

SPOTMOD I

Theoretical background and hydrological consistency validation

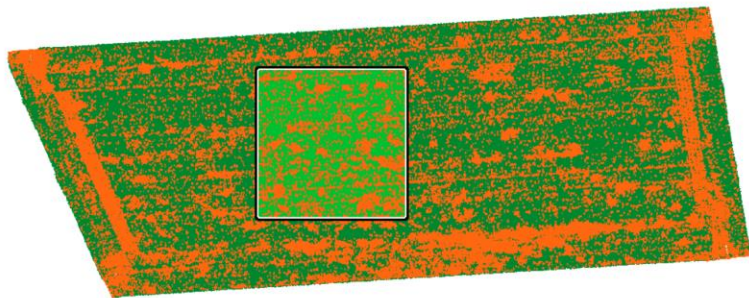
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XVIII Symposium on Pesticide Chemistry · Cremona, Italy · Session III · Friday 4 September 2026, 09:40



Why runoff needs its own framework



Real thistle infestation in a French sugar beet field, with a 1-hectare FOCUS-scale tile marked. Treated area is neither uniform nor random.

The state of play

Drift reduction from precision application is being actively quantified — including this morning in this session. Runoff reduction is not, and it does not scale linearly with treated area.

Objectives of this talk

i

Present the theory

The 2D mechanistic framework coupling PRZM, VFSMOD and a TOXSWA metamodel to quantify pesticide runoff from precision (spot) applications and derive long-term PEC_{sw}.

ii

Establish hydrological consistency

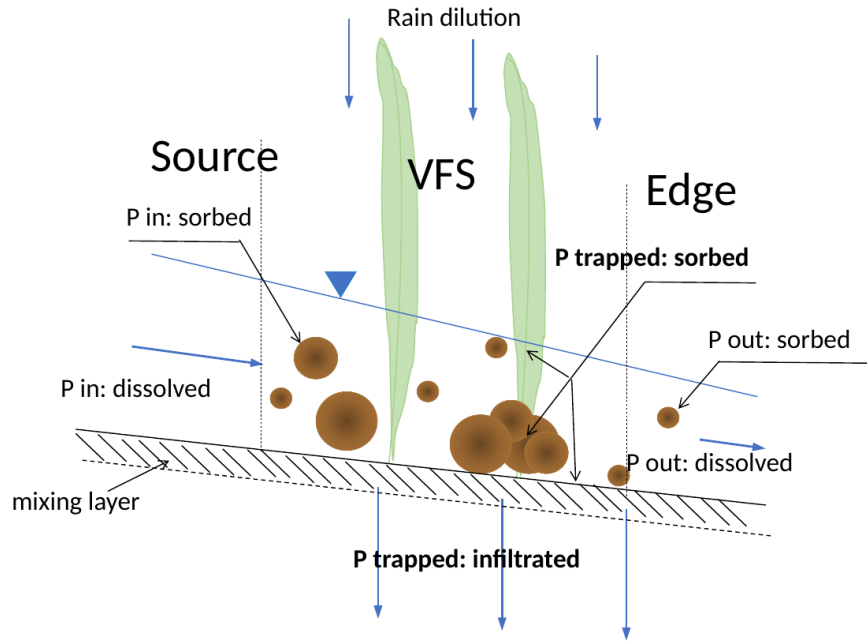
Validate SPOTMOD hydrology against full-field PRZM runoff across the FOCUS R1–R4 surface-water scenarios, before any claim is made about pesticide.

What this talk is not

It is not the case studies. Real application maps — scattered thistles in France, a dense weed map in Ohio, band applications — are Jorge Olivares-Rivas at 10:00, immediately after this.

The idea: the untreated field is its own buffer

THEORY



Sources

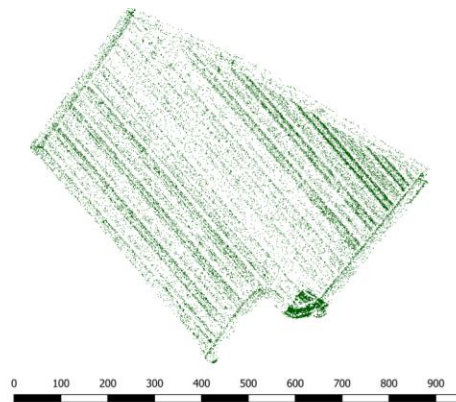
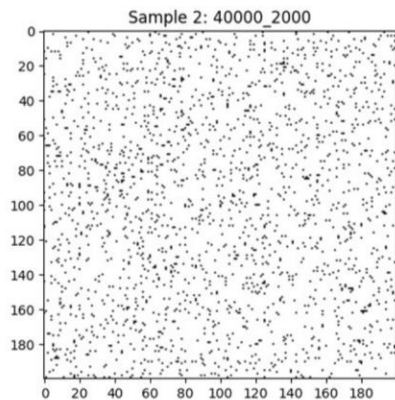
Runoff generated on treated spots, carrying dissolved and sediment-bound pesticide — a small fraction of the field area.

Sinks

Every untreated downslope segment behaves as a vegetative filter strip: infiltration, sedimentation and pesticide trapping, with the mixing-layer processes that go with them.

The consequence

Reduction comes from two effects at once — less mass applied, and mitigation of what is applied.



Left: a random realization for a 1 ha field, 0.5×0.5 m spots, 5 % treated area. Right: real thistle maps in sugar beet, tractor-mounted cameras, French field sites.

Why the pattern is an input, not an assumption

Treated area fraction is not the same thing as infestation rate: re-sampling a fine infestation map onto a larger spot grid conservatively marks a whole cell as treated if any pixel in it is infested, so the treated fraction grows with spot size.

Option 1 — generated

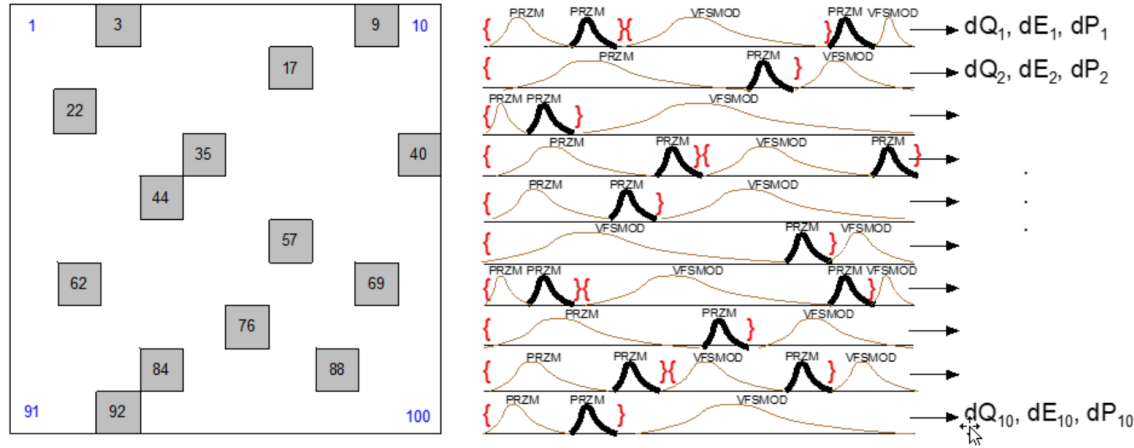
Random, quasi-random or biased patterns built from a chosen spot size and treated-area fraction. Spatial autocorrelation (Moran's I) controls how clustered the infestation is.

Option 2 — observed

Real infestation maps from remote or proximal sensing, resampled to the modelled spot grid. More realistic: they capture features a random draw never will, such as heavier infestation in driving lanes and at field edges.

Steps 2–3 · Strips along the flow direction

THEORY



Each row is one spot wide; treated cells (PRZM) and untreated cells (VFSMOD) alternate along the flow path; hydrographs and pollutographs are convolved down the row.

The decomposition

The field is divided into strips of the width of the treated spots, running down the main slope. Flow and transport are contained within each strip.

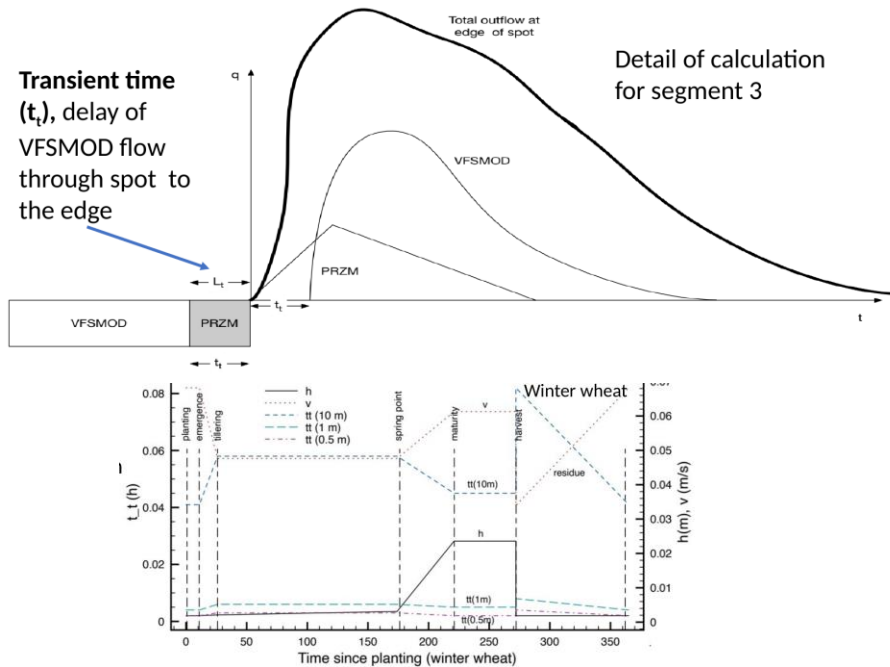
Sources: PRZM

On treated segments, the 20-year FOCUS Step 4 PRZM outputs are scaled from the 100×100 m field down to the spot footprint.

Sinks: VFSMOD

Each untreated segment is routed as a buffer of its own length.

Figure 1 of the submitted summary · flow direction left to right, water body at the right-hand edge



What is convolved

The outflow hydrograph and pollutograph from an upslope untreated segment are added to the runoff generated on the next treated spot, then routed on. The sum, not the maximum, reaches the edge.

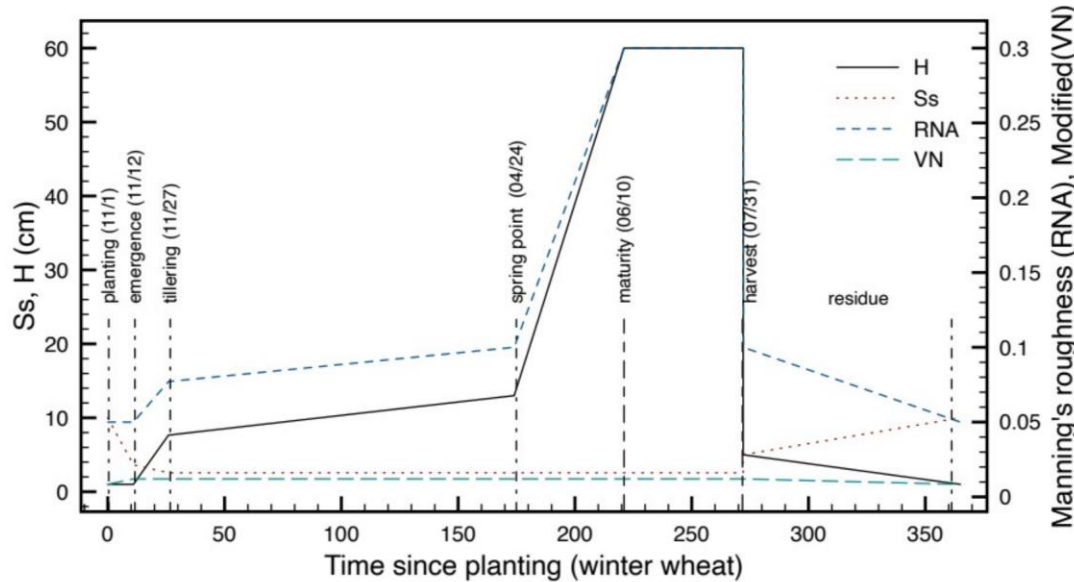
Transient time (t_t)

The delay for upslope runoff to cross a treated spot, set by runoff depth and velocity — which depend in turn on slope and on how much crop cover is present at that point in the season.

Order of magnitude

For a 2 % slope, crossing a 1 m spot takes seconds to tens of seconds; a 10 m segment, minutes.

The sink is not the same all season



Winter wheat: crop height H , stem spacing S_s , Manning roughness RNA and stem roughness VN from planting through residue.

Why it has to vary

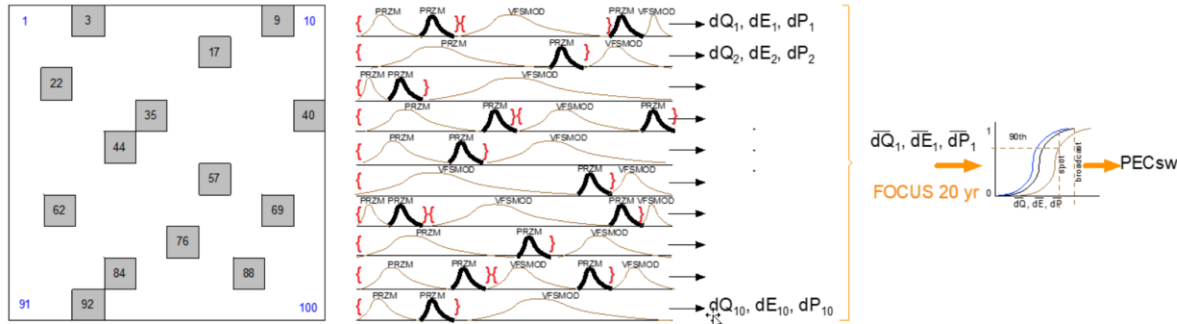
The same untreated segment is a poor filter at emergence and a good one at maturity. Holding vegetation constant across a 20-year assessment would misplace mitigation relative to the spray calendar.

What changes

Hydraulic resistance to overland flow, infiltration opportunity time, and the sedimentation that carries sorbed pesticide out of suspension.

Where it enters

Both the PRZM and the VFSSMOD parameterization, event by event.



Step 4 · Summation

Runoff (dQ), erosion (dE) and pesticide (dP) from the edge of every strip are summed over the field and passed to a TOXSWA metamodel to give the surface-water concentration.

Step 5 · A distribution, not a single number

For a given infestation rate, spot size and scenario, many application patterns are drawn and the whole procedure repeated. What comes out is a probability distribution of PEC_{sw} over the 20-year period — which is what lets a percentile, rather than one realization, carry the regulatory answer.

Comparison basis

Every SPOTMOD result is expressed against a standard FOCUS PRZM broadcast simulation with the same soil, scenario and substance properties, normalized to a 1-hectare field.

What had to change to make this possible

VFSMOD was built for vegetation segments of metres, not segments of centimetres. Two fixes made the small-segment case work; two further changes improved the engine generally:

Sediment and pesticide mass balance

closes at segment lengths well below the tested range

Green-Ampt infiltration fixes

stable for very short contact times

Automatic Courant-based node selection

general improvement — discretization no longer a user choice

Bivariate Petrov-Galerkin stabilization

general improvement — non-oscillatory transport at small Péclet and Courant numbers

VFSMOD 4.6.2.1

Implementation

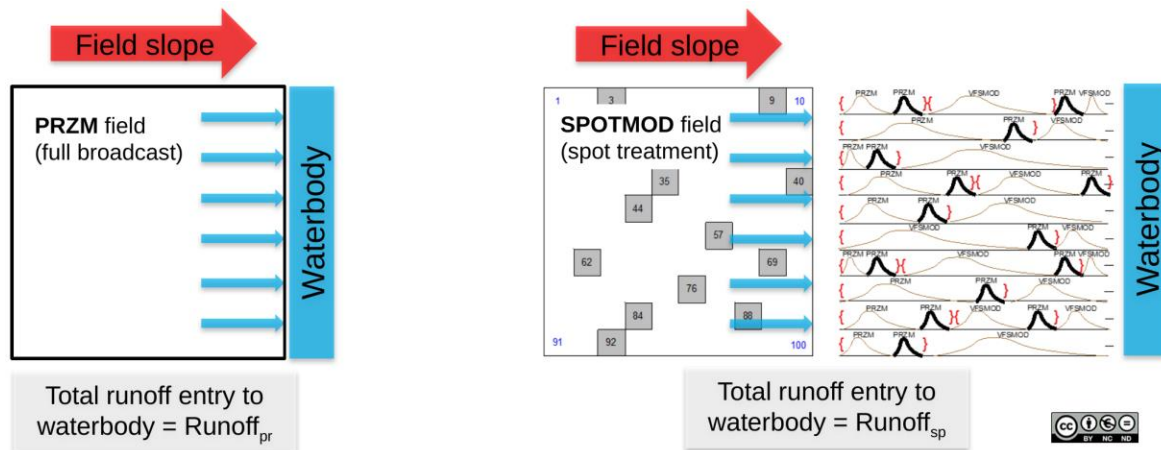
SPOTMOD is written in Python, open-source, and fully modular — the same code runs one 1-hectare map on a laptop and millions of simulations on a cluster. Simulations are configured from a JSON file.

Scaling

Multiprocessing plus MPI for multi-node parallelization on UF HiPerGator, with SCRATCH storage for I/O. Field rows, runoff days and random layouts all parallelize independently.

Why it matters here

The metamodel on the next-to-last slide is only reachable at this scale.



The metric

$$\Delta R_{sp} (\%) = (1 - \text{Runoff}_{sp} / \text{Runoff}_{pr}) \times 100$$
, evaluated event by event over the 20-year record.

Why this comes first

PRZM is the accepted basis for regulatory runoff entries. If SPOTMOD's hydrology drifted from it, no reduction factor derived from SPOTMOD would be defensible — whatever the pesticide algorithms did.

Hypothesis

Total field runoff entering the water body in SPOTMOD (sp) is comparable to a full-field PRZM simulation (pr) of the same scenario. Set the treated fraction to 100 % and the two must agree.

How the comparison was set up

VALIDATION

Scenarios	All four FOCUS surface-water runoff scenarios, R1 to R4
Crops	Maize, potatoes and field beans, each with a bare-soil counterpart
Calibration events	11 representative runoff events per scenario, spanning the storm-magnitude distribution, for both the cropping season and bare soil
Calibrated parameters	Three VFSMOD soil parameters: vertical saturated hydraulic conductivity (VKS), average suction at the wetting front (SAV), and saturated water content (OS)
Then — the test	That single parameterization is then held fixed and SPOTMOD run over the full 20-year record. Every event in those two decades is compared with PRZM, not just the 11 that were fitted.
Spot sizes	From 5×5 cm to 1×1 m, at an infestation rate of 11 % — treated rate rising to roughly 60–70 % at the largest spots, depending on the infestation pattern

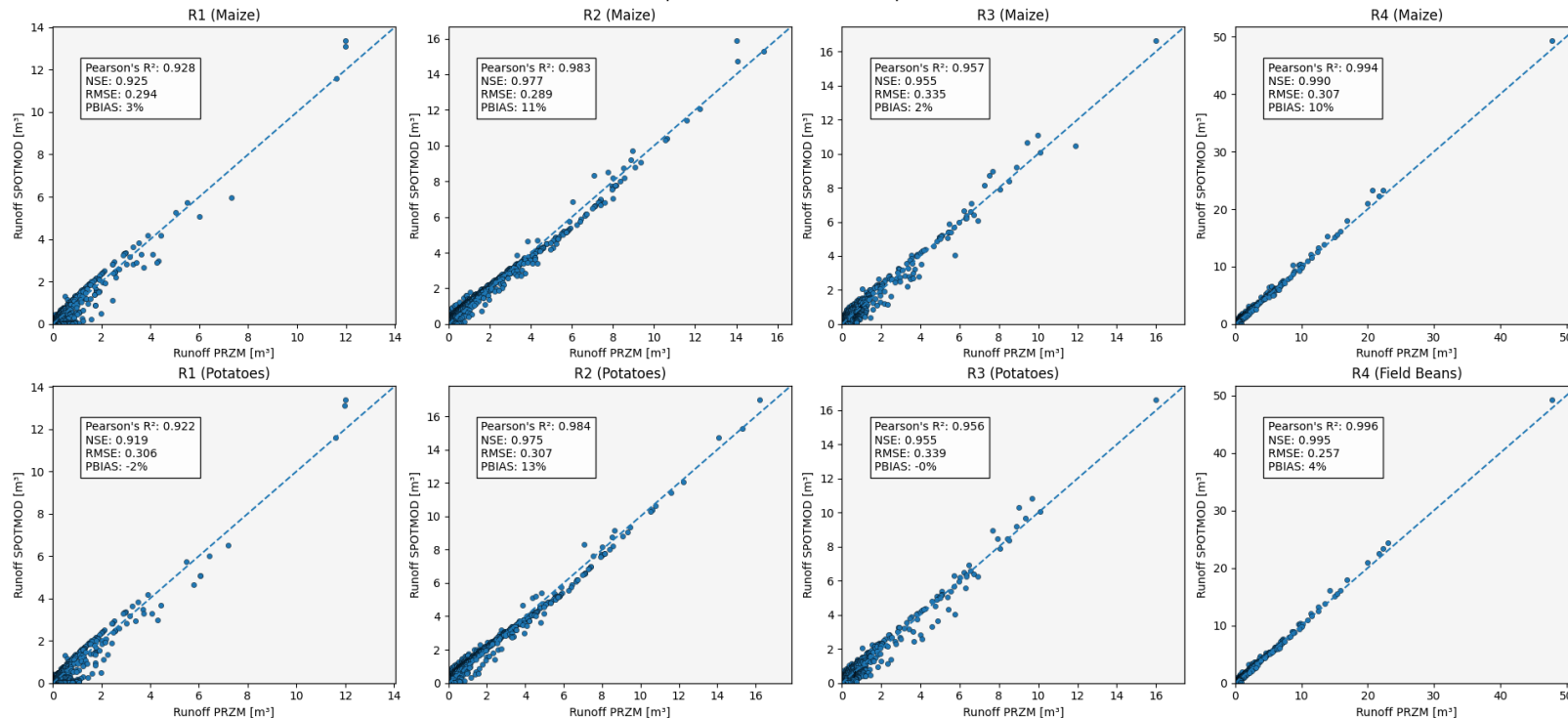
Calibration is of VFSMOD soil hydrology against PRZM runoff volumes — not of the pesticide algorithms, which are unchanged.

Full-field SPOTMOD reproduces PRZM across R1–R4

VALIDATION

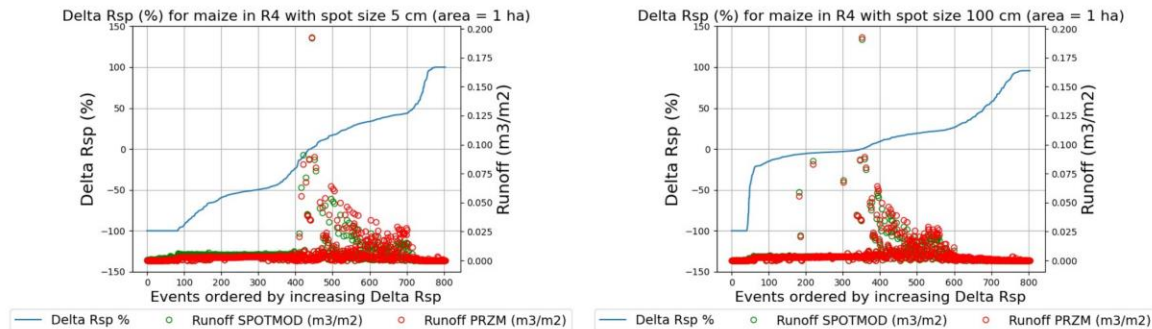
NSE 0.919–0.995 · **RMSE 0.257–0.339 m³** · **|PBIAS| ≤ 13 %** · **R1–R4 × 3 crops × 20 years**

Crop & Scenario Runoff Comparison



Spot size does not drive the hydrology

VALIDATION



Variable	Value	
Spot size	5 x 5 cm	100 x 100 cm
Runoff volume (SPOTMOD)	46,000 m ³	44,000 m ³
Runoff volume (PRZM)	49,000 m ³	

Maize, R4, 1 ha tile — 5 × 5 cm spots (left) and 100 × 100 cm spots (right); ΔR_{sp} capped at -100 % in the plots

The test

A twenty-fold change in spot side length, from 5 cm to 1 m, holding the scenario and infestation fixed.

The result

Total 20-year runoff volume differs by about 4.5 % between the two spot sizes: 46,000 m³ at 5 cm and 44,000 m³ at 1 m, against 49,000 m³ for PRZM — 6 % and 10 % below it respectively.

Why it matters

The framework is not quietly resolution-dependent.

Where the two components differ — and why that is informative

VALIDATION

Two different hydrologies

PRZM uses the empirical curve-number approach with an initial abstraction. VFSMOD solves Green-Ampt infiltration with kinematic-wave overland flow — a genuinely different description of the same water.

The open question

Over 20 years the volumes match. On individual peak events they need not — and in a case study the two models can disagree about whether a particular PEC peak occurs at all.

Large events agree better

Initial abstraction (I_a) is simulated empirically in PRZM but mechanistically in VFSMOD, so the two diverge most on small events — where the absolute volumes, and the risk, are smallest. Snowmelt runoff generated in PRZM is passed through to VFSMOD; those events are small and low-risk too.

Which one is right?

Not yet settled. VFSMOD is the physically consistent description; PRZM is the accepted regulatory baseline. For an assessment driven by the peak event, that distinction is not academic.

What this test is, and is not

Three soil parameters were fitted per scenario; the 20-year record then tests that fit. It is not an independent validation.

Coming next

Jorge shows exactly this in Case Study 3 at 10:00.

Factor	Number of values	Values	Comments
Koc (L kg ⁻¹)	11	10, 50, 100, 200, 500, 1000, 2000, 5000, 10000, 100000, 1000000	Large spread including highly-sorbed compounds (e.g., pyrethroids, etc.)
DegT ₉₀ in soil (d)	9	10, 25, 50, 100, 180, 250, 360, 500, 1000	Spaced values from 10 to 1000 days
Application dates (-)	5	BBCH 00, 10, 20, and 30; and 10 days after harvest	FOCUS PAT was used to select dates that avoid meteorological outliers
FOCUS Scenarios (-)	4	R1 – R4	All four FOCUS runoff scenarios
Crops (-)	5	Winter cereals, maize, sugar beets, potatoes, field beans	Only field crops are considered in the current metamodel development
Infestation rates (%)	5	<10, 10-15, 15-20, 20-25, 25-30	Infestation rate is not equivalent to the treated area fraction, since spot size re-sampling results in a larger treated area
Spatial autocorrelation (Moran's I)	3	< 0.71, 0.71-0.73, >0.73	Moran's I was used to determine the autocorrelation, which impacts increase in treated rate with spot size
Spot size [side length] (m)	10	0.05, 0.15, 0.25, 0.35, 0.45, 0.55, 0.65, 0.75, 0.85, 1.0	Length of the spot size (all spots are assumed square); 0.05 to 1 m to include new machinery
Number of map patterns for each combination of the three above factors	25 (tentative)	Distinct 1 ha tiles	Based on the fine-resolution thistle maps provided by Corteva Agriscience



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Factor space behind the metamodel under development

Machine-learning surrogates trained on the full simulation, with the goal of a lightweight, portable implementation that executes quickly compared with running the full model.

For end users

A metamodel giving the expected reduction in pesticide runoff loss and PEC_{sw} for a substance, crop, scenario, spot size and infestation rate.

For refinement

Running actual SPOTMOD field simulations locally, taking a PRZM simulation as input so it drops into a standard FOCUS surface-water workflow.

Delivered through

A user-friendly GUI intended to support both regulatory use and scientific analysis.

Conclusions and outlook

1 A 2D mechanistic framework now exists for spot applications

Sources on treated spots (PRZM) and sinks on untreated downslope segments (VFSSMOD), joined by convolution along field strips and closed to PEC_{sw} through a TOXSWA metamodel.

2 The hydrology is consistent with the regulatory baseline

NSE 0.919–0.995 and RMSE 0.257–0.339 m³ against full-field PRZM across FOCUS R1–R4 and three crops, with bias within 13 % — and the result is not sensitive to spot size.

3 Realism is an input, not an assumption

Variable spot size, treated fraction, spatial pattern and seasonal crop cover are all set from data, which is what makes a worst-case assessment meaningful.

4 Next: sediment, drift, and flow paths

Refine the sediment-phase comparison and run a Morris screening of the coupled model; couple to a mechanistic drift model so both entry routes are mitigated together; allow non-parallel and joining flow paths.

Thank you

Acknowledgements

Olivier de Cirugeda Helle, Vincent Guth and Anne Alix (Corteva Agriscience) for the observed weed maps
USDA National Institute of Food and Agriculture, Hatch projects 1024705, 1024706 and 1028045
University of Florida High-Performance Computing Center (HiPerGator)

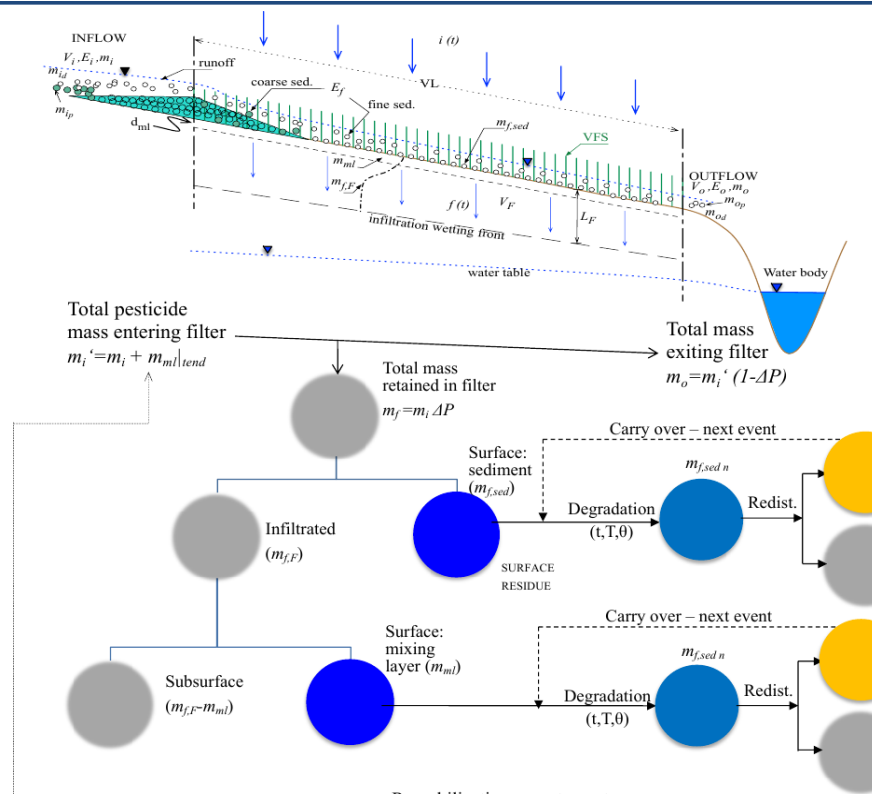
References

Muñoz-Carpena, Parsons & Gilliam (1999) J. Hydrol. 214:111–129 · Ritter, Muñoz-Carpena et al. (2023) CERSA, doi:10.5281/zenodo.7789811 · FOCUS (2001) SANCO/4802/2001-rev.2 · Carsel et al. (2003) PRZM-3 User's Manual · Adriaanse et al. (2017) Sci. Total Environ. 584, doi:10.1016/j.scitotenv.2016.12.001

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Backup



Within one segment

Runoff partitioning and transport, sediment filtration, mixing-layer leaching with dissolved and sorbed redistribution, degradation, remobilization from the mixing layer, and carry-over to the next event.

Why the mixing layer matters here

Residues trapped in an untreated segment do not stay put: they can be remobilized by the next storm, which is why a storm-based model needed multi-event bookkeeping before it could support 20-year assessments.

Reference

Muñoz-Carpena et al. (2015) Chemosphere 139:410–421

Technique	Section width	Spot size minimum
Field sprayer (1)	1,0m	100x80cm ²
Feldspritze (1)	0,5m	50x80cm ²
Amazone Smart Sprayer (2)	0,25m + PWM	25x45cm ²
ARA Ecorobotix (3)	0,04m	6x10cm ²

Quelle: Eike Hunze, Uni Göttingen, 2023



Section width falls from 1.0 m on a retrofitted field sprayer to 0.04 m on a smart micro-applicator; minimum spot footprint from $100 \times 80 \text{ cm}^2$ to $6 \times 10 \text{ cm}^2$.

Why the range matters

The modelled spot sizes run from 5 cm to 1 m — the upper end matches retrofitted sprayers, and the lower end sits below the finest device in this table, so the framework does not have to be re-derived as the machinery gets finer.

Savings depend on more than the machine

Weed density, weed distribution, technical resolution and driving speed all affect what a given applicator actually saves — which is the argument for driving the assessment from observed maps rather than a nominal application rate.