



Advances in VFS Modeling to Mitigate Pesticides

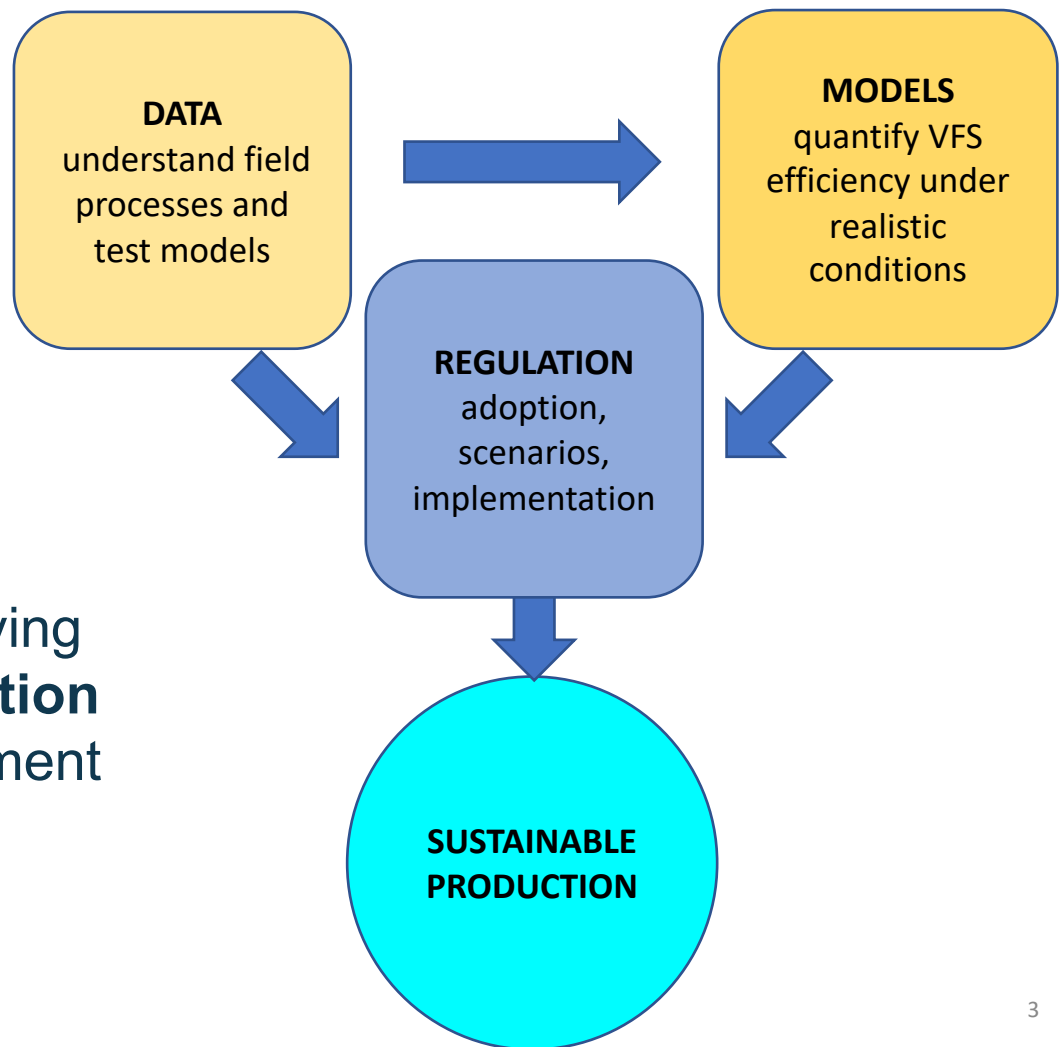
Rafael Muñoz-Carpena

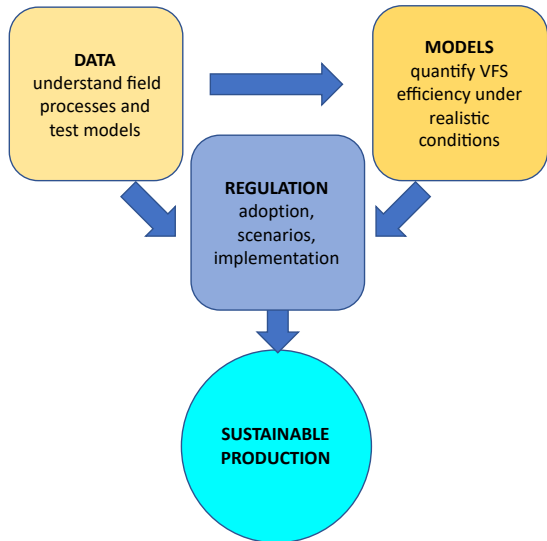
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ACKNOWLEDGEMENTS: (America) G. Fox, A. Ritter, I. Rodea, O. Perez-Ovilla, Bin Gao; (EU): S. Reichenberger, R. Sur, K. Hammel, S. Sitting, M. Campo-Bescos...



Collaborative efforts of multiple stakeholders driving **quantitative VFS mitigation** in regulatory risk assessment





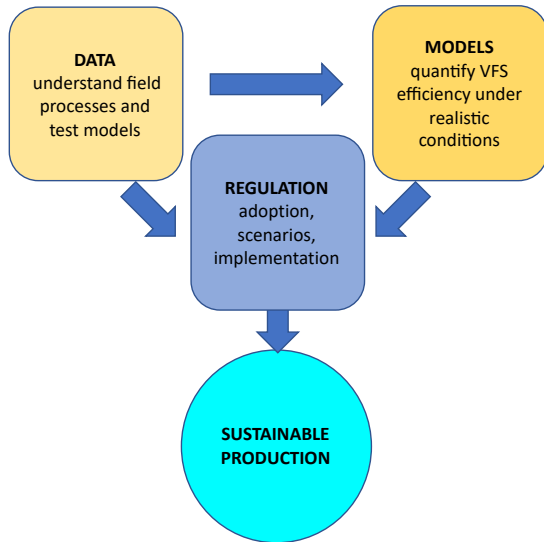
- Stakeholder transfer

2020 VFS workshops in the European Union (EU)

- Following 2018 VFS CERSA, a special seminar was organized at 2019 Conference of American Society for Agricultural and Biological Engineers (ASABE), followed by two 2020 EU stakeholder VFS workshops.
- Focus of EU stakeholder workshops: VFS **quantitative mitigation of pesticides** in surface runoff with VFSSMOD.
- 130 participants: First **industry**-targeted (80 industry representatives of 27 different entities) followed by a second for EU **regulators and agencies** (50 representatives from 7 EU Southern Region countries).
- These workshops aimed at **shifting the paradigm from qualitative, empirically based VFS pesticide mitigation approaches** to the adoption of quantitative, process-based models as part of the higher-tier pesticide risk regulatory framework.

EU summary: Adoption of SWAN-VFSMOD for STEP 4 Quantitative Mitigation

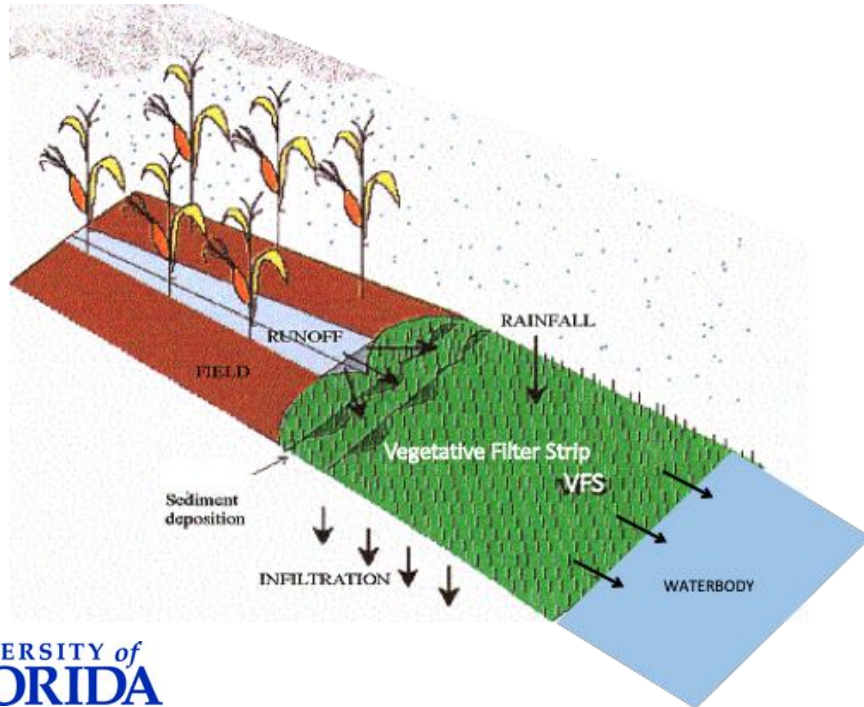
- VFSMOD, integrated in the EU STEP 4 Surface Water Assessment eNabler tool (SWAN), is a widely published and validated model and represents the “**state-of-science**” in VFS pesticide quantitative mitigation efficiency,
- In contrast to empirical EU FOCUS L&M factors, SWAN-VFSMOD **predicts more realistically** low VFS efficiency for large rainfall/runoff events and events dominated by snowmelt or seasonal water table.
- It is “**the right thing to do**”. Cases that pass the regulatory process based on stringent science- based quantitative mitigation offer transparent arguments on why they should pass. This gives both the registrant and agency a transparent, sound science-based decision and protection for litigation and responsibilities.
- It is “**the smart thing to do**” as is a “**win-win-win**” situation for regulators and the public in terms of improving water quality and for the industry in terms of identifying critical uses that require more scrutiny and mitigation.
- **Emerging farm digitalization** will likely impact site-specific risk assessments. Spatial compound distribution, diagnosis and mitigation advice will likely be needed. A mechanistic model such as VFSMOD can be run targeting individual landscape patches.
- Adoption and harmonization of advanced mitigation technologies by risk assessors and regulators in existing exposure assessment **is a current need at the global level.**



- VFSSMOD: processes advances – realistic representation

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)

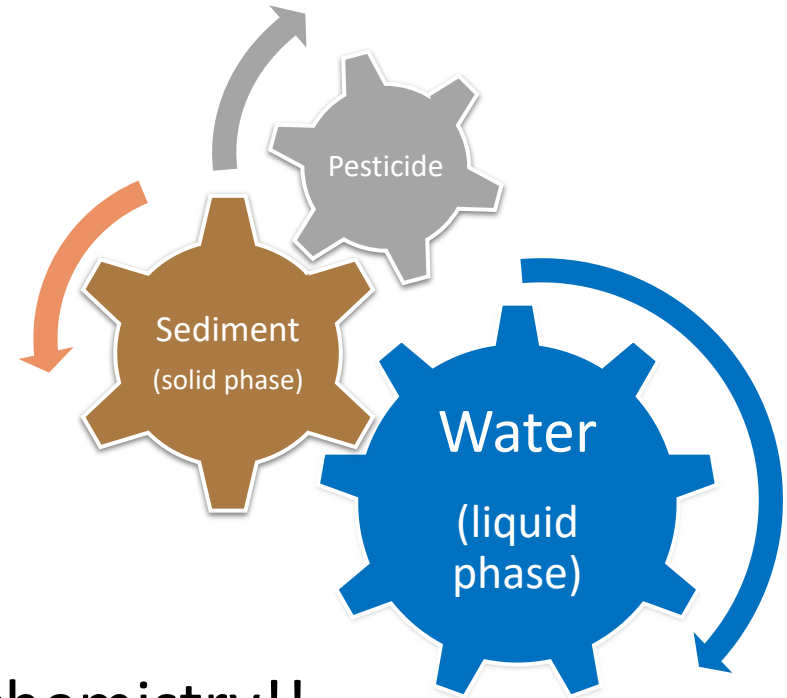
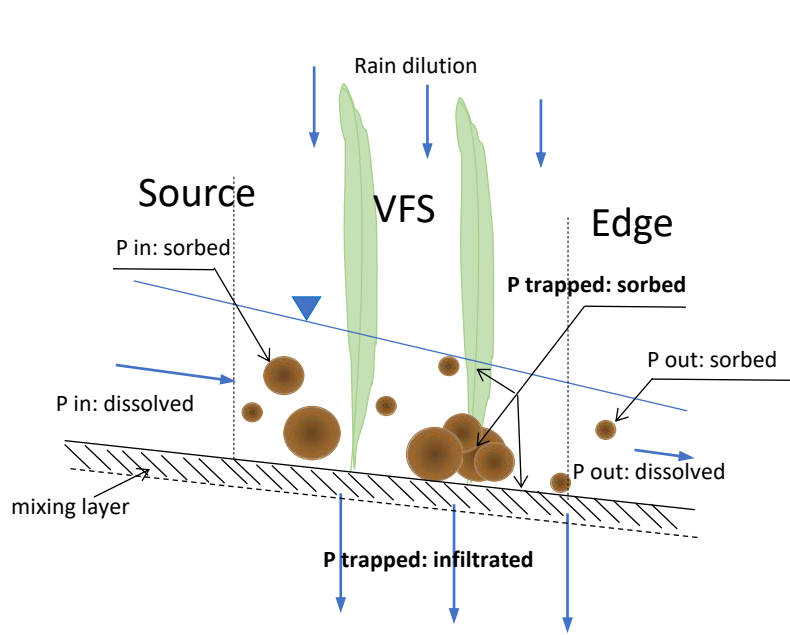


Delay settles sediment/particles (and sorbed pollutants)



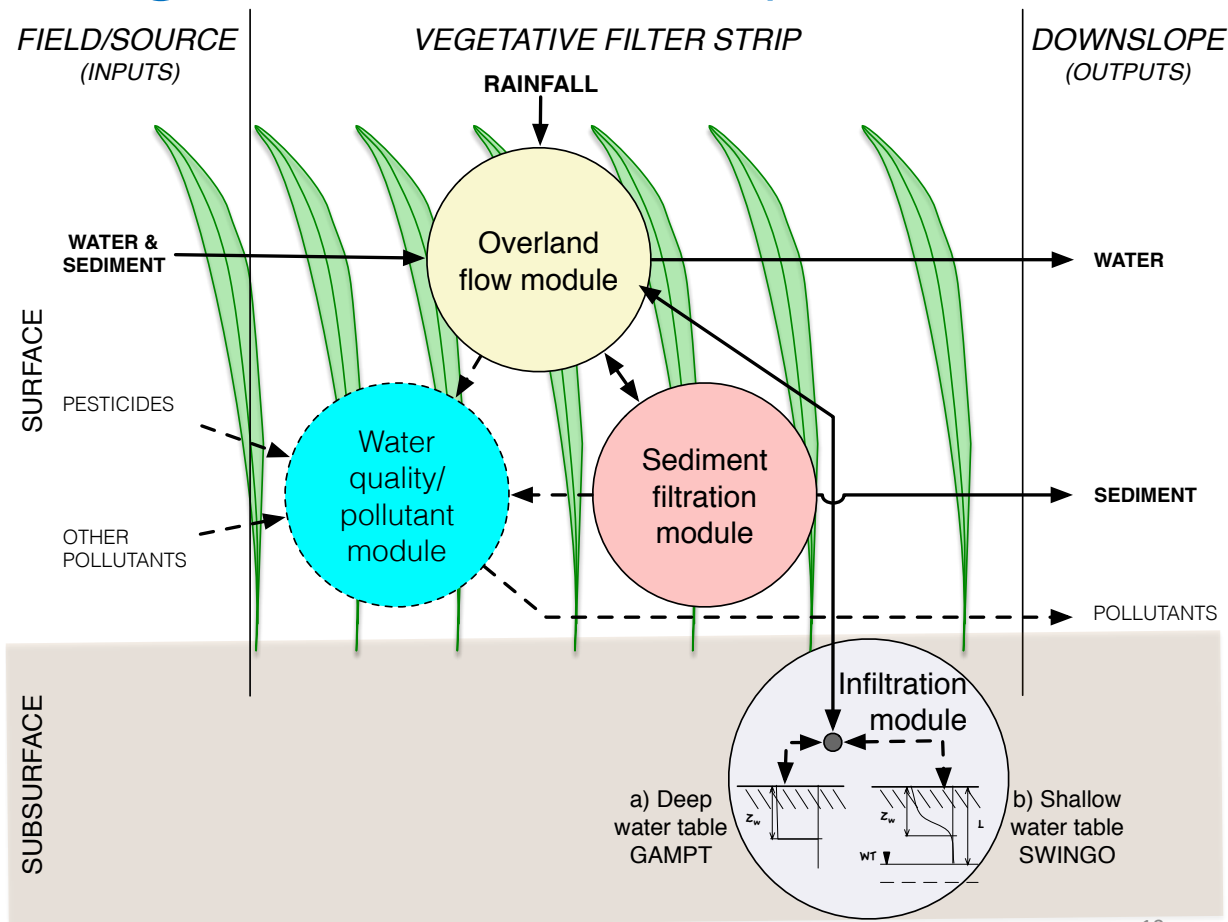
Final reduction in runoff volume, sediment, and dissolved and sorbed pollutants

Quantitative VFS Mitigation: Mechanistic View



Is not about (just) chemistry!!

VFSMOD: Vegetative filter strip model



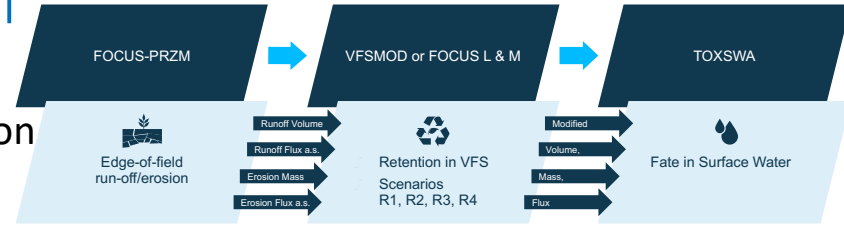
Public domain distribution
web site:

<https://abe.ufl.edu/vfsmod>

(Google: VFSMOD)

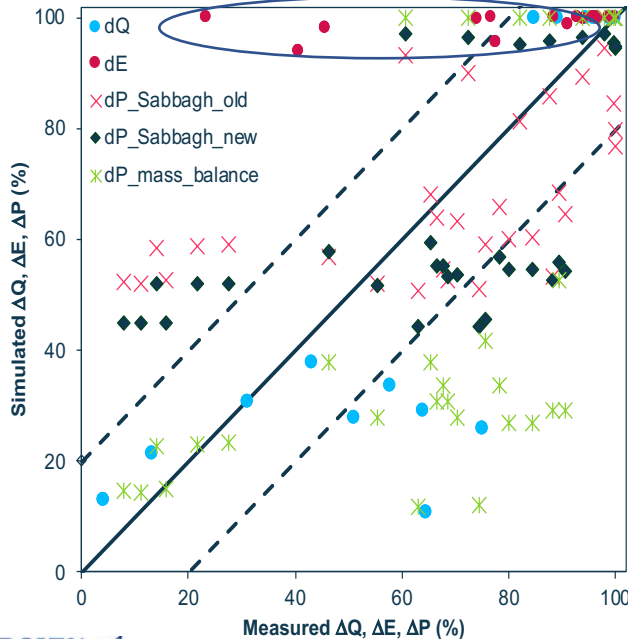
Improved Sediment parametrization

- EU FOCUS: crude single sediment for all mitigation scenarios (Brown et al., 2015). Leads to ΔE overestimation
- Need to identify scenario relevant sediment properties



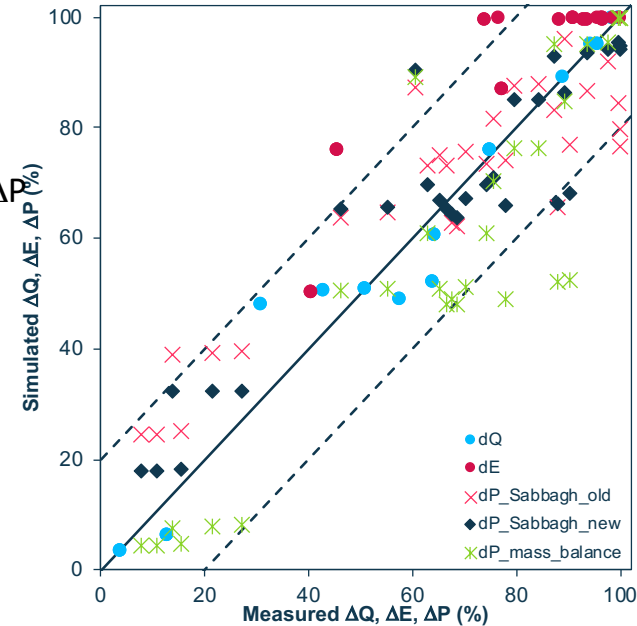
Default EU FOCUS sediment

→ Overestimated ΔE propagates to ΔP



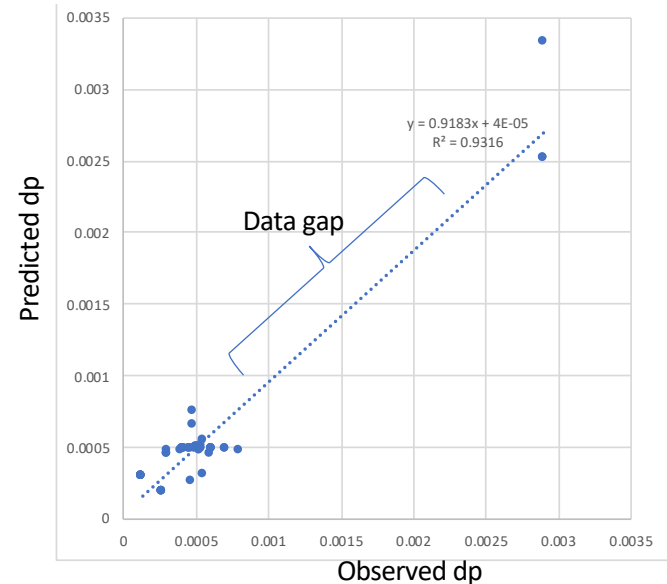
Default EU FOCUS optimized sediment (DREAM)

Mass balance equation
Provides conservative estimates
→ ΔE and in turn ΔP well improved

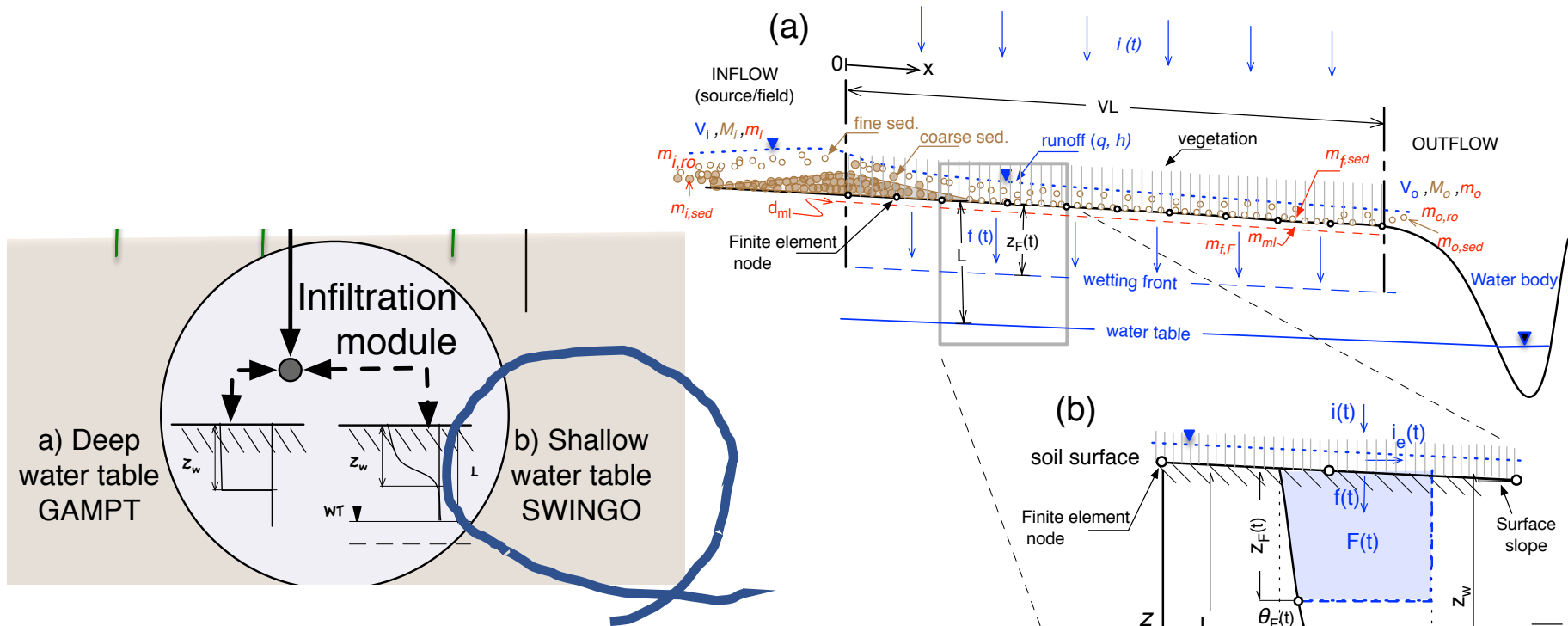


Incoming particle size (dp) prediction

- Assemble a large set of field events dataset from published and new studies with measured incoming dp into VFS.
- Predictors: sediment inflow concentration (C_i), precipitation (P), runoff and runoff reduction (V_i , V_o), runoff reduction (ΔQ), incoming and outgoing sediment mass (E_i , E_o), sediment trapped (ΔE), field soil texture.
- Preliminary results with best predictors
- Filling gap in range with new studies

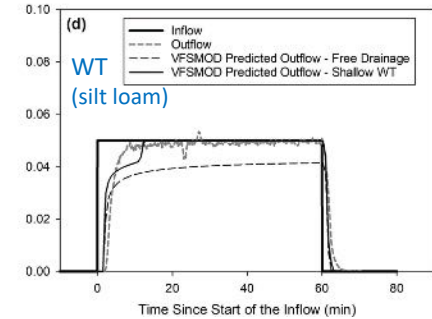
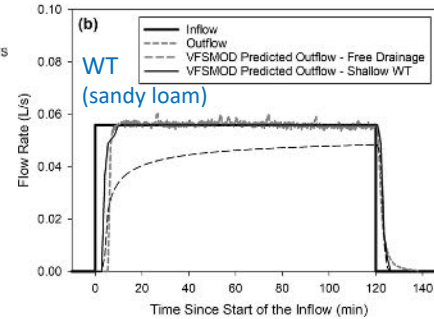
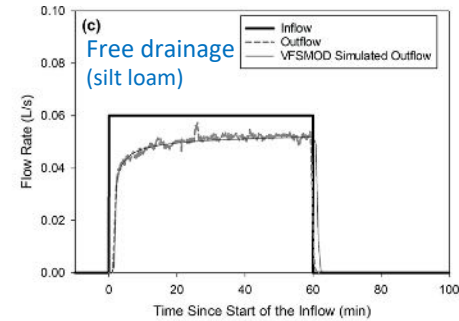
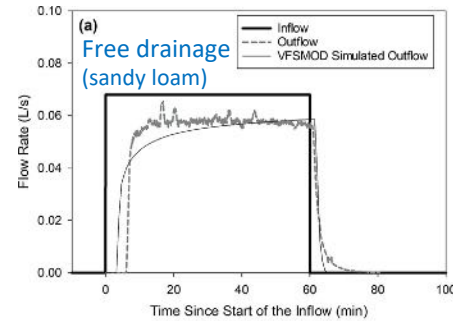
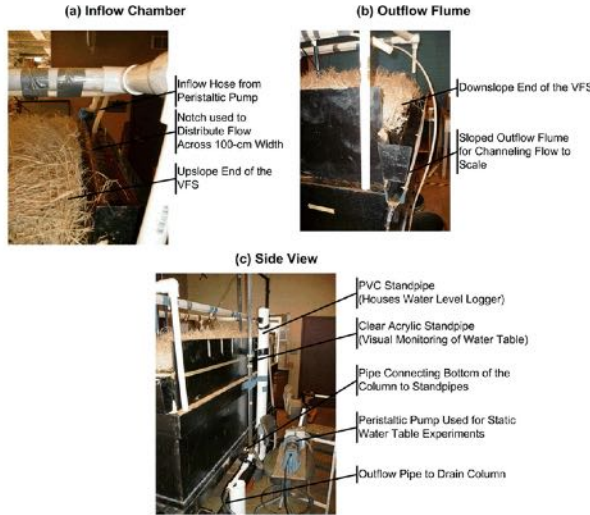


Soil infiltration module: seasonal water table



[Muñoz-Carpena, R., Lauvernet, C., and Carlier, 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](https://doi.org/10.5194/hess-22-53-2018)]

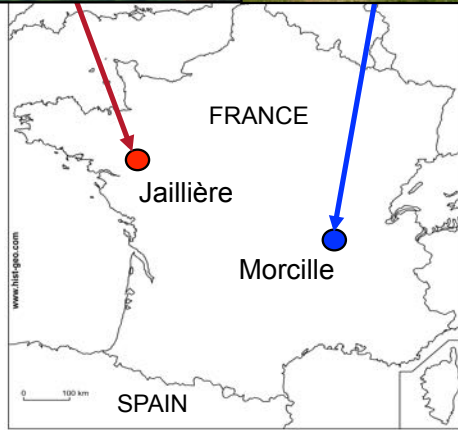
Shallow water table: laboratory testing



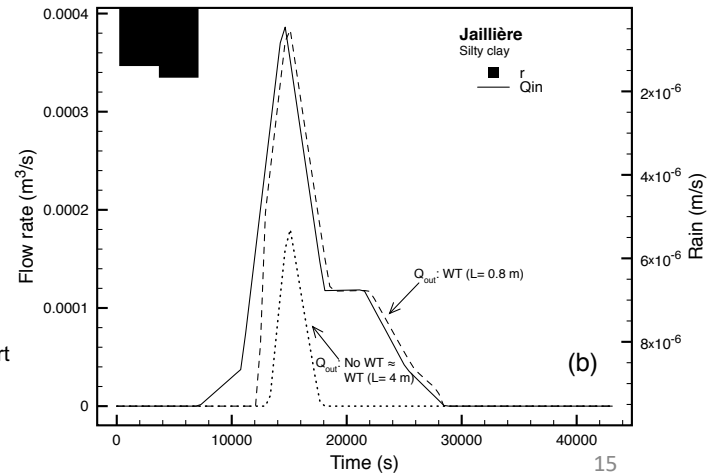
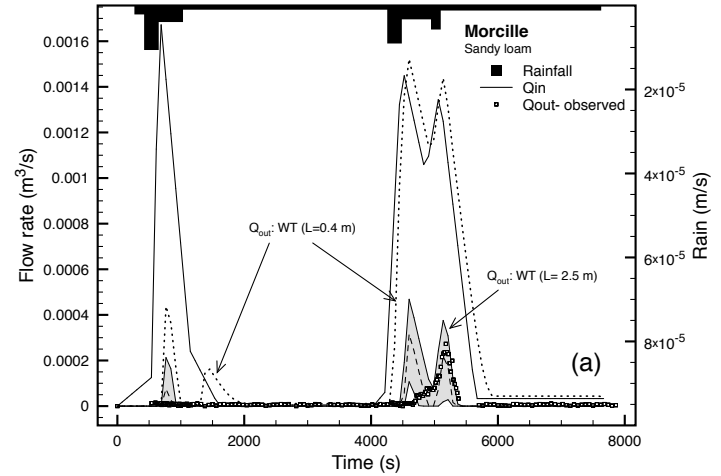
Observed versus VFSMOD-predicted runoff from the simulated vegetative filter strip for a silt loam (a and b) and sandy loam (c and d) soils with free drainage (a and c) and shallow water table WT (depths = 0.4 and 0.3 m below ground surface for the silt loam (b) and sandy loam (d) soils, respectively).

Shallow water table: initial field testing

Testing and application – shallow water table

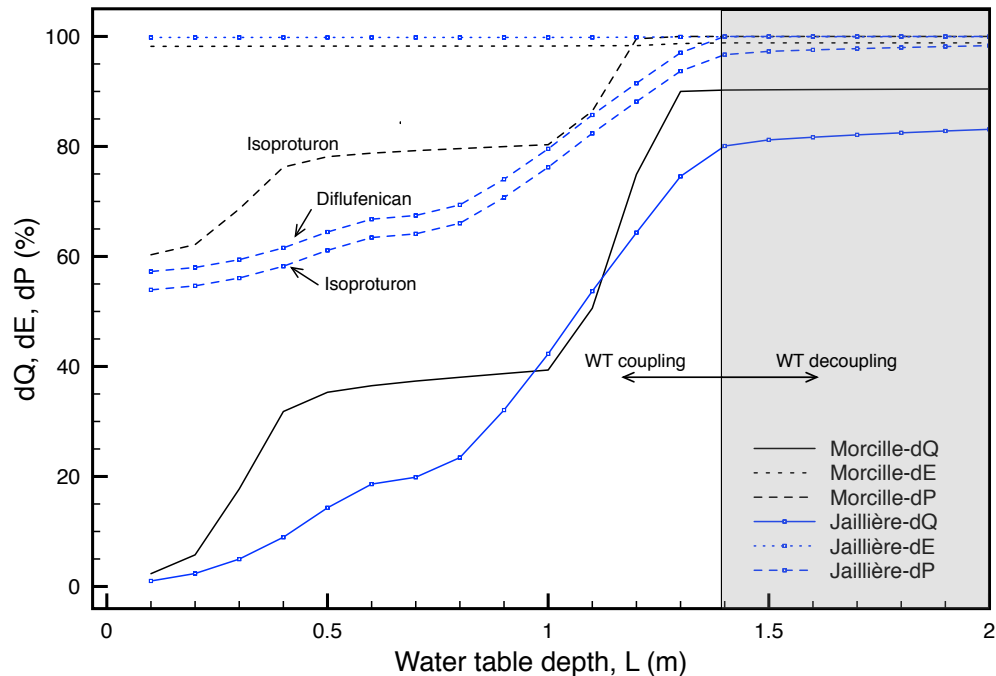


Lauvernet, C. and Muñoz-Carpena, R.. 2018. Shallow water table effects on water, sediment and pesticide transport in vegetative filter strips: Part B. model coupling, application, factor importance and uncertainty, *Hydrol. Earth Syst. Sci.* 22:71-87. [doi:10.5194/hess-22-71-2018](https://doi.org/10.5194/hess-22-71-2018)

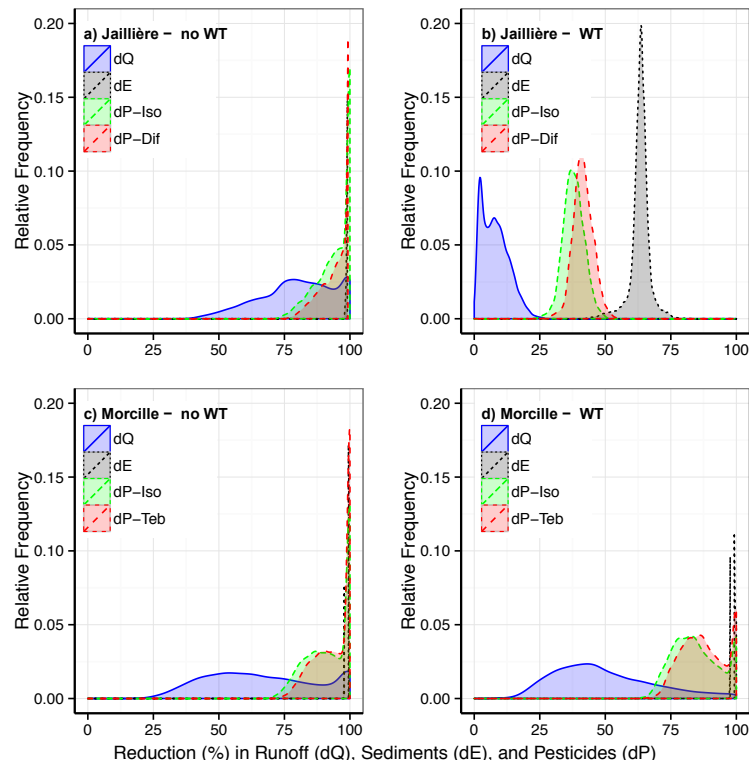


Shallow water table: pesticide reduction

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

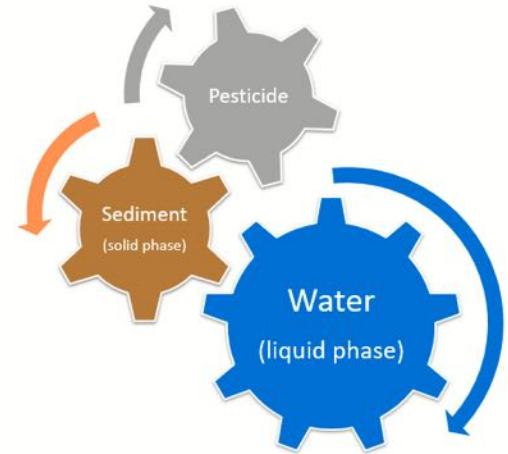


Uncertainty Analysis



Pesticide Trapping Efficiency Calculation

- VFS functions mainly through two mechanisms: infiltration and sedimentation
- Mobility (K_{oc}) determines chemical distribution in water and sediment phase
- Infiltration is the dominant process to retain water soluble compounds
 - Infiltration rate and capacity are controlled by soil characteristics, soil water content and rainfall intensity, therefore pesticide trapping efficiency is event based and dynamic
- VFSMOD, as a process-based model, captures hydrological processes governing infiltration, sedimentation and pesticide trapping



Pesticide Trapping Efficiency Calculation

- **Sabbagh equation** (2009) using 47 data points

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

- **Sabbagh-recalibrated** using 244 data points (Reichenberger et al, 2018)

- **New Mass balance** (Reichenberger et al, 2018)

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

with V_i = incoming run-on volume (L)

where ΔP = relative reduction (%) of total pesticide load,

ΔQ = relative reduction (%) of total inflow,

ΔE = relative reduction (%) of incoming sediment load,
 $\%C$ = clay content (%) of field The phase

F_{ph} = phase distribution coefficient (ratio of dissolved and particle-bound pesticide mass in inflow),

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

where Q_i = total water inflow into the VFS (run-on + rainfall + snowmelt (L)), E_i = incoming sediment load (kg), K_d = linear sorption coefficient (L kg⁻¹).

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](https://doi.org/10.1016/j.scitotenv.2018.07.429)

Pesticide Trapping Efficiency Calculation

Validation with measured data shows good model performance

- Sabbagh-recalibrated: $r^2 = 0.82$
 - 5 regression parameters and 6 independent variables: ΔQ , ΔE , Q_i , E_i , K_d , %clay
- **Mass balance:** $r^2 = 0.74$
 - **NO (0)** regression parameters, 5 independent variables: V_i , K_d , E_i , ΔE and ΔQ

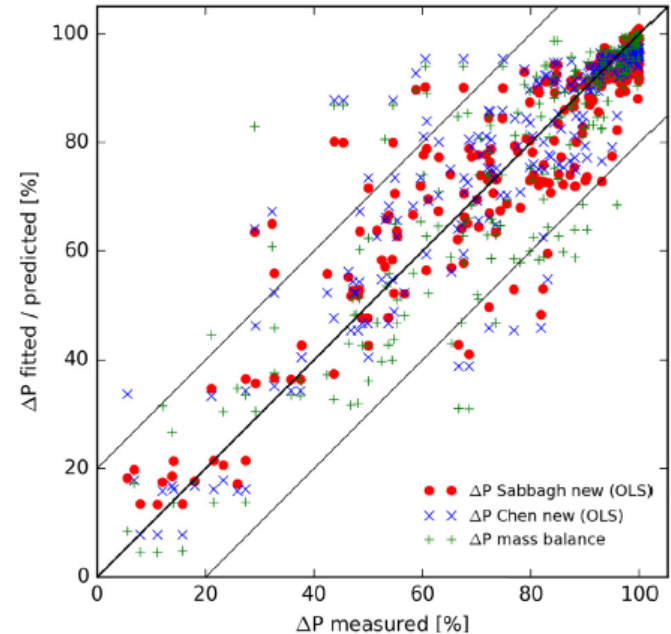
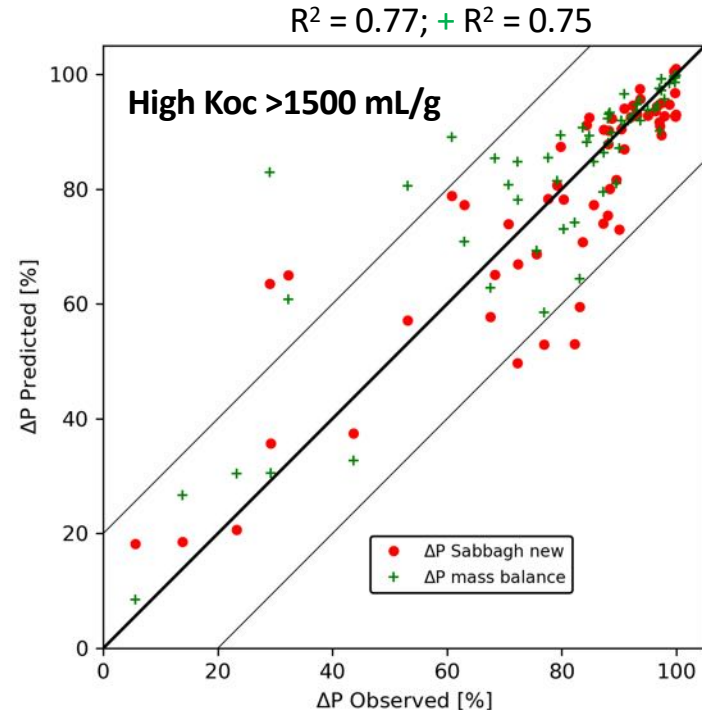
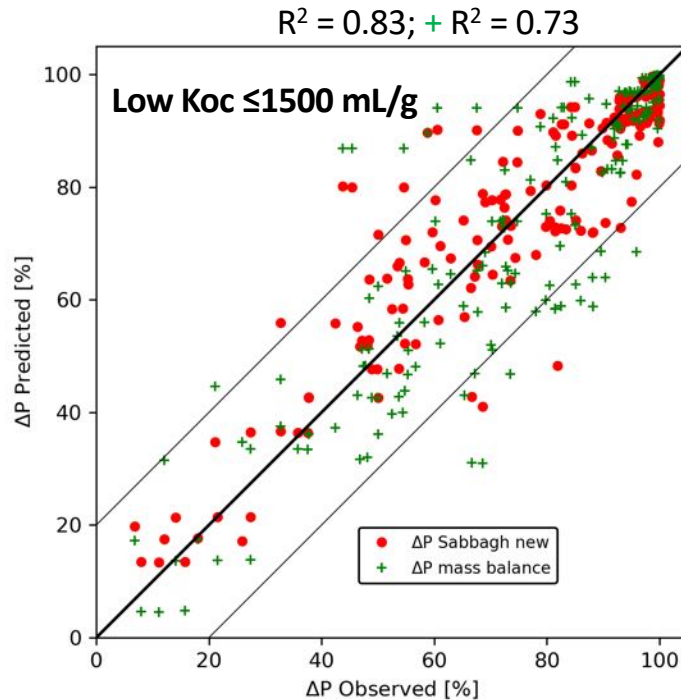


Fig. 1. Measured ΔP vs. ΔP fitted with the Sabbagh and Chen equations (OLS regression) and ΔP predicted with the mass balance approach for the full test dataset ($n = 244$).

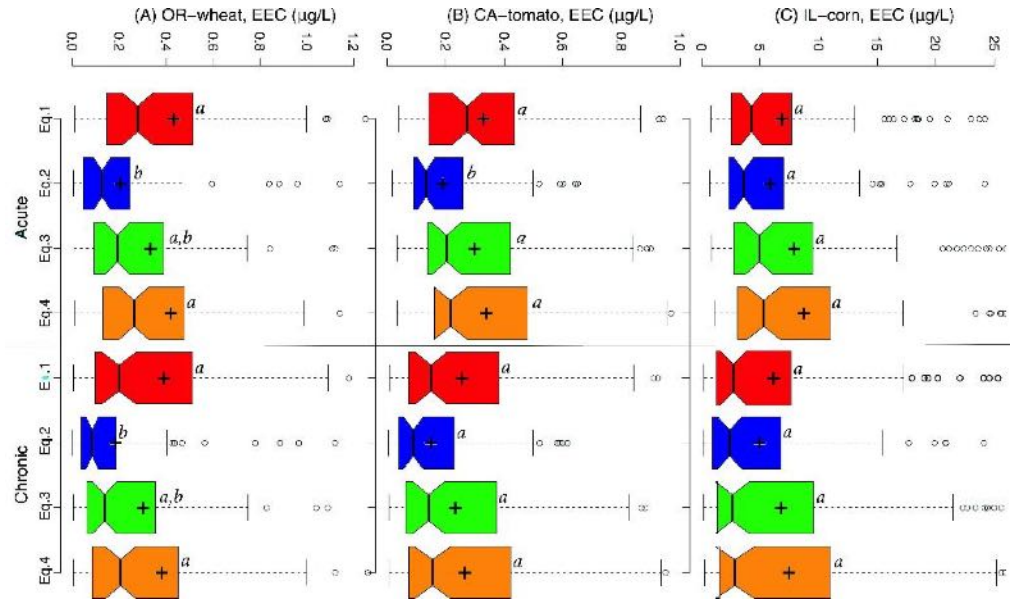
Pesticide Trapping Efficiency Calculation

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



VFS Eq. Comparison in Long-Term EPA Exposure Assessments

- Ranking the equations based on EEC medians: Chen(E4) <> Orig. Sabbagh (E1) > Mass balance (E3) > Refit Sabbagh (E2)
- 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
 $(\alpha=0.05)$

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

VFS Eq. Comparison: EU FOCUS SWAN VFSSMOD vs. LM

- **Methods:** SWAN-VFSSMOD 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.
- **Findings:** Because it accounts for environmental conditions SWAN-VFSSMOD describes VFS performance (dQ, dE, dP) more realistically (“higher-tier”) than FOCUS LM fixed efficiency approach.
- In contrast to FOCUS LM, SWAN-VFSSMOD 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.

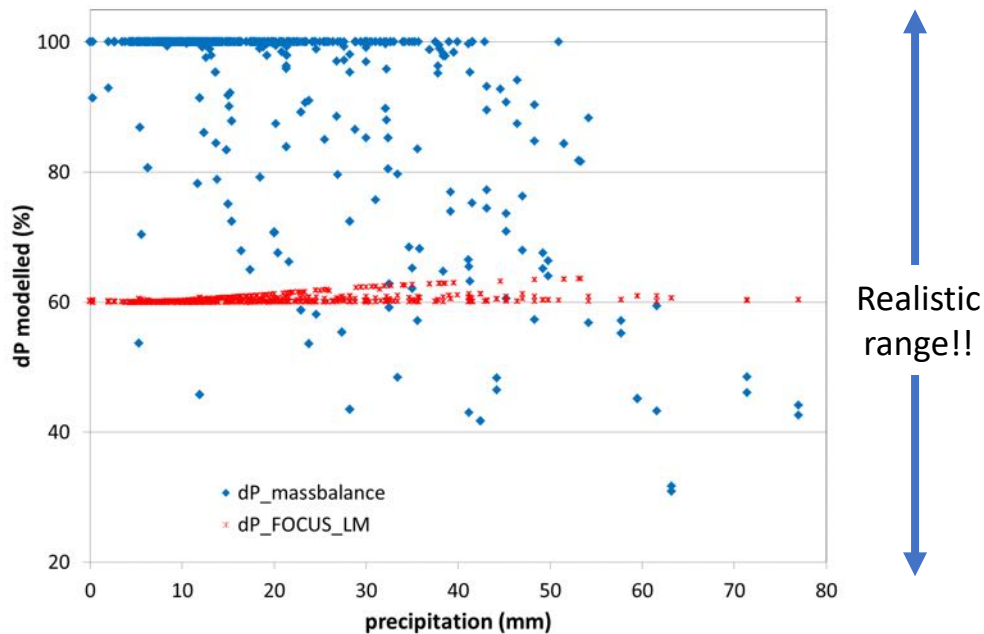
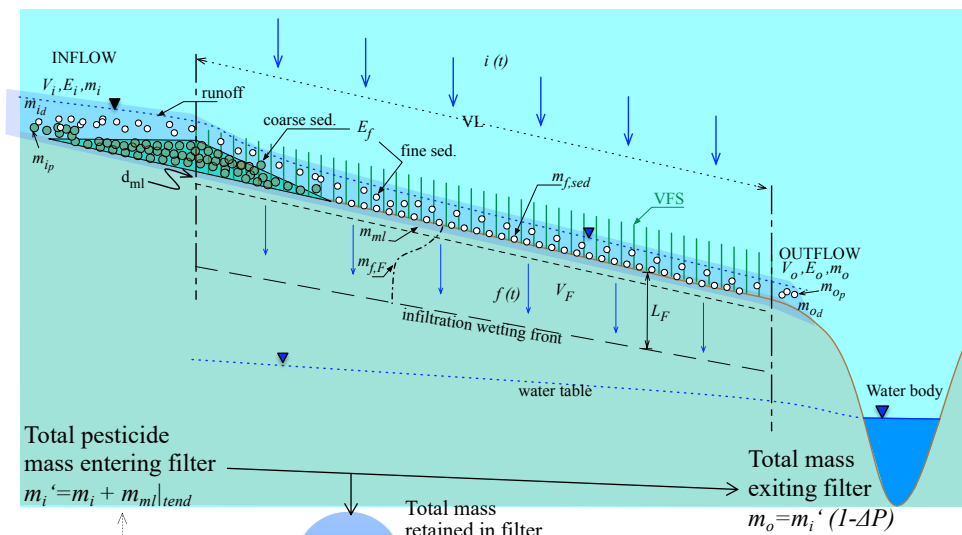


Fig. 1: Predicted pesticide reduction efficiency (ΔP) by a 10m-VFS for a dummy compound with $K_{oc} = 1000$ L/kg. dP FOCUS LM: fixed efficiencies according to FOCUS (2007). dP mass balance: SWAN-VFSSMOD simulation with a mechanistic mass balance trapping equation (Reichenberger et al., 2019)

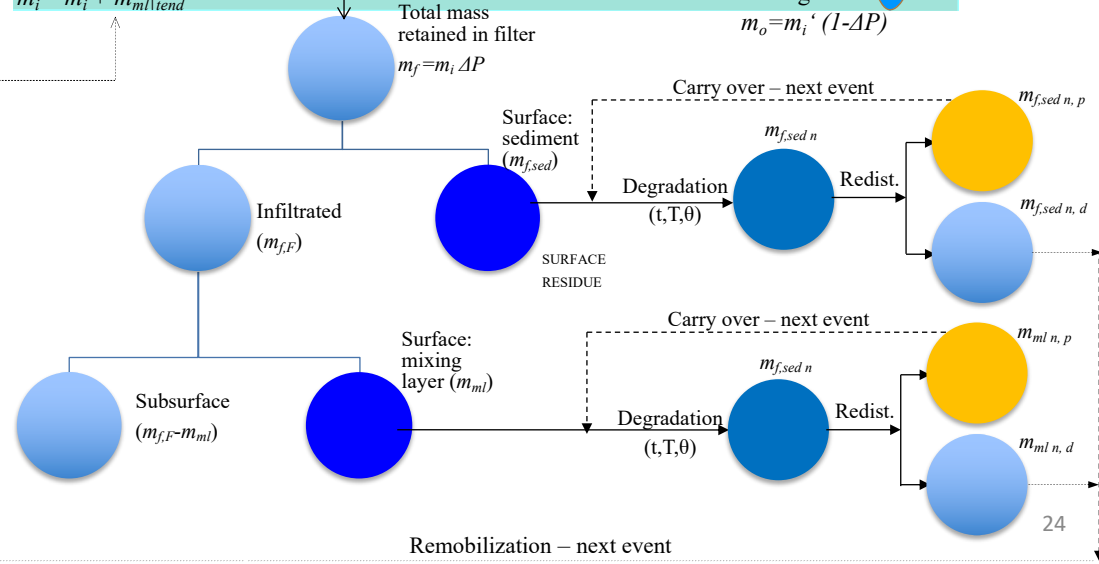
Fate of VFS pesticide residues

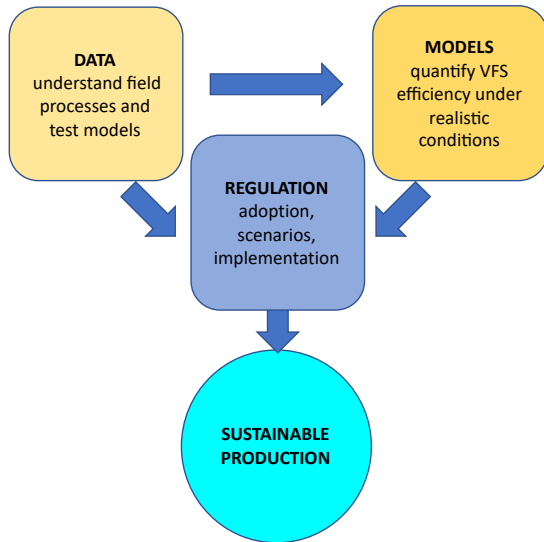
- Mixing layer and deposited sediment
- Dissolve and sorbed redistribution
- Degradation
- Remobilization
- Carry over



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](https://doi.org/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 Environment* 619-620:977-987, [doi:10.1016/j.scitotenv.2017.11.093](https://doi.org/10.1016/j.scitotenv.2017.11.093)

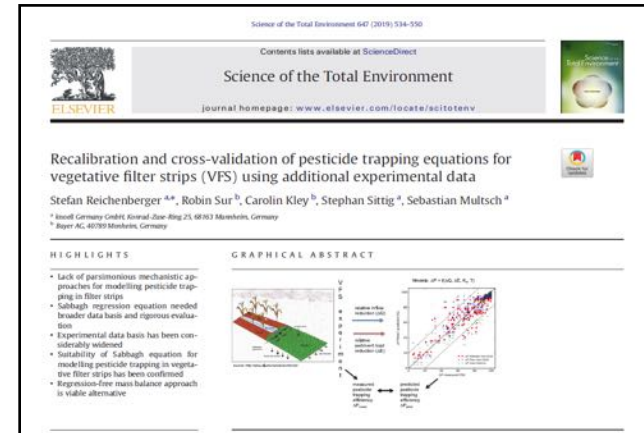
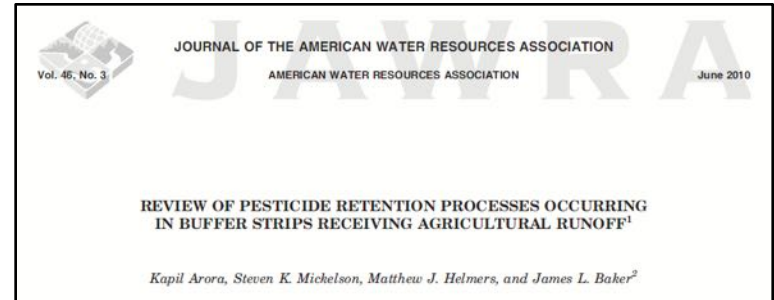




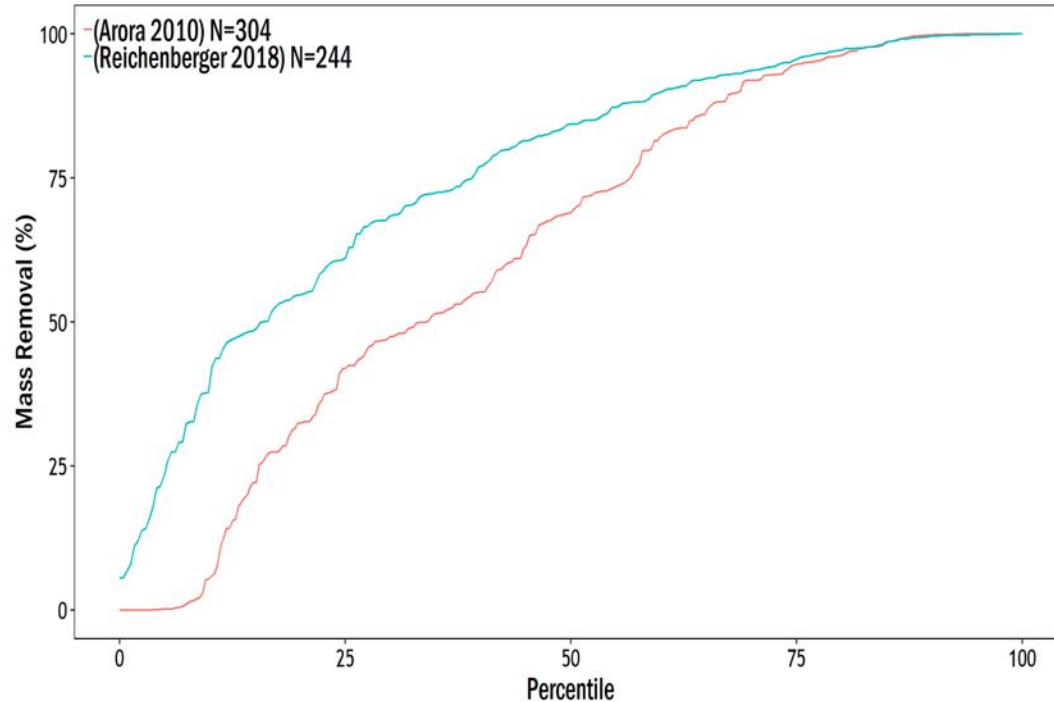
- Field Data and Model Testing

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, 2019) compiled published data for evaluations of pesticide trapping efficiency equations
- 15 studies and 244 individual test results for 18 pesticides and metabolites



VFS Pesticide Removal Effectiveness

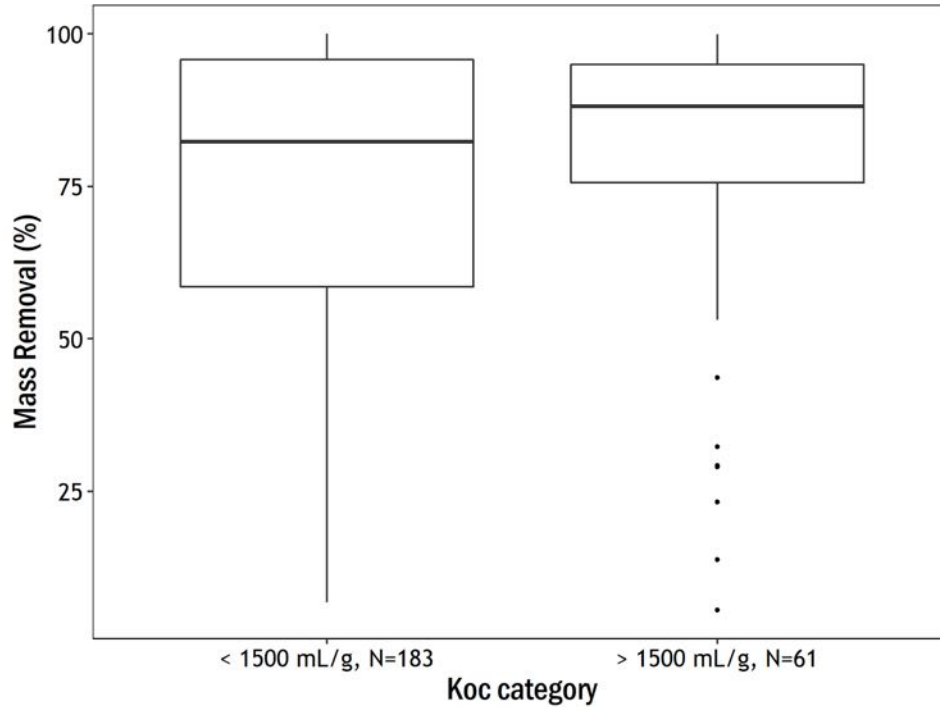


Mass removal:

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

Cumulative distribution of pesticide mass removal

Field Data: VFS efficiency with Koc Water Soluble Compounds



- Group data in Reichenberger et al, 2019 into two categories by pesticide property
 - $K_{oc} \geq 1500$ (mL/kg) and solubility ≤ 1 mg/L
 - $K_{oc} \leq 1500$ (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

Redux: Independent VFS Model Comparison Study

- 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)
 - REMM:USDA-ARS
 - VFSSMOD: 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.

Redux: 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
- VFSSMOD

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

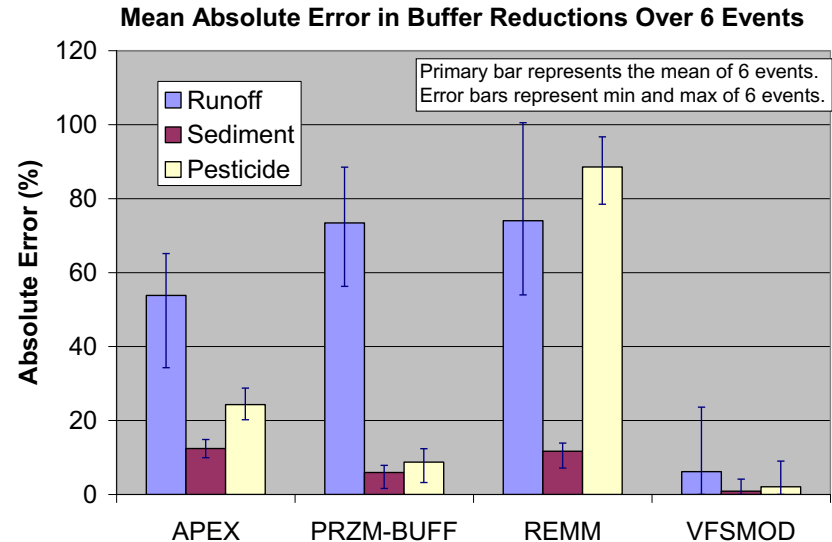
Redux: Independent VFS Model Comparison Study

VFSMOD Performs Best

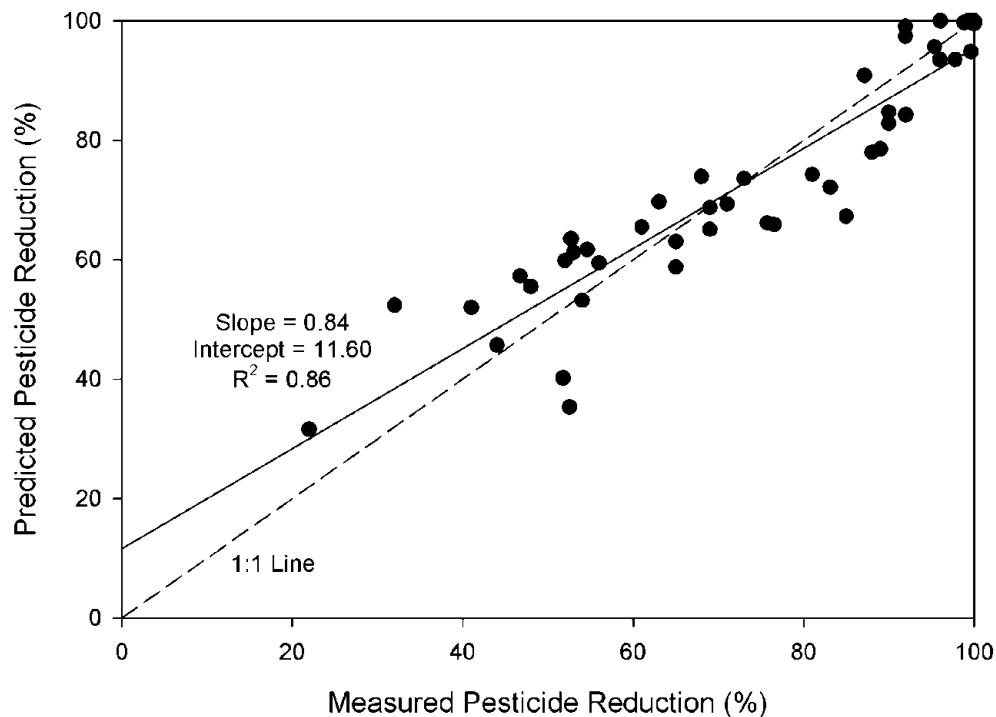
Ranking by Mean Absolute Error (%)

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)

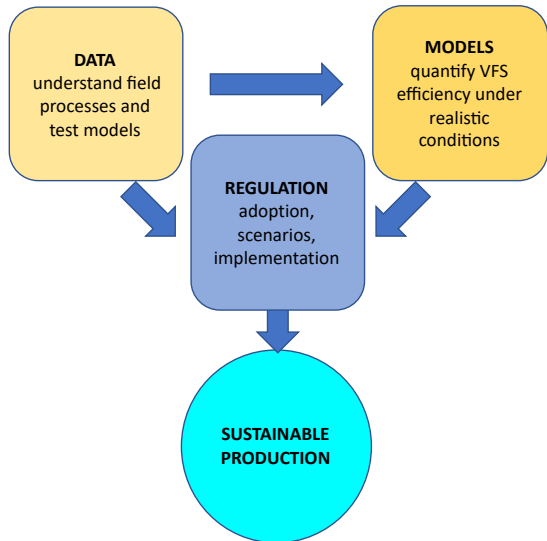
Number in parentheses is the standard deviation



...more model testing



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



- Quantitative Mitigation with VFSSMOD in high-tier assessments

VFS Consideration in Regulatory Process

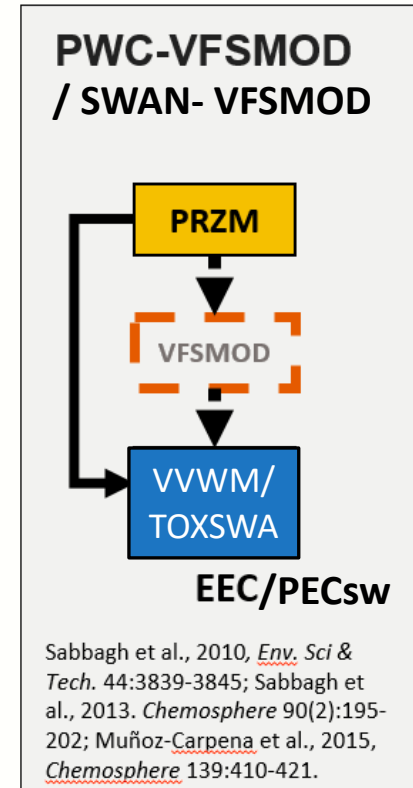
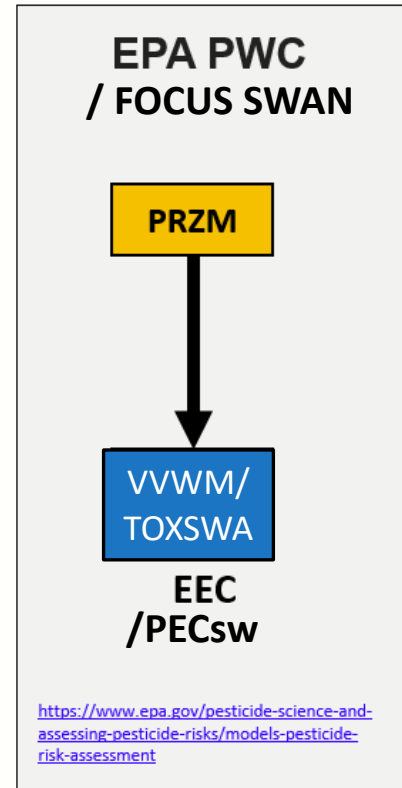
- VFS has long and widely been used for soil erosion control and runoff mitigation
- Currently, EPA /PMRA/FOCUS considers VFS as a product-label mitigation approach to reduce off-site pesticide transport to surface water
 - A result of risk/benefit decision
 - Often not based on quantitative risk assessment



Riparian buffer strips in Airlie Gardens, Wilmington, NC , constructed between 1906 and 1937

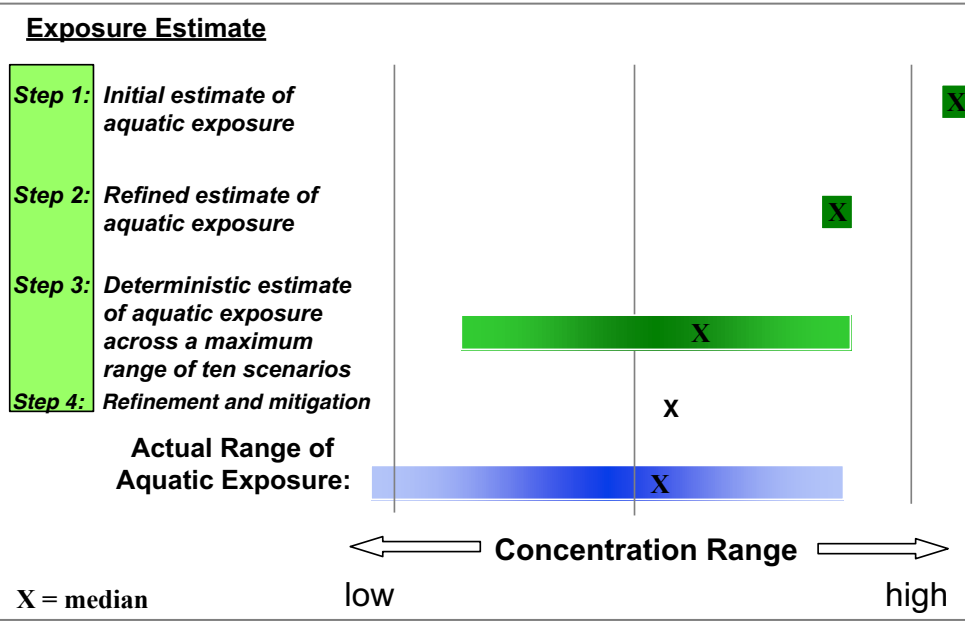
Application of VFSSMOD in Risk Assessment

- Buffer efficiency is considered in risk assessment by integrating VFSSMOD with regulatory models (PRZM/VVWM or TOXSWA) using existing FOCUS or EPA standard scenarios for long term simulations
 - Calculate necessary buffer strip width to achieve required exposure endpoint
 - Calculate reductions for a set of standard buffer widths
 - Develop PEC/EEC reduction factors
- Surface water exposure with **quantitative** VFS mitigation framework based on high-tier SWAN-VFSSMOD or EPA PWC (Pesticide in Water Calculator)

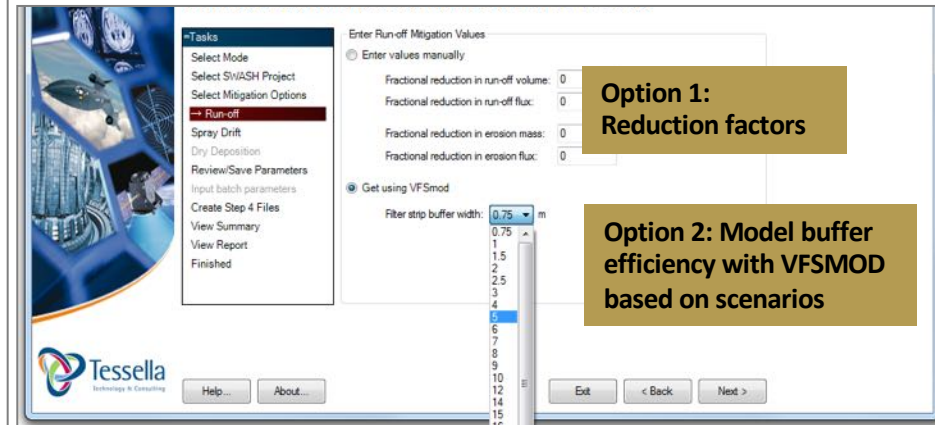


EU FOCUS Pesticide Exposure Framework: PECsw ranges at Steps 1-4

Conceptual relationship between the desired PEC at Steps 1, 2 and 3 and the actual range of exposure (FOCUS, 2015) and STEP 4 SWAN tool



FOCUS Step 4 – SWAN input



[Slide from D. Kane, Knoell, 2020 EU VFS Workshops]

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

- SWAN-VFSMOD: 1031 runoff events (27 combinations of crop (corn/winter cereals) x 4 FOCUS R1-R4 scenarios x 2 water body (stream and pond). VFS length in flow direction: 10 m, Koc values: 10 to 10^7 L/kg
- Because it accounts for environmental conditions SWAN-VFSMOD describes VFS performance (dQ, dE, dP) more realistically ($\rightarrow \Delta P$: 30% and 100%) than FOCUS LM fixed efficiency approach ($\rightarrow \Delta P$: 60% and 85%).
- 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.

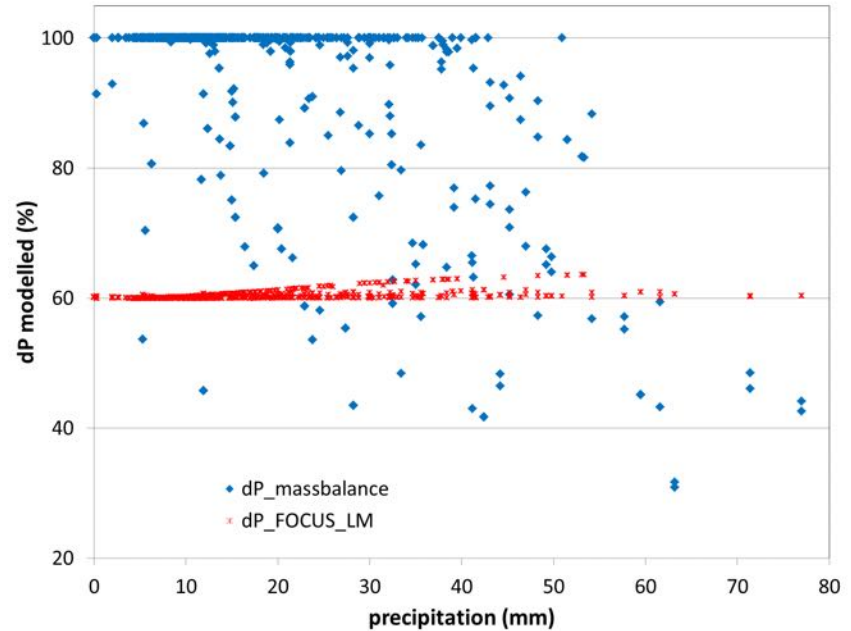


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Regulatory Status of VFSSMOD

- America: Adopted by California DPR (PREM tool), soon in Canada PRMA. EU: accepted in Poland, EFSA cases under consideration by state members, Norway management tool.
- EU Report: Mitigating the Risks of Plant Protection Products in the Environment (**MAGPIE**), 2013 (Brown et al., 2017) concluded that VFSSMOD is recommended because of scientific status but raises questions on generality of initial Sabbagh et al. (2009) pesticide trapping equation.
- Recent work (Reichenberger et al. 2019; Muñoz-Carpena et al., 2019) fully addresses the MAGPIE concern introduced by the semi-empirical VFS pesticide trapping algorithm. The new mass balance equation or the semiempirical refitted equation with a larger dataset proved efficient across large field dataset to quantitatively predict VFS pesticide mitigation.

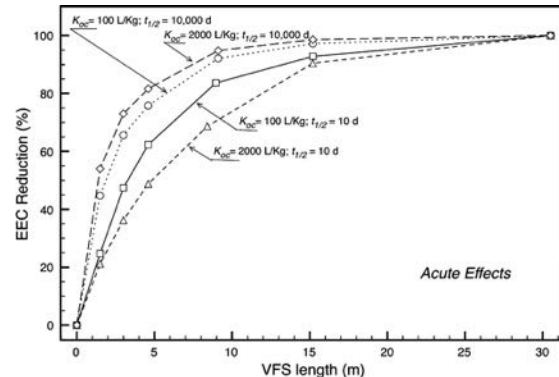
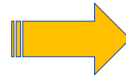
Brown, B., V. Laabs, N. Mackay, A. Alix, R. Bradascio, J. Dyson, B. Golla, K. Knauer, D. Rautmann, B. Roepke, M. Röttele, M. Strelake, J. Van de Zande. 2017. Risk mitigation measures to protect surface waters. Mitigating the Risks of Plant Protection Products in the Environment, Proceedings of the MAGPIE Workshop, 978-1-880611-99-9, Society of Environmental Toxicology and Chemistry (SETAC), Pensacola, Florida (2017).

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

Look-up tables and response curves for initial mitigation practice

- Initial screening based on response curves from PWC-VFSMOD simulations.
- Contrasting EPA scenarios (or the full set) could be used to screen initial VFS mitigation efficiencies expected.
- User selects from lists or pull-down menus a combination of characteristics.
- Based on results, quantitative refinements would follow by running full PWC-VFSMOD for specific conditions.

- Scenario (Ca-To/IL-corn/OR-Wheat...)
- Koc (low/medium/high)
- Degradation t_{1/2} (low/medium/high)
- Maintenance/channeliz. (normal/low)
- Effects (acute/chronic)
- Seasonal water table (no/yes)
- Other...

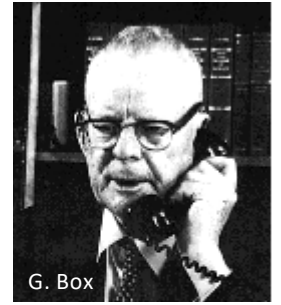


Conclusions

- System-wide assessment of important factors controlling pesticide mitigation is critical in risk assessment (complex problem)
- New advances in sediment parametrization, seasonal shallow water, mechanistic pesticide trapping, pesticide residues, field testing.
- Must move away from qualitative, empirical preconceptions of important drivers in favor of quantitative evaluations considering wide range of field conditions.
- Consideration of in-situ field characteristics leads to realistic assessment of mitigation efficiency
- VFSSMOD integrated in current regulatory tools (EU SWAN, PRMA, CA-DPR) produces modeling frameworks suitable for quantification mitigation of pesticides within regulatory high-tier assessments.

‘...all models are wrong, some are useful’

‘... and remember – GIGO!!’



G. Box



W.E. Deming

Thank you for your attention