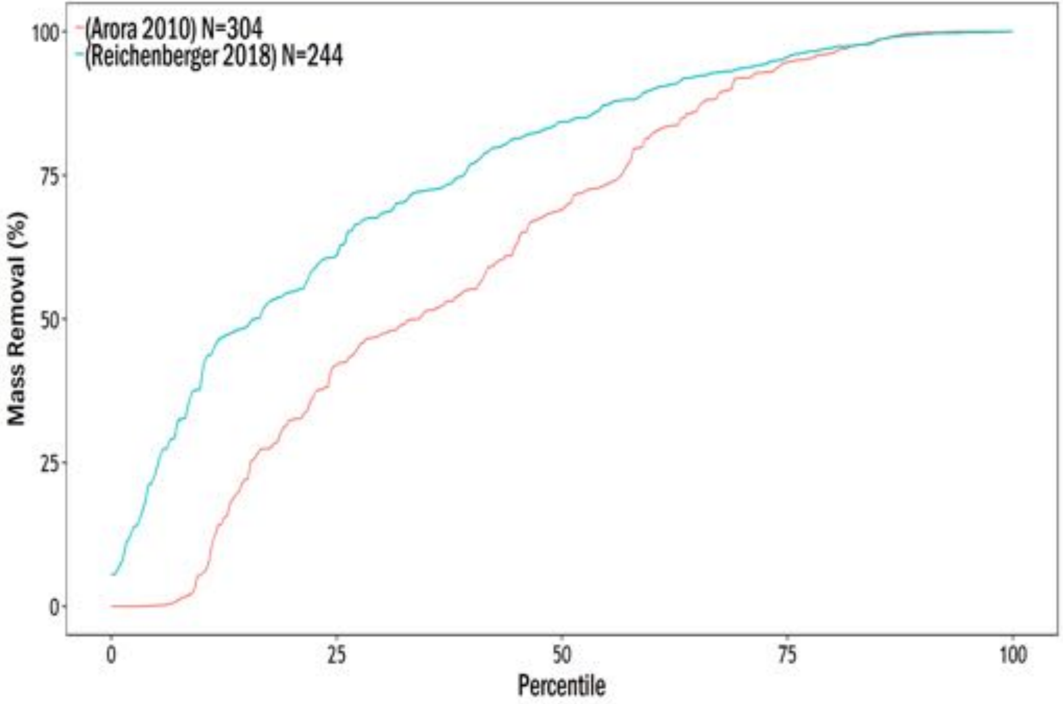
HIGHLIGHTS

- Lack of parsimonious mechanistic approaches for modelling pesticide trapping in filter strips
- Sabbagh regression equation needed broader data basis and rigorous evaluation
- Experimental data basis has been considerably widened
- Suitability of Sabbagh equation for modelling pesticide trapping in vegetative filter strips has been confirmed
- Regression-free mass balance approach is viable alternative

GRAPHICAL ABSTRACT

VFS Pesticide Removal Effectiveness

Wide range!!



Cumulative distribution of pesticide mass removal

Mass removal:

- Wide range (0-100%)
- Mean: 60% for the Arora dataset (304 data points)
- Mean: 76% for the Reichenberger dataset (244 data points)

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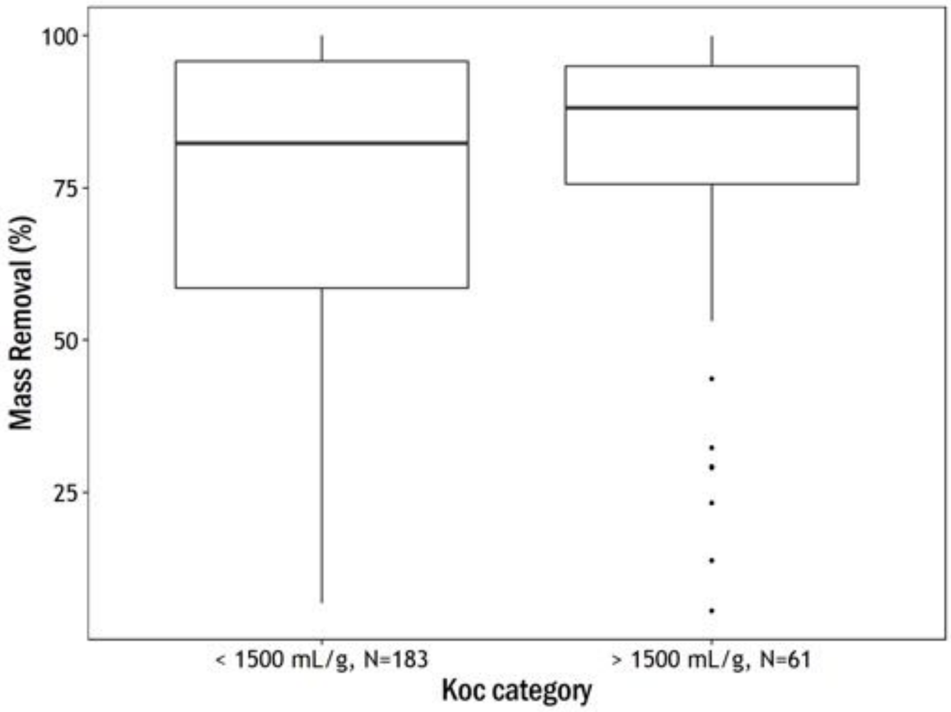
Field Data: VFS efficiency with Koc Water Soluble Compounds



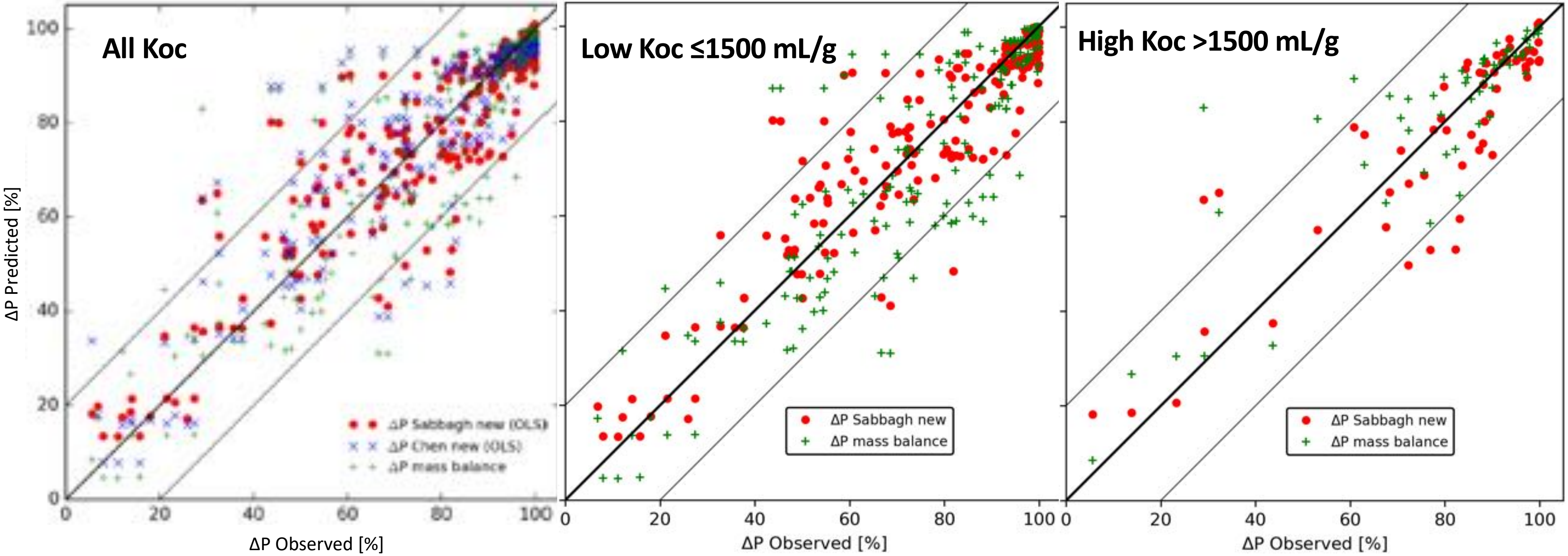
- Group data in Reichenberger et al, 2008 into two categories by pesticide property
  - Koc ≥ 1500 (mL/kg) and solubility ≤ 1 mg/L
  - Koc ≤ 1500 (mL/kg) and solubility ≥ 1 mg/L and
- For individual event-based trapping efficiency under experimental conditions, no statistically significant difference is observed for the two categories

Good VFSMOD performance of pesticide trapping efficiency ΔP equations for water soluble compounds across Koc values (low and high adsorption)

● NSE = 0.82; + NSE = 0.74

● NSE = 0.83; + NSE = 0.73

● NSE = 0.77; + NSE = 0.75



Reichenberger, S., R. Sur, C. Kley, S. Sittig, S. Multsch. 2019. Recalibration and cross-validation of pesticide trapping equations for vegetative filter strips (VFS) using additional experimental data. *Science of the Total Environment* 647 (2019) 534–550 doi:10.1016/j.scitotenv.2018.07.429

Independent VFS Model Comparison Study (report for EPA)

- In the past 15 years several organizations have started to develop mechanistically-based buffer strip models for removal of pesticides or to expand mechanistically-based nutrient models to pesticides.
- US-EPA commissioned an independent evaluation of "**uncalibrated**" VFS models
  - APEX: Texas Blacklands Research and Extension
  - PRZM-BUFF: Waterborne Environmental
  - SWAT: USDA-ARS (discarded after initial evaluation – not field)
  - REMM:USDA-ARS
  - VFSMOD: U. of Florida

Winchell, M.F., R.L. Jones and T.L. Estes. 2011. Comparison of Models for Estimating the Removal of Pesticides by Vegetated Filter Strips. In: Goh et al.(eds.), Pesticide Mitigation Strategies for Surface Water Quality. Chapter 17. Pp. 273-286. ACS Series. American Chemical Society: Washington, DC.

Independent VFS Model Comparison Study

Industry sponsored a study to compare predictions of four models on three common (U.S. and European) data sets in an uncalibrated simulation mode

- APEX
- PRZM-BUFF
- REMM
- VFSMOD

Location	Sponsor	Pesticide	Data points
Georgia: Gibbs Farm	USDA	Alachlor	2 R, 2S, 3 P
North Rhine-Westphalia: Verlbert-Neviges	University of Bonn	Pendimethelin	6 R, 6S, 6 P
Iowa – Sioux County	Dow AgriSciences	Chlorpyrifos atrazine	12 R, 12 S, 24 P

R: runoff, S: sediment, P: Pesticide

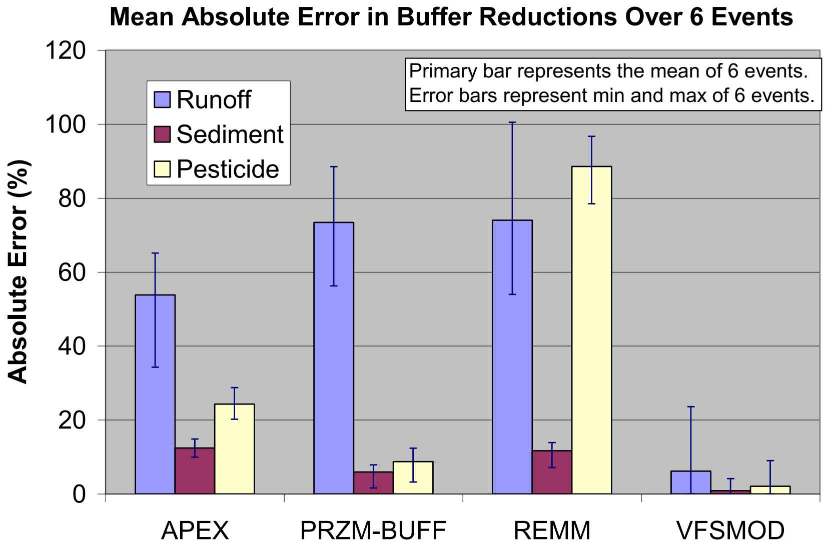
Independent VFS Model Comparison Study

VFSMOD Performs Best

Ranking by Mean Absolute Error (%)

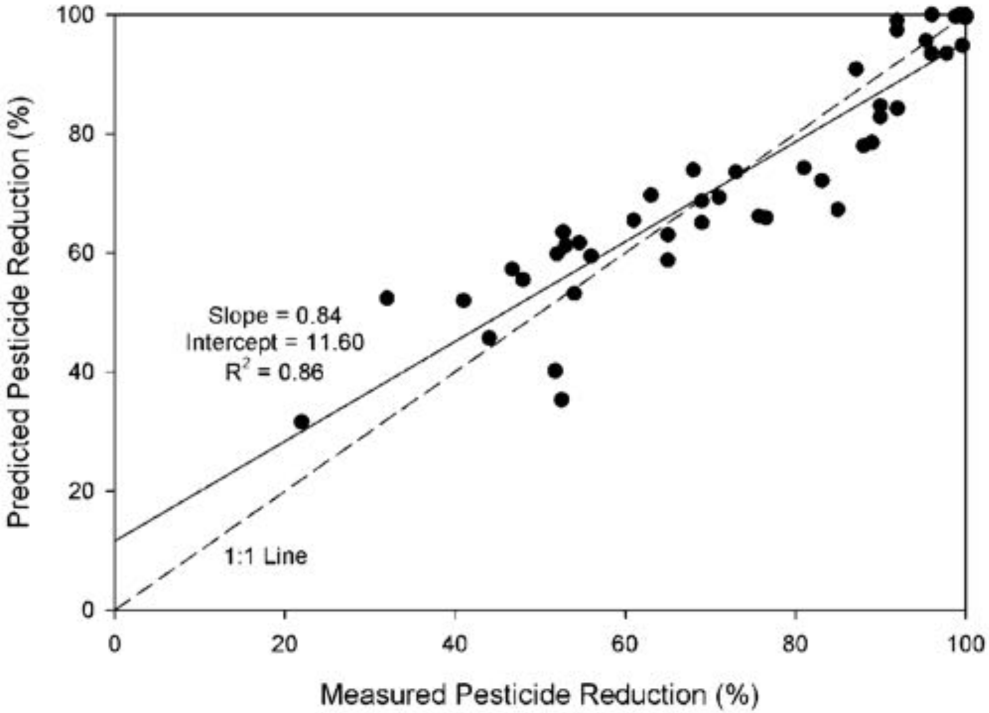
Model	**APEX**	**PRZM BUFF**	**REMM**	**VFSMOD**
Pesticide	15.6 (10)	16.3 (14)	31.2 (31)	8.5 (8)
Runoff	30.4 (20)	36.9 (28)	34.5 (32)	12.3 (9)
Sediment	19.4 (17)	31.0 (31)	30.3 (24)	12.2 (17)

Number in parentheses is the standard deviation



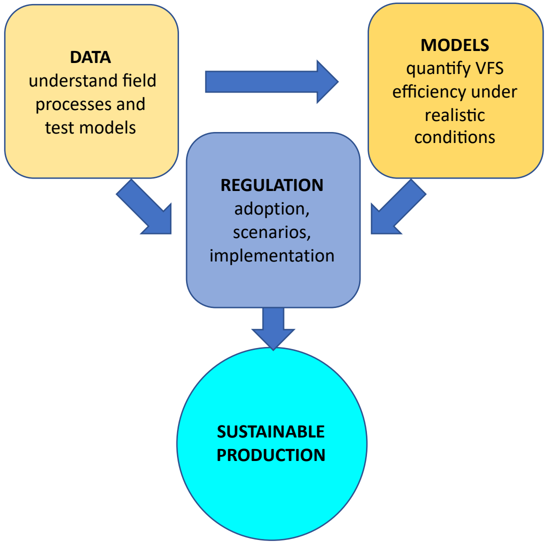
Winchell, M.F., R.L. Jones and T.L. Estes. 2011. Comparison of Models for Estimating the Removal of Pesticides by Vegetated Filter Strips. In: Goh et al.(eds.), Pesticide Mitigation Strategies for Surface Water Quality. Chapter 17. Pp. 273-286. ACS Series. American Chemical Society: Washington, DC.

…more model testing



See collection of other model testing and application publications at: https://abe.ufl.edu/faculty/carpena/vfsmod/citations.shtml

(Sabbagh, Fox et al., 2009, J. Env. Qual. 38(2):762-771)



DATA
understand field processes and test models

MODELS
quantify VFS efficiency under realistic conditions

REGULATION
adoption, scenarios, implementation

SUSTAINABLE PRODUCTION

- Factors controlling VFS efficiency under field conditions

The important question:

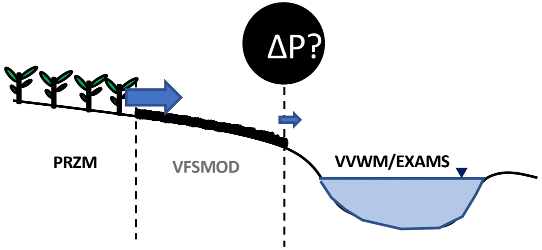
~~Do VFS reduce runoff pesticides?~~

or

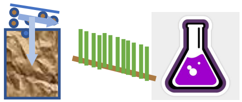
What factors control VFS pesticide mitigation efficiency under realistic field settings?

A simple question?

What are the most IMPORTANT factors for VFS pollutant mitigation efficiency?

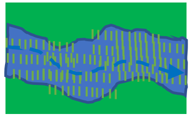


ΔP= Pesticide trapping in VFS



Common factors (hydrology, soil, vegetation, chemical)

Muñoz-Carpena et al. 2010. *J. Environ. Qual.* 39(1):630-641. doi:10.2134/jeq2009.0300

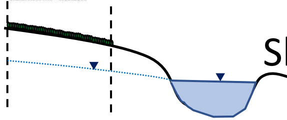


Surface channelization

Fox G.A., R. Muñoz-Carpena, G.J. Sabbagh. 2010. *J. of Hydrology* 384:164-173. doi:10.1016/j.jhydrol.2010.01.020; Lambrechts, T., S. François, S. Lutts, R. Muñoz-Carpena, C.L. Bielders.2014. J.of Hydrology 511:800–810. doi:10.1016/j.jhydrol.2014.02.030

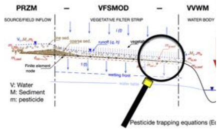
Timing of application

Sabbagh G.J., R. Muñoz-Carpena, G.A. Fox. 2013. *Chemosphere* 90:195–202. doi:10.1016/j.chemosphere.2012.06.034



Shallow water table

Lauvernet C. and R. Muñoz-Carpena, 2018. *Hydrol. Earth Syst. Sci.*, 21:1–17, doi:10.5194/hess-21-1-2017;



Long-term VFS pesticide trapping processes (empirical/mechanistic)

Muñoz-Carpena et al. 2019. *Water Research* 165:1149833. doi:10.1016/j.watres.2019.114983

Pesticide residues, degradation and remobilization

Muñoz-Carpena et al., 2015. *Chemosphere* 139:410-421. doi:10.1016/j.chemosphere.2015.07.010
Muñoz-Carpena et al., 2018. *Sci. Tot. Env*. 619–620:977–987 doi:10.1016/j.scitotenv.2017.11.093

…

Others (non-uniform/preferential soil drainage)

Orozco-López et al., 2018. *Vadose Zone* J. 17:180031. doi:10.2136/vzj2018.02.0031

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Maintenance is Important to Maintain VFS Performance

- Buffers must be properly managed to maintain performance
  - Minimize concentrated flow
  - Avoid compaction and promote infiltration
- Maintenance plan: regular mowing, weed prevention/removal, exclude cattle and vehicle traffic on VFS to avoid compaction, Reset (plough, level and reseed) VFS after major event (typically T>10 yr) or every 5 years as vegetation ages.
- Studies show that without proper maintenance, VFS can degrade and loose efficiency over time (Dillaha et al, 1989)
- Other studies (for example, Dosskey et al.; 2007) show that the performance of well managed buffer strips generally improve over time
  - Enhanced filtration due to increasing density of vegetation and changes in soil structure

Conclusions

- System-wide assessment of important factors controlling VFS pesticide mitigation is critical in risk assessment (complex problem)
- Must move away from qualitative preconceptions of important VFS efficiency drivers in favor of quantitative evaluations.
- Objective identification of important VFS efficiency drivers requires consideration of all factors present.
- Consideration of in-situ field characteristics leads to realistic assessment of mitigation efficiency
- VFSmod for mechanistic quantification mitigation of pesticides mitigation within regulatory high-tier assessments.

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Fox, G.A., R. Muñoz-Carpena, B. Brooks, T. Hall. 2020. Advancing surface water pesticide exposure assessments for ecosystem protection. *Trans. ASABE* (accepted).

‘…all models are wrong, some are useful’

‘… and remember – GIGO!!’


G. Box

Additional VFSMOD references:
https://abe.ufl.edu/faculty/carpena/vfsmod/citations.shtml

W.E. Deming

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Thank you!