VFS Effectiveness to Mitigate Pesticides: Mechanistic Analysis with VFSMOD

Identifying important drivers in pesticide mitigation exposure assessments

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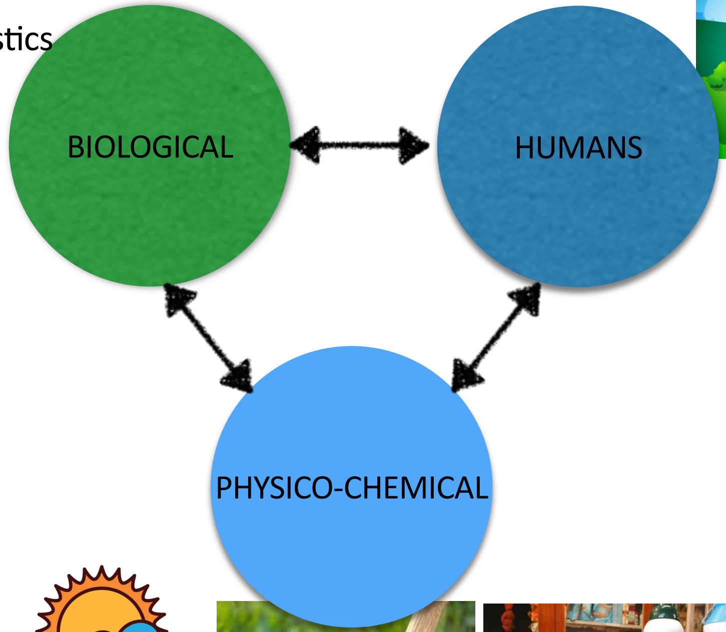
Pesticide Mitigation: Complex System

Vegetation characteristics



Land use
Socio-economic

Unknown components

+

Unknown Interactions

||

EMERGENT BEHAVIOUR

||

UNCERTAINTY

Climate Soil Chemicals

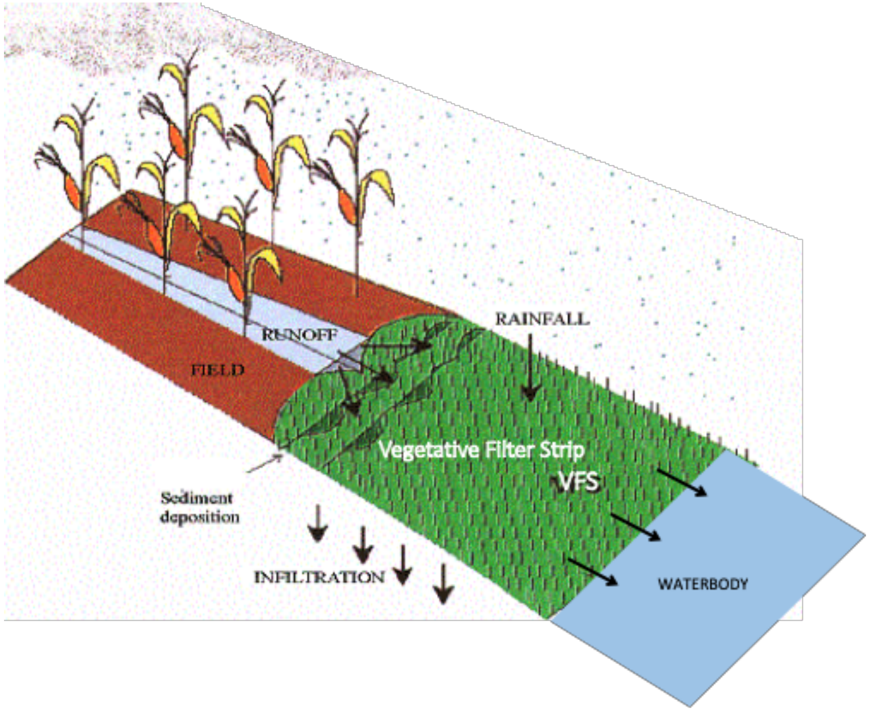
Complex systems: What can we do?

- Apply "systems thinking"- integration
- Develop data, tools and strategies to capture the complex system behavior
- Analyze important factors driving the system behavior (dimension reduction)
- Develop management strategies around important factors to influence positive behavior or reduce risk.

Modeling to understand, reproduce, forecast and control (management and planning) the system behavior

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

VFS Mitigation Efficiency: approaches

simplicity

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

transparency

Occam: simpler is better (but only if it works!)

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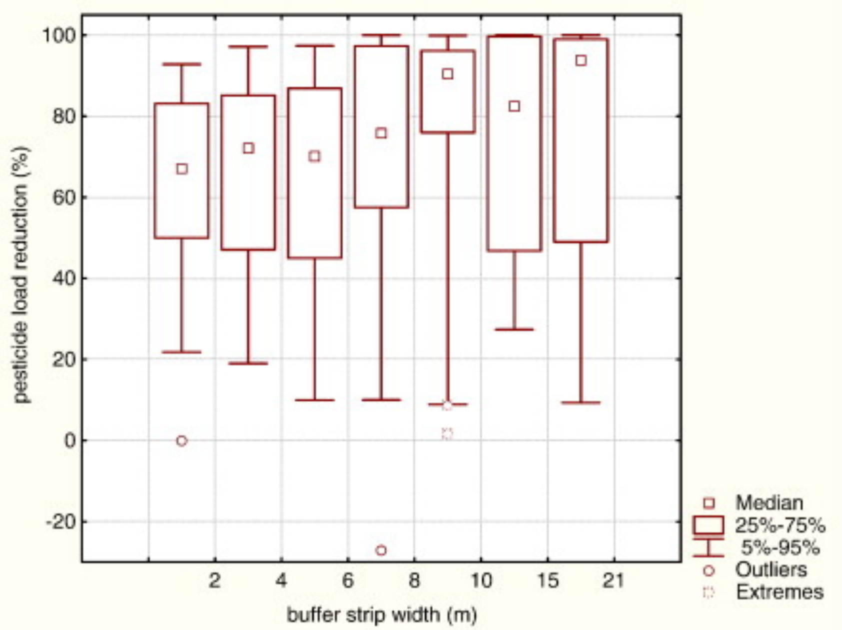
VFS Efficiency- Bigger is better?

International review (Reichenberger et al., 2007):

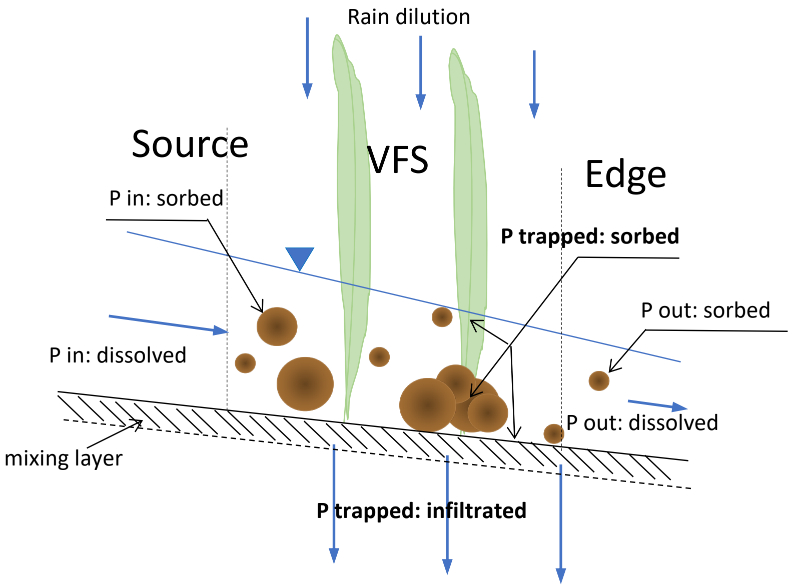
- Individual events trapping efficiency ΔP = 0-99 %.
- Long-term ΔP > 50%.
- Variability driven by site characteristics (hydrology, sedimentology and pesticide)
- Infiltration is the main process of this control (followed by sedimentation and surface adsorption)

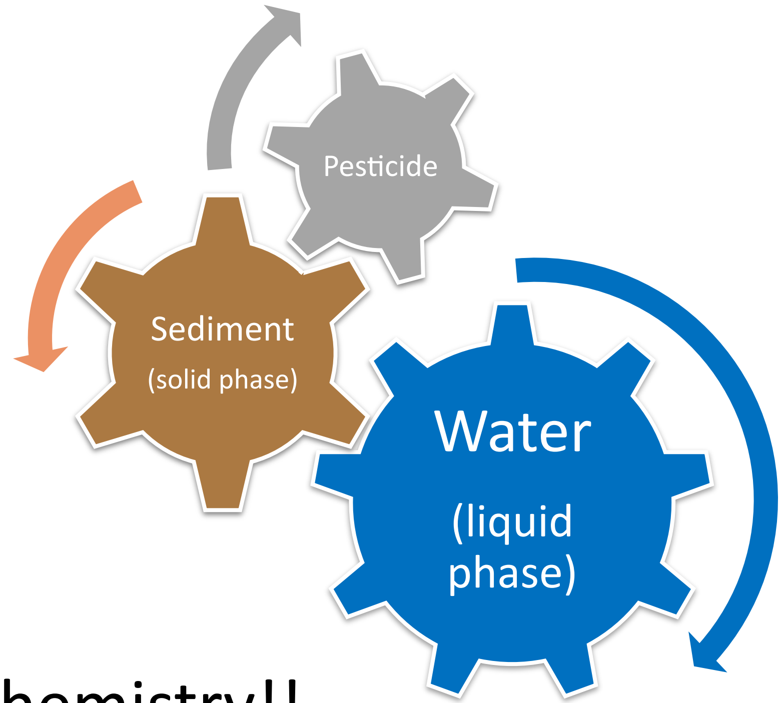


- Aggregated data insensitive to filter size → Other processes!!

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

VFS Mitigation: Mechanistic View

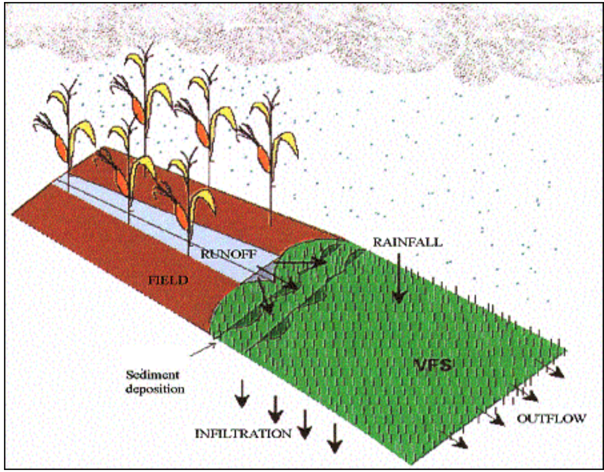




Is not about (just) chemistry!!

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)

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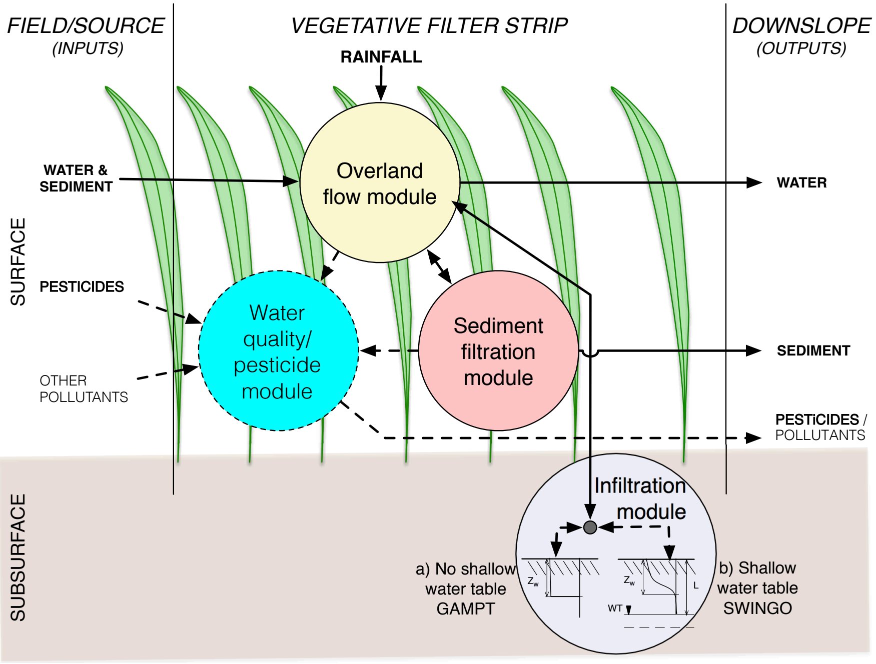
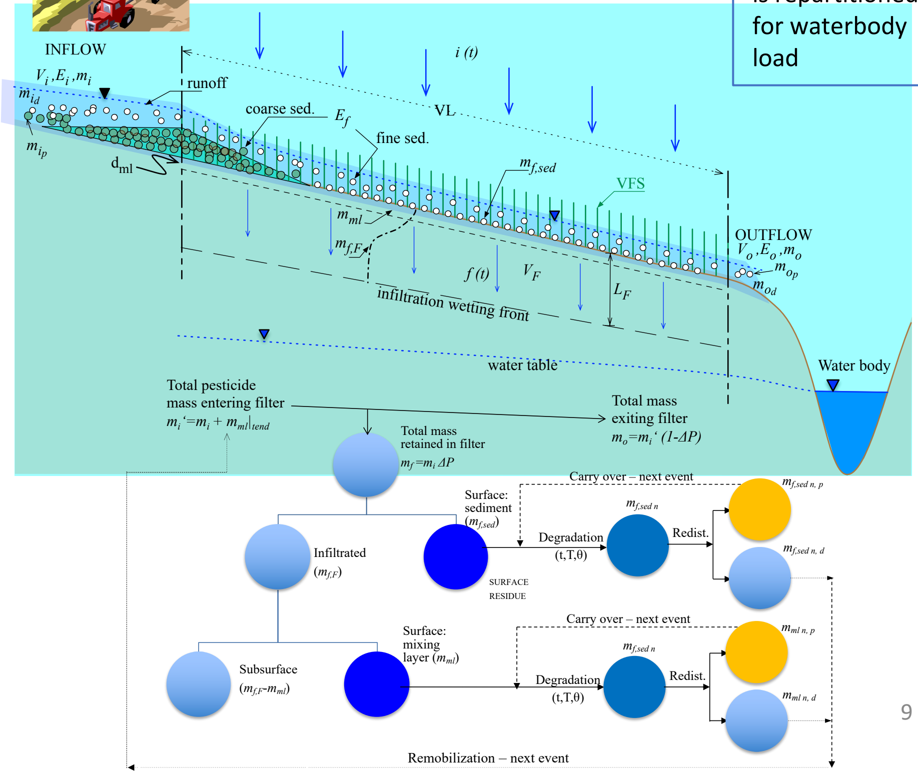
Pesticide runoff mitigation - buffers

VFSMOD: Vegetative filter strip modeling system



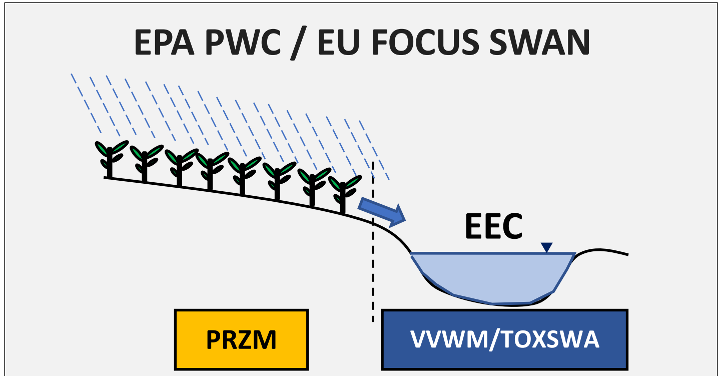
[Muñoz-Carpena et al. 1999. *J Hydrol*. 214:111– 129]



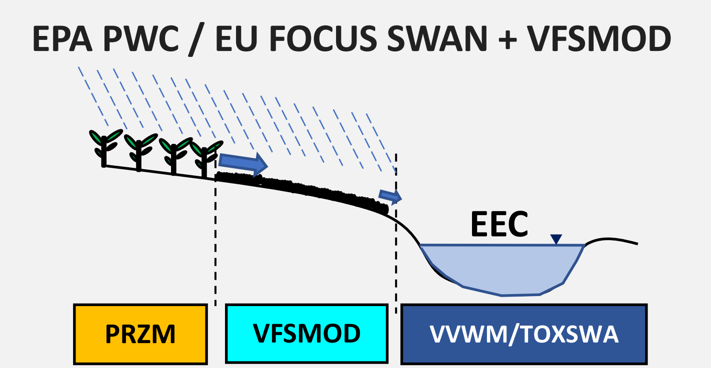
Total mass not trapped in VFS is repartitioned for waterbody load

Higher-Tier Risk Assessment: PWC/FOCUS-SWAN

Surface water exposure with **quantitative** VFS mitigation framework based on high tier EPA PWC (Pesticide in Water Calculator) or SWAN and VFSMOD



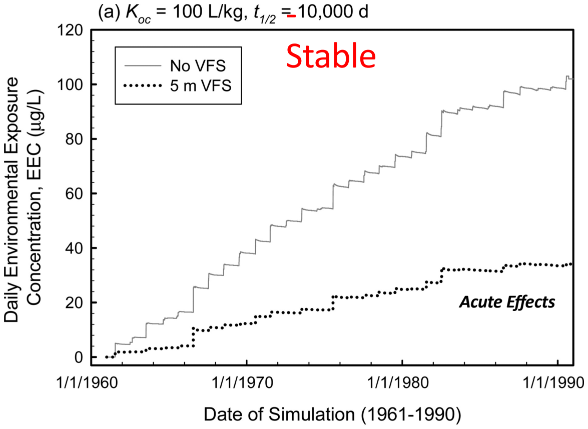
https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/models-pesticide-risk-assessment

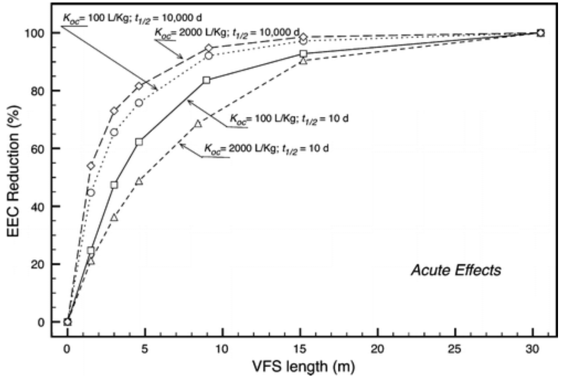


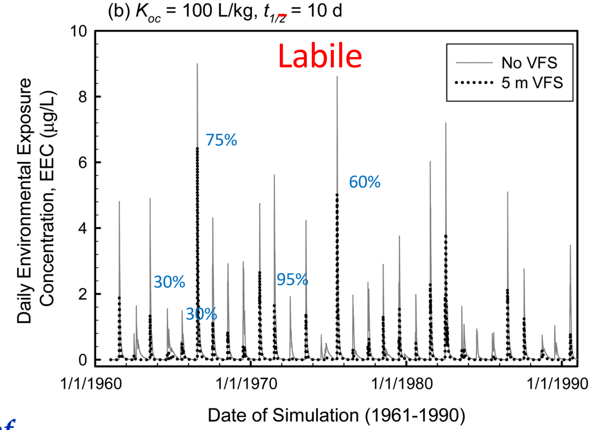
Sabbagh et al., 2010, *Env. Sci & Tech.* 44:3839-3845; Sabbagh et al., 2013. *Chemosphere* 90(2):195-202; Muñoz-Carpena et al., 2015, *Chemosphere* 139:410-421.

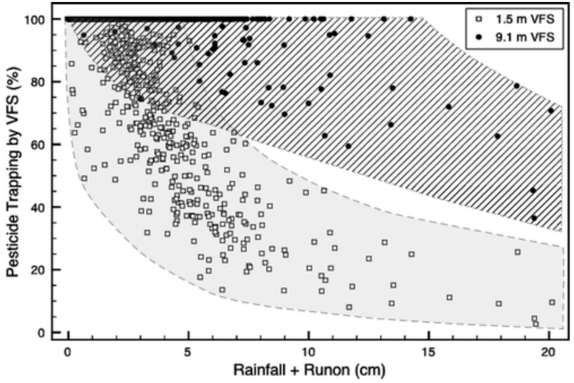
30 (10) years, daily simulations, EEC 90th percentile

Risk Assessment with Buffer Mitigation: EPA PWC-VFSMOD









Sabbagh, G., G. Fox, G., R. Muñoz-Carpena and M. Lenz. 2010. A revised framework for pesticide aquatic environmental exposure assessment that accounts for vegetative filter strips. Environmental Science & Technology 44:3839–3845 . doi: 10.1021/es100506s.

Risk Assessment with Buffer Mitigation: EU FOCUS SWAN-VFSMOD vs LM

Issue: EU FOCUS LM (higher-tier VFS mitigation) table of fixed pesticide reductions factors

Objective: evaluate the impact of the choice of SWAN-VFSMOD vs. FOCUS LM on reduction of pesticide inputs (ΔP) into surface water.

Methods: SWAN-VFSMOD run for 1031 runoff events in total (27 combinations of crop (corn/winter cereals) x 4 FOCUS R1-R4 scenarios x 2 water body (stream and pond) x runoff events in application season), VFS length in flow direction: 10 m.

ΔP was calculated from:

- SWAN-VFSMOD hydrological output (Koc values: 10 to 10^7 L/kg), with 3 pesticide trapping equations: (1) the empirical multiple regression equation by Sabbagh et al. (2009); (2) the revised Sabbagh equation (Reichenberger et al., 2019); (3) a mechanistic mass balance approach (Reichenberger et al., 2019) →ΔP: 30% and 100%
- FOCUS LM fixed reduction efficiencies (60% for runoff, 85% for eroded sediment) and pest. phase distribution → ΔP: 60% and 85%

[R. Sur, S. Reichenberger, P. Srinivasan, H. Meyer, C. Kley. 2019. Effectiveness of vegetated filter strips based on modeling with VFSMOD or fixed reduction percentages from the European regulatory framework. Paper no. AGRO 302, 2019 ACS Meeting, August 25-29, San Diego, CA (USA).]

Risk Assessment with Buffer Mitigation: EU FOCUS SWAN-VFSMOD vs LM

Findings: Because it accounts for environmental conditions SWAN-VFSMOD describes VFS performance (dQ, dE, dP) more realistically than FOCUS LM fixed efficiency approach. In contrast to FOCUS LM, SWAN-VFSMOD can predict low VFS efficiency for large rainfall/runoff events and events dominated by snowmelt. Nevertheless, the LM approach is well suited as a lower tier approach.

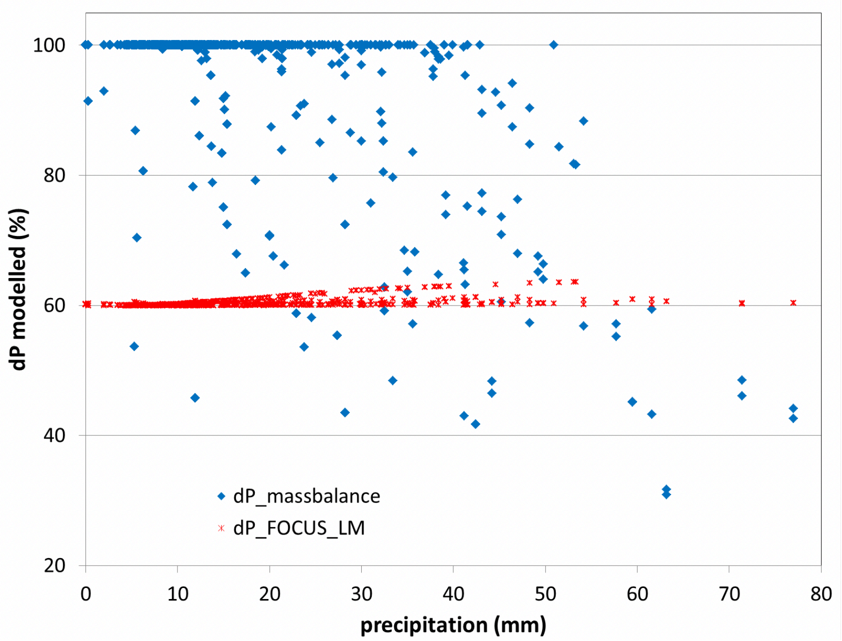


Fig. 1: Predicted pesticide reduction efficiency (ΔP) by a 10m-VFS for a dummy compound with Koc = 1000 L/kg. dP FOCUS LM: fixed efficiencies according to FOCUS (2007). dP mass balance: SWAN-VFSMOD simulation with a mechanistic mass balance trapping equation (Reichenberger et al., 2019)

[R. Sur, S. Reichenberger, P. Srinivasan, H. Meyer, C. Kley. 2019. Effectiveness of vegetated filter strips based on modeling with VFSMOD or fixed reduction percentages from the European regulatory framework. Paper no. AGRO 302, 2019 ACS Meeting, August 25-29, San Diego, CA (USA).]

Regulatory Status of VFSMOD

- America: Adopted by California DPR (PREM tool), under testing in Canada PRMA, US EPA working group. EU: accepted in Poland and EFSA cases under consideration by state members

- Mitigating the Risks of Plant Protection Products in the Environment (MAgPIE), 2013 (Brown et al., 2017).

"The model is recommended for use here given its general validation status in the scientific literature and because it is able to reflect changes in buffer efficacy based on e.g. changes in antecedent moisture conditions. Additional work is recommended outside of the MAgPIE process to reach a conclusion on the regulatory acceptability of the model in the EU. A particular issue is evaluation of coupling of the basic VFSMOD code with the regression equation for pesticide transfer across vegetated filter strips reported by Sabbagh et al. (2009).”

Evaluation of VFSMOD pesticide trapping equations

A) Experimental data evaluation with extended dataset (Reichenberger et al., 2019)

1. Original regression equation (Sabbagh)

$$\Delta P = 24.79 + 0.54\Delta Q + 0.52\Delta E - 2.42ln\left(\frac{Q}{K_d E_i} + 1\right) - 0.89\%C$$

2. Reparameterized regression equation (Refit Sabbagh)

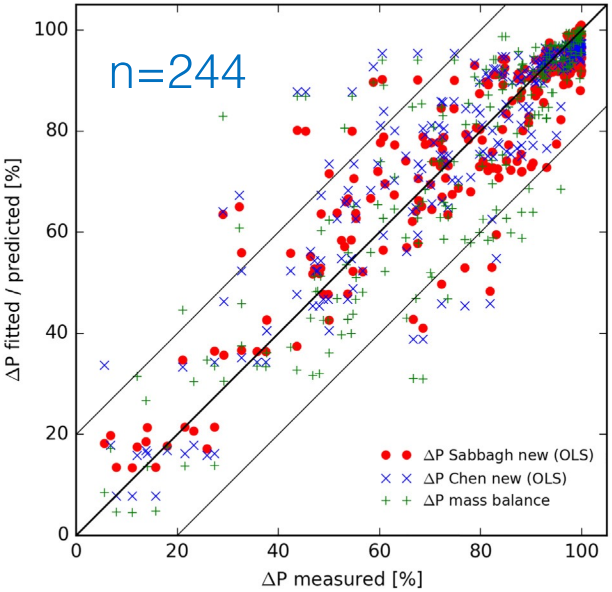
$$\Delta P = -11.5 + 0.59\Delta Q + 0.49\Delta E - 0.38ln\left(\frac{Q}{K_d E_i} + 1\right) + 0.20\%C$$

3. Mechanistic equation (Mass balance)

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

4. Regression equation (Chen)

$$\Delta P = 101 - (8.06 - 0.07\Delta Q + 0.02\Delta E + 0.05\%C - 2.17Cat + 0.02\Delta QCat - 0.0003\Delta Q\Delta E)^2$$



R^2 (Nash):

- Orig. Sabbagh: 0.528
- Refit Sabbagh: 0.82
- mass balance approach: 0.74
- Chen: 0.79

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

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Evaluation of VFSMOD pesticide trapping equations

B) Higher-tier long-term EEA evaluation (Muñoz-Carpena et al, 2019)

- 3 distinct agroecological EPA scenarios for 30-year assessments:
  - Illinois-Corn, Oregon-Wheat, California-Tomato
- Soils, land-use and climate from USEPA prescribed scenarios
- VFS grass mixture, good stand, filter lengths VL=0 (no filter), 1, 5 and 9 m (0-30 ft).
- 2-5 applications at typical insecticide timings and rates for each crop scenario.
- Pesticides compared: K_{oc} (20, 200, and 2000 L/kg) , t_s (aerobic soil metabolism half-life 10, 100, 1000 d), t_w (half-life in water and sediment 10, 100, 1000 d)
- Pesticide residue calculations, aerobic soil decay rate only (IDG=2)
- Pesticide trapping eqs: Orig. Sabbagh (1), refit Sabbagh (2), mass balance (3), Chen (4)
- 1053 (30-yr) simulations: scenario/efate/equation/VFS length combinations

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Muñoz-Carpena, R., A. Ritter, G. Fox. 2019. Comparison of empirical and mechanistic equations for vegetative filter strip pesticide mitigation in long-term environmental exposure assessments. *Water Research*. doi:10.1016/j.watres.2019.114983

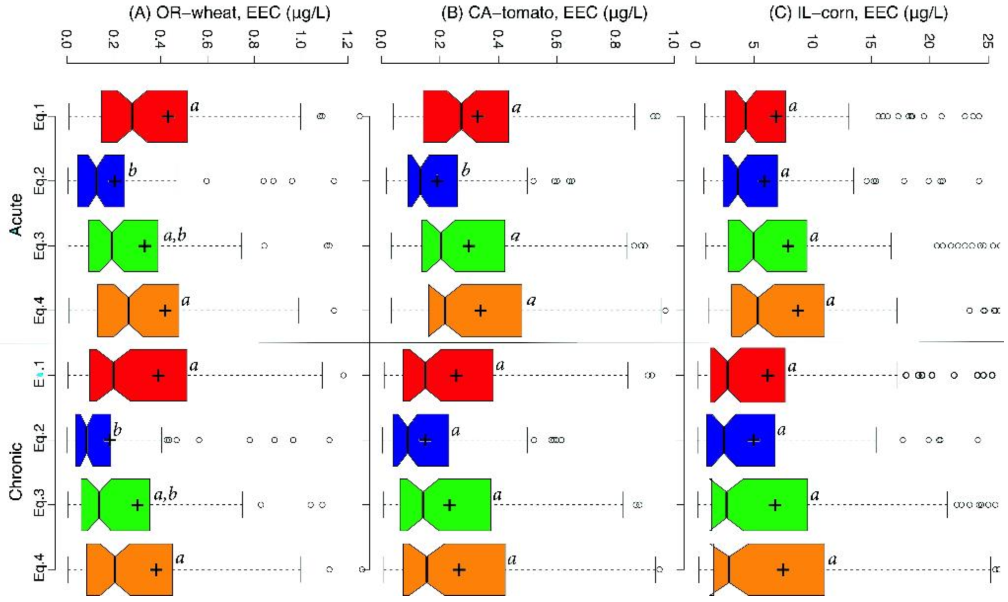
Evaluation of VFSMOD pesticide trapping equations

B) Higher-tier long-term EEA evaluation (Muñoz-Carpena et al, 2019)

Summary: best predicting eq. (refit Sabbagh, Eq2) produce smaller but not significantly different EEC than mechanistic mass balance (Eq3)

Details:

- Statistical tests on the medians:
  - No significant differences in EEC results for Eq. (1) and (4).
  - No significant differences in EEC results for Eq. (2) and (3), except for the CA-tomato acute EEC scenario.
- Variability (interquartile range):
  - Eq. 2 smallest in all cases – indicates the equation selection is likely the most important in this case compared to other factors.
  - Eq. 4 largest in all cases – other factors are likely to be more influential



n = 81 for each boxplot
a, b = groups of significantly different medians
(α=0.05)

Eq. 1 – original Sabbagh
Eq. 2 – refit Sabbagh
Eq. 3 – mass balance
Eq. 4 - Chen

Muñoz-Carpena, R., A. Ritter, G. Fox. 2019. Comparison of empirical and mechanistic equations for vegetative filter strip pesticide mitigation in long-term environmental exposure assessments. *Water Research*. doi:10.1016/j.watres.2019.114983

MAgPIE and VFSMOD in High-Tier Exposure Assessments

- The combined work of Reichenberger et al. (2019) and Muñoz-Carpena et al. (2019) fully address the MAgPIE issue of potential limitations introduced by semi-empirical VFS pesticide trapping algorithms.
- A mechanistic approach to quantitative pesticide mitigation with VFS in high-tier risk assessments is realized with VFSMOD because of its consideration for a wide range of VFS processes (i.e., shallow water table, degraded vegetation with channelization, wide range of land use, soils, hydrological, vegetation and agrochemical characteristics).
- VFSMOD allows for robust assessments of VFS quantitative mitigation for under realistic field conditions suitable for EEAs.

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The important question:

~~Do VFS reduce runoff pesticides?~~

or

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

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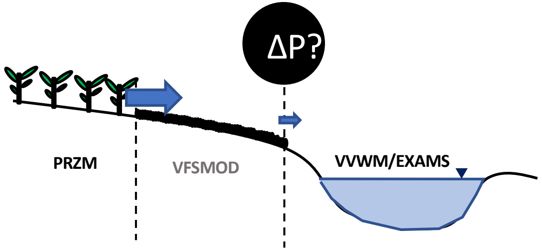
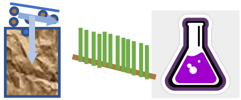
A simple question?

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

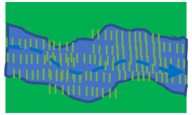


ΔP= Pesticide trapping in VFS



Common factors (hydrology, soil, vegetation, chemical)

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

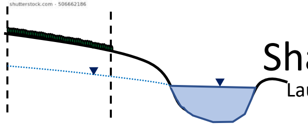


Surface channelization

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

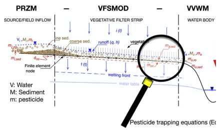
Timing of application

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



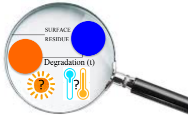
Shallow water table

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, urban heavy metal urban runoff)

Orozco-López et al., 2018. *Vadose Zone* J. 17:180031. doi:10.2136/vzj2018.02.0031; Muñoz-Carpena et al., . 2019. AGU Abstract H13I-1803

Conclusions

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

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'…all models are wrong, some are useful'

'… and remember – GIGO!!'