Comparison of TOXSWA and AGRO-2016 as receiving water models for European pesticide exposure assessment

Lauren Padilla[1], Scott Jackson[2], Michael Winchell[1]

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1. Stone Environmental, Inc.
2. BASF Corporation

Introduction

Aquatic exposure modeling for EU pesticide registration and regulation follows similar approach to that used in US

- Landscape model coupled to receiving water model
- Scenarios define input parameters for different regions and agricultural uses
- But uses different models

A limitation of the receiving water model, TOXSWA (Toxic Substances in Surface Waters), is that eroded soil loadings and suspended sediment are not not explicitly modeled which can impact the partitioning of pesticides in the water body

For hydrophobic chemicals, (which strongly sorb to soil and sediment), sediment processes influence the overall fate and transport of a pesticide in the water body and the proportion available for uptake by organisms

We present a comparison of TOXSWA with a Canadian aquatic exposure model, AGRO, that explicitly accounts for the sediment mass balance

FOCUS aquatic exposure modeling

FOCUS (Forum for the Coordination of Pesticide Fate Models and their Use) exposure models:

- Landscape processes: PRZM (runoff) or MACRO (drainage)
- Receiving water body: TOXSWA

Pond, stream, ditch type water bodies

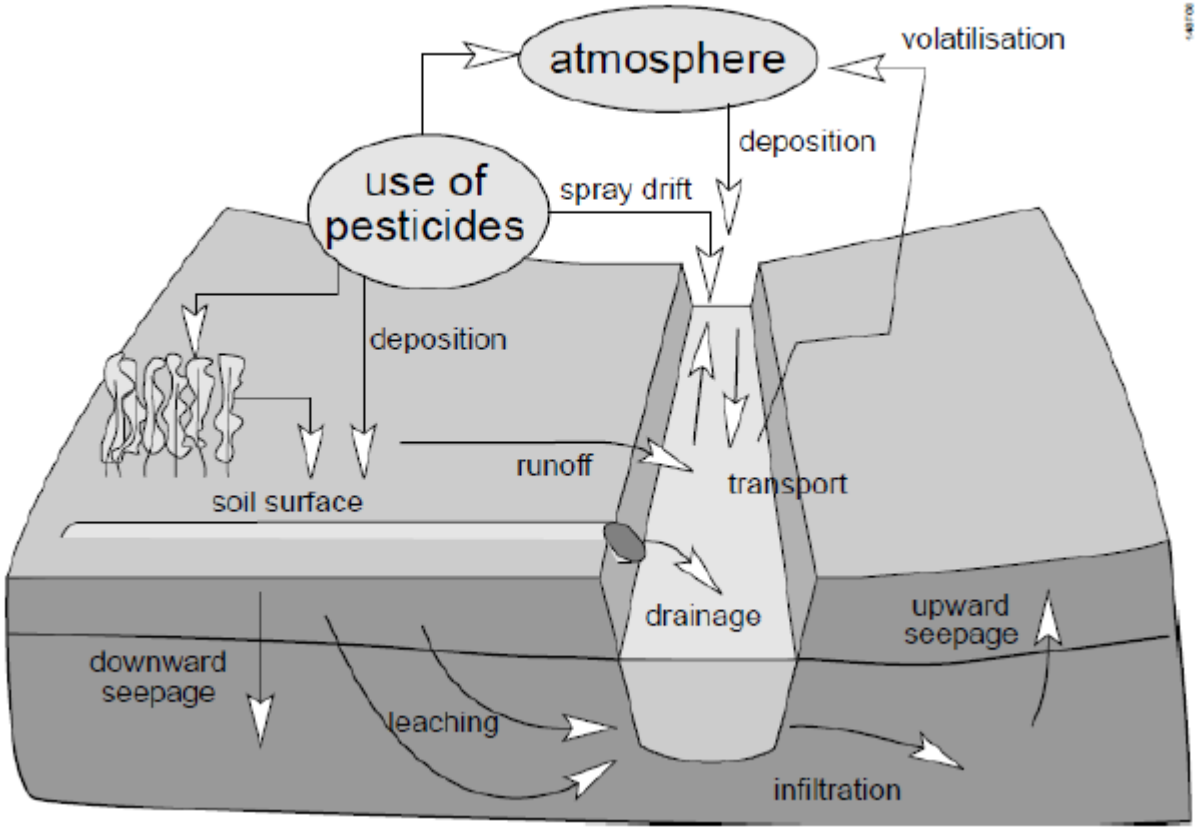
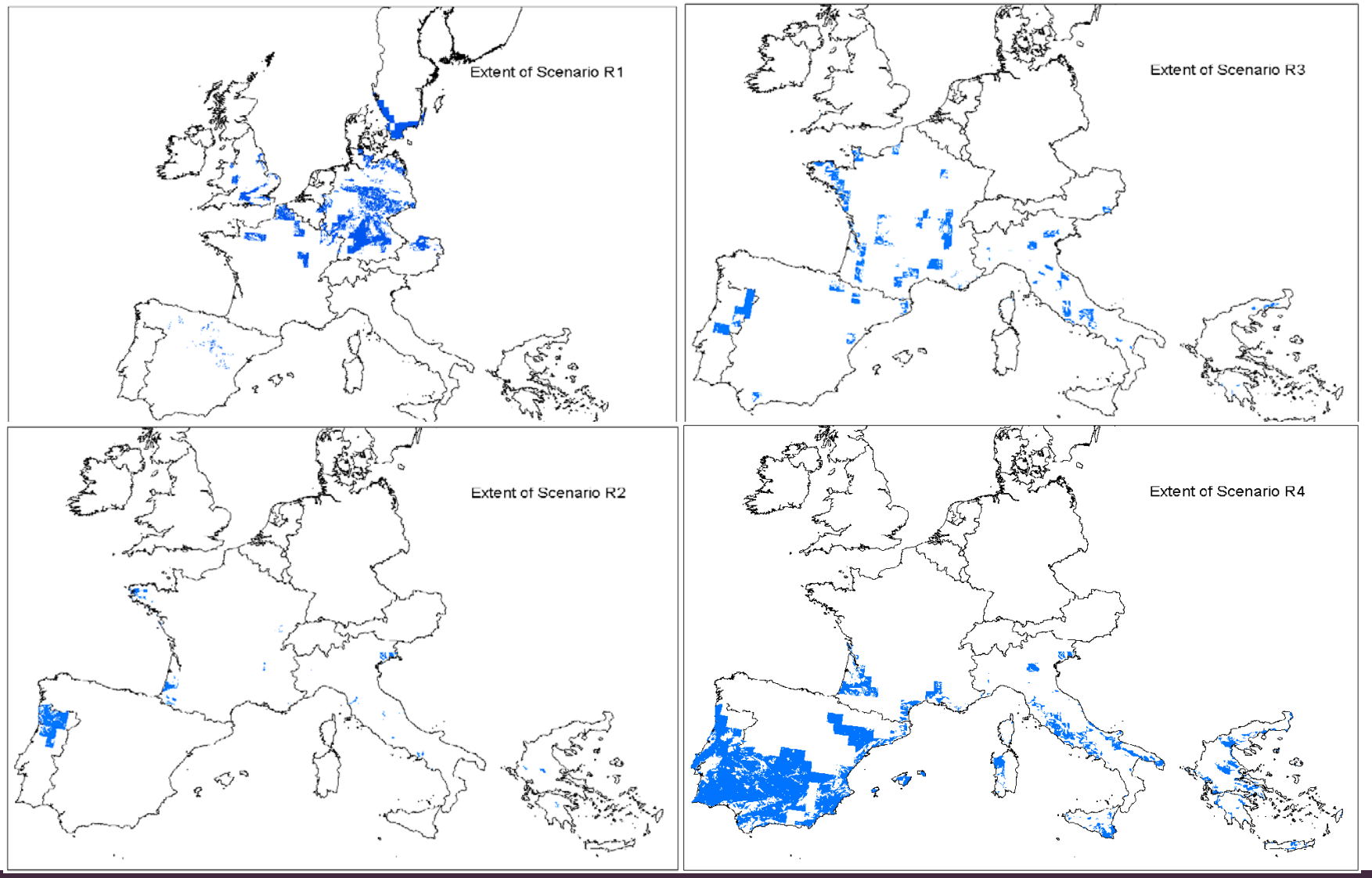


Figure 2.3 FOCUS TOXSWA User Manual

FOCUS PRZM simulations

4 regional scenarios for runoff

Pond water body - R1 loadings, Stream water bodies - R2, R3, R4 loadings



Brief history of AGRO

AGRO (2008), water quality module based on the Canadian Environmental Modeling Center (CEMC) Quantitative Water, Air, Sediment Interaction (QWASI) Fugacity model (Mackay, 2001)

- Simulation of sediment dynamics, including settling/resuspension of incoming sediment and burial; important for high Koc compounds

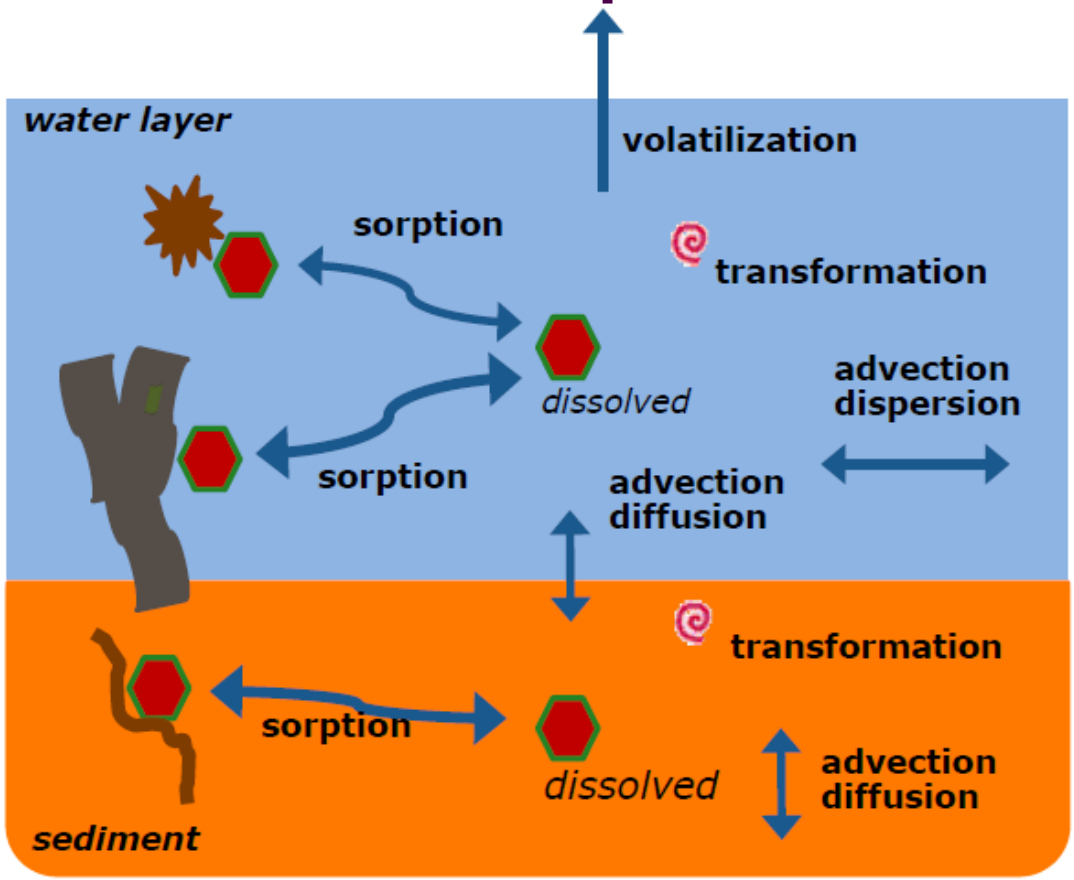
AGRO-2014, Pyrethroid Working Group improvements to AGRO (2008) that preserve sediment dynamics while making more physically realistic

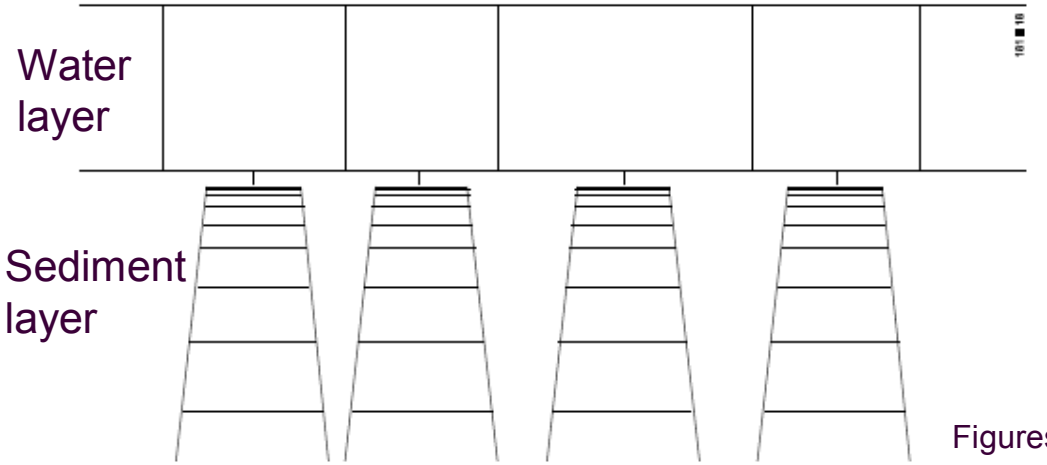
- Improved parameterization of water-sediment diffusive exchange coefficient based on pyrethroid mesocosm data

AGRO-2016, update of AGRO-2014 to make compatible with FOCUS scenarios

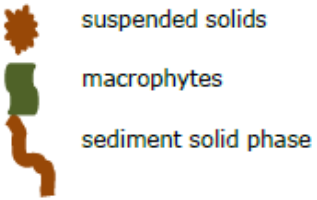
- Improved numerical integration scheme to improve numerical stability
- Options for FOCUS water body dimensions and environmental characteristics

TOXSWA conceptual model





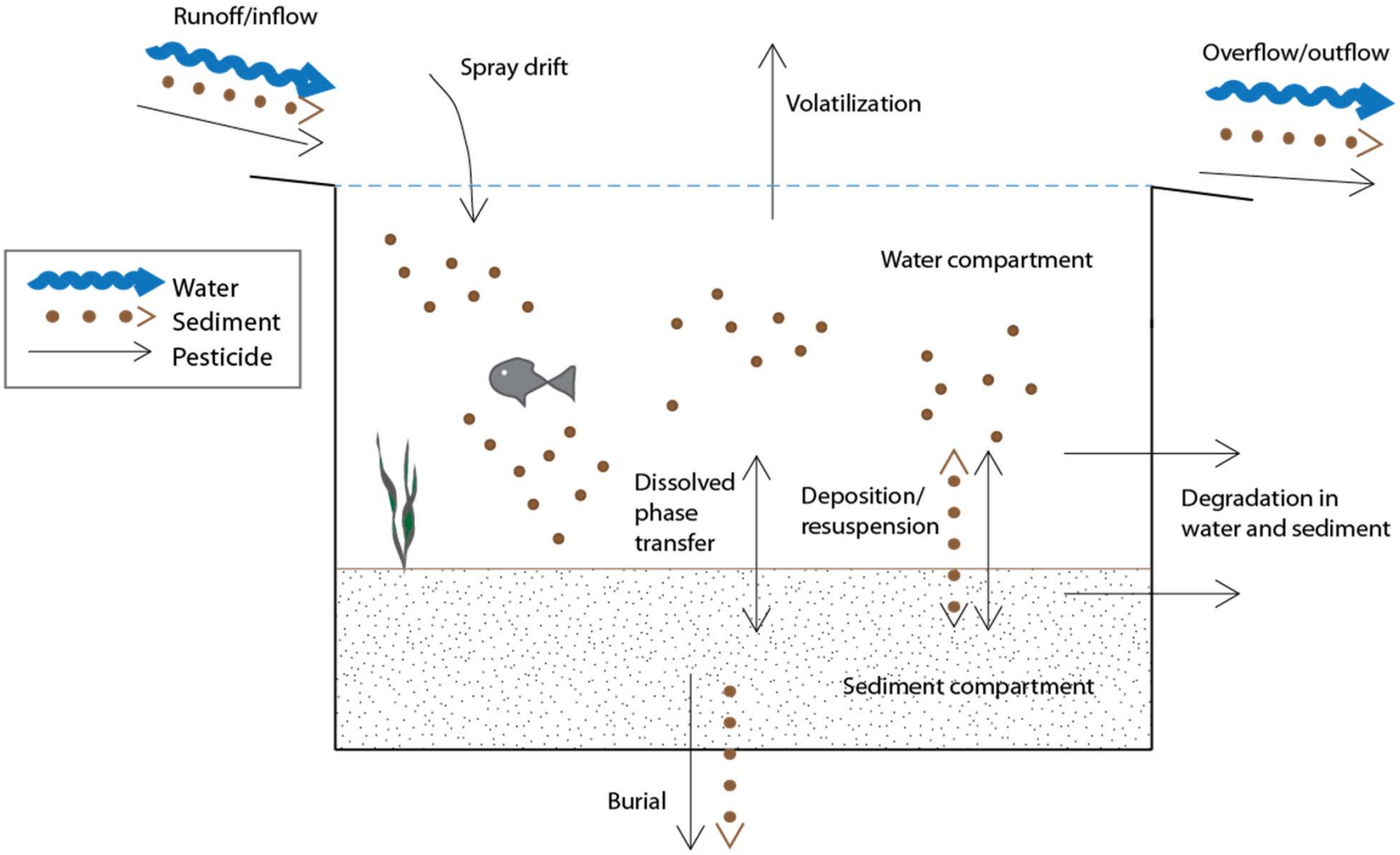
- Multiple water nodes in horizontal direction
- Vertical array of sediment nodes below each water node
- Variable volume
- Spray drift and runoff loadings
- Degradation, water-sediment advection-diffusion processes
- Pesticide sorbed to sediment determined by fixed sediment characteristics



Figures 2.1 and 2.2 FOCUS TOXSWA User Manual

AGRO conceptual model

Two compartment box-model with sediment mass balance
Pesticide sorbed to sediment moves with sediment
Fixed volume (inflow = outflow)



Conceptual model comparison

Key differences in model processes:

Model feature	TOXSWA	AGRO	Impact
Sediment compartment discretization	multilayer sediment profile 	single well-mixed layer 	**Major.** Controls exchange of pesticide from water to sediment with TOXSWA exchange slower than AGRO
Entry point for pesticide load adsorbed to eroded soil	sediment layer 	water layer 	**Major.** Controls initial condition for processes that redistribute pesticide.
Suspended sediment concentration	fixed	variable, depends on PRZM loading	**Minor.** FOCUS PRZM scenarios have low eroded soil loadings (erosion zone limited to 20 m buffer)
Deposition/resuspension	not modeled	variable, depends on PRZM loading	**Major.** Provides additional pathway for water-sediment exchange in AGRO

Conceptual model comparison

Model differences control the distribution of pesticide in the water body which has a major impact on its fate and transport, including:

- whether pesticide is available to organisms for uptake
- degradation rate (faster in water, slower in sediment in this case study)
- whether pesticide overflows/outflows

	Bioavailable	Not bioavailable
Degradation Overflow/outflow	Dissolved in water	Sorbed to suspended sediment
No overflow/outflow	In pore water	Sorbed to bed sediment

Input parameters

Simulations conducted for variety of regions, crops, application patterns, and receiving water bodies

Scenario	R1	R2	R3	R4
Water body	pond	highest flow stream	lowest flow stream	moderate flow stream
Crops	leafy veg field beans vines-early legumes	leafy veg	field beans fruting veg	leafy veg fruiting veg

TOXSWA and AGRO provided with identical FOCUS-PRZM loadings

Water body dimensions and other characteristics matched as closely as possible

Chemical properties for a hypothetical, moderately persistent pesticide (268d half life in water, stable in sediment) with low solubility (0.035 mg/L)

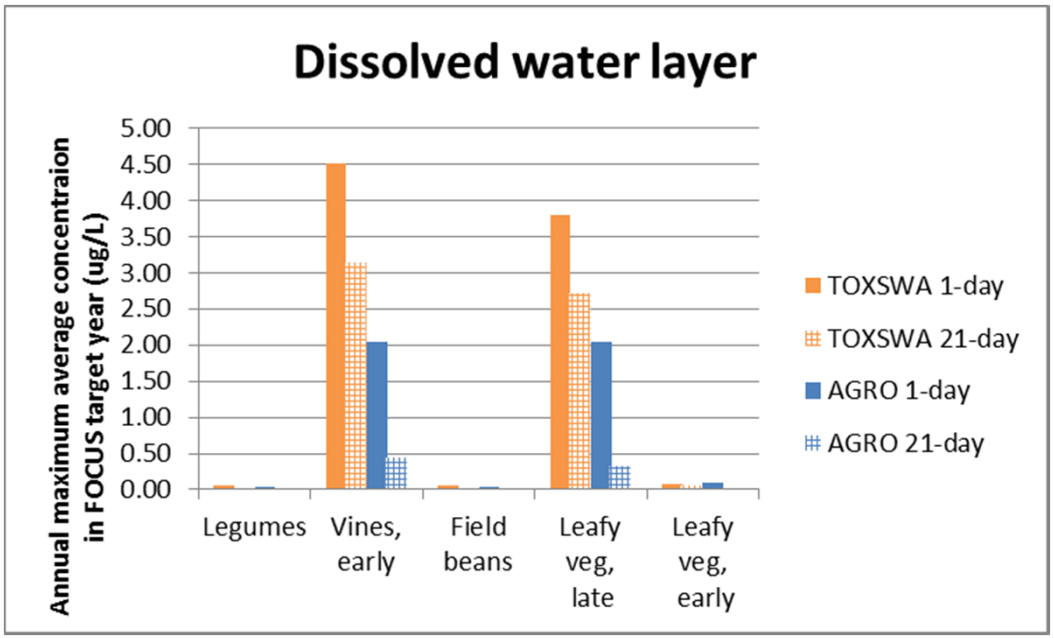
Two organic carbon partition coefficients:

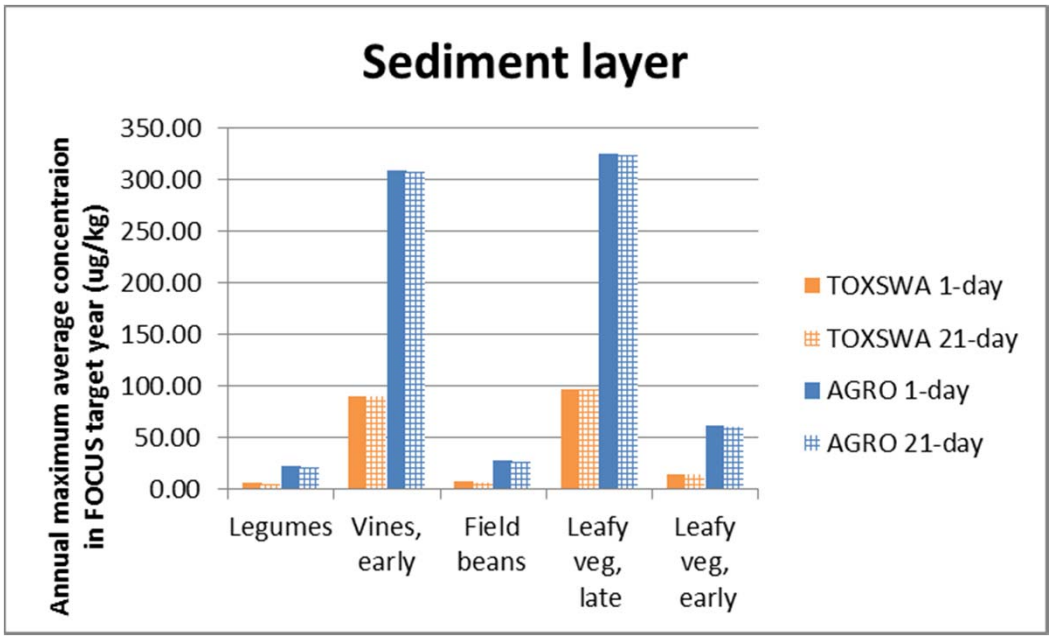
- hydrophobic compound (high Koc, 30,753 L/kg),
- more typically mobile compound (low Koc, 30 L/kg)

TOXSWA and AGRO pond concentrations – high Koc

With the exception of early season leafy vegetables, AGRO water concentrations lower than TOXSWA but same order of magnitude

AGRO sediment concentrations were higher than TOXSWA

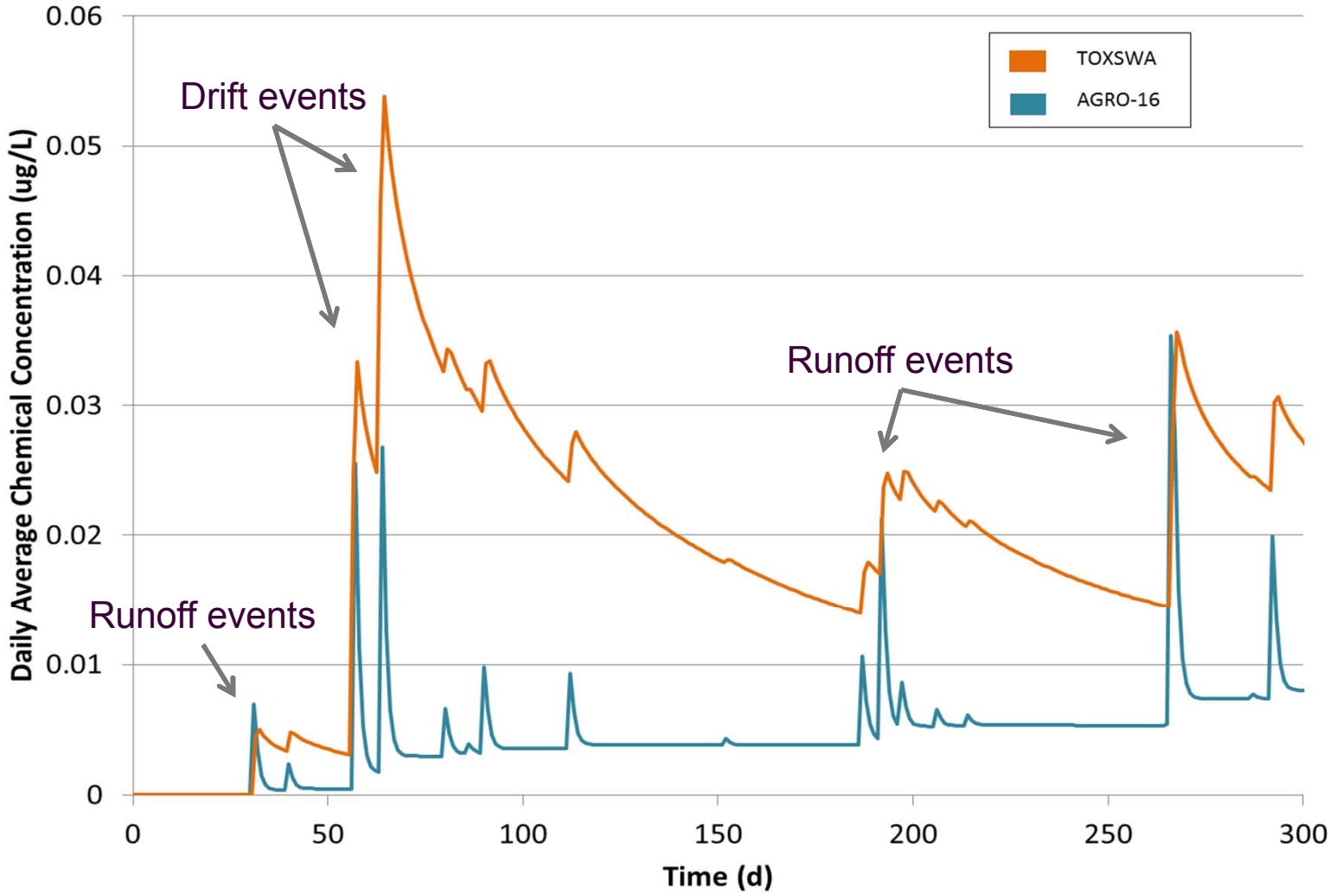




TOXSWA and AGRO dissolved pond concentrations – high Koc

Pesticide resides in water layer longer in TOXSWA due to slower water-sediment diffusion

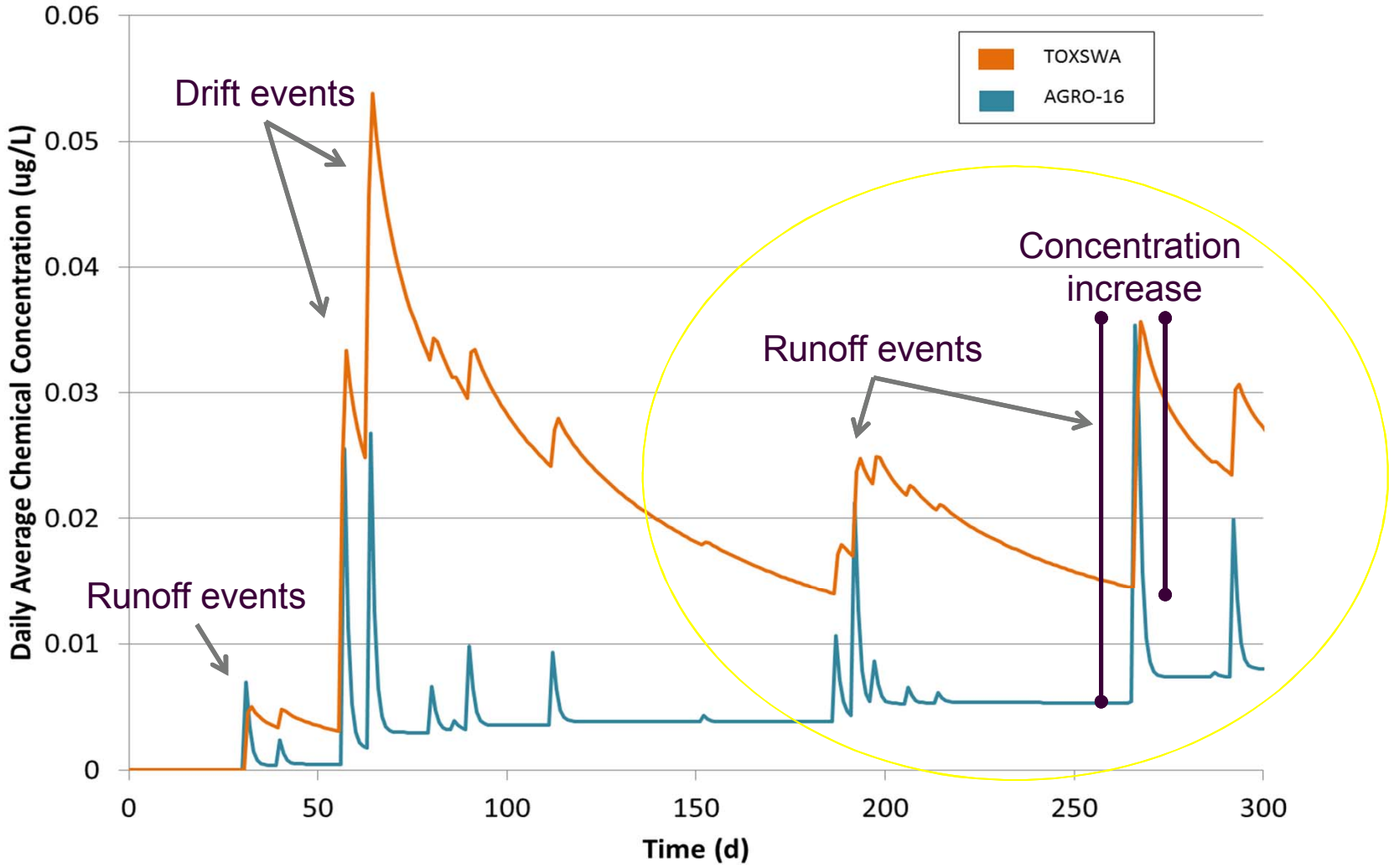
Causes water column concentration to build up in TOXSWA



TOXSWA and AGRO dissolved pond concentrations – high Koc

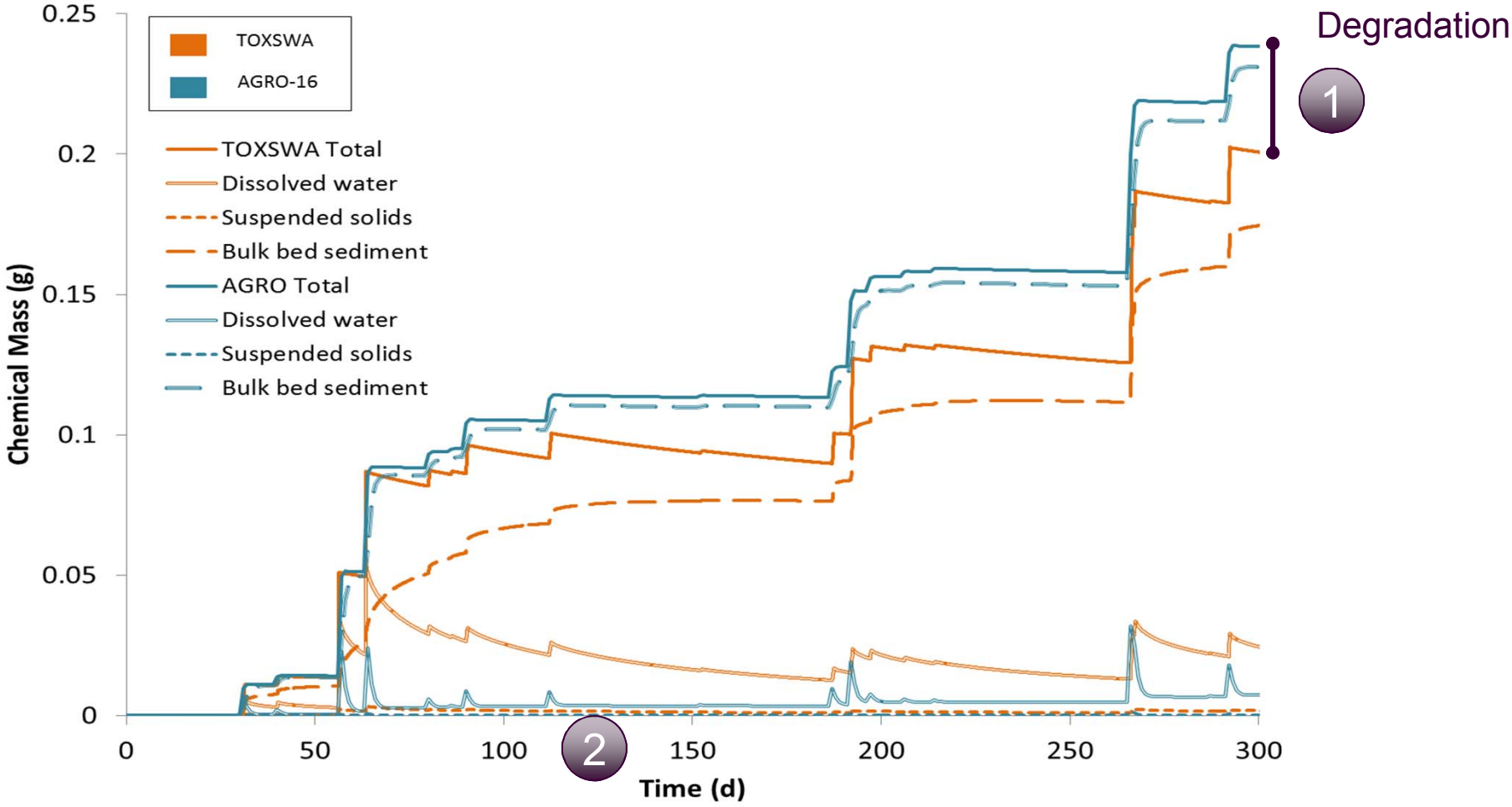
All pesticide loadings added to water layer in AGRO while only dissolved pesticide loadings added to water layer in TOXSWA

Results in smaller concentration increases after runoff events in TOXSWA



TOXSWA and AGRO pond pesticide mass balance – high Koc

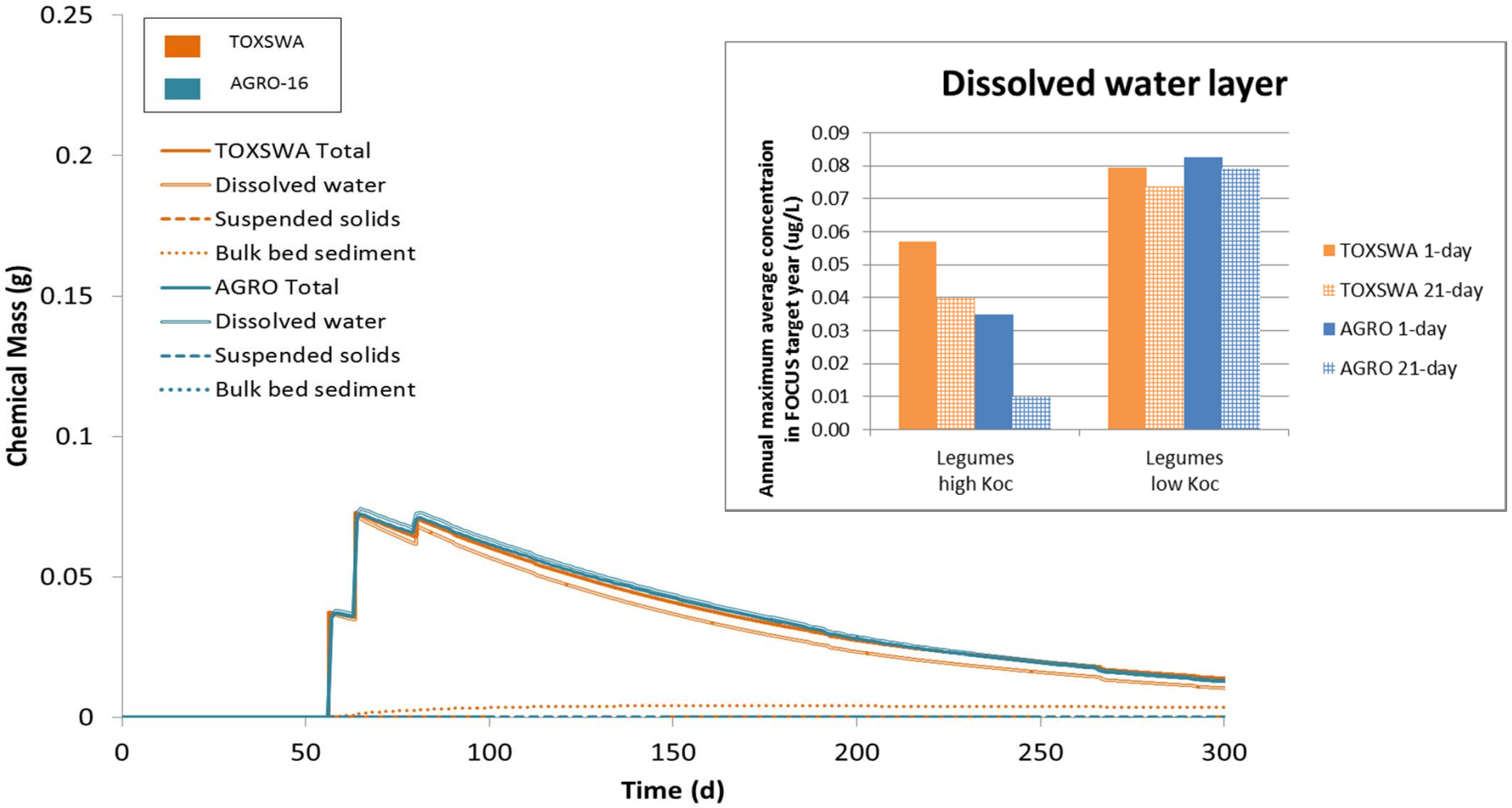
1. With pesticide residing in water layer longer in TOXSWA, cumulative degradation is greater. Most pesticide mass in AGRO resides in bed sediment where no degradation takes place
2. Pesticide adsorbed to suspended solids minimal in both models



TOXSWA and AGRO pond pesticide mass balance - low Koc

Pesticide predominantly resides in water layer where it decays in both models.
Distribution of pesticide mass and concentrations very similar

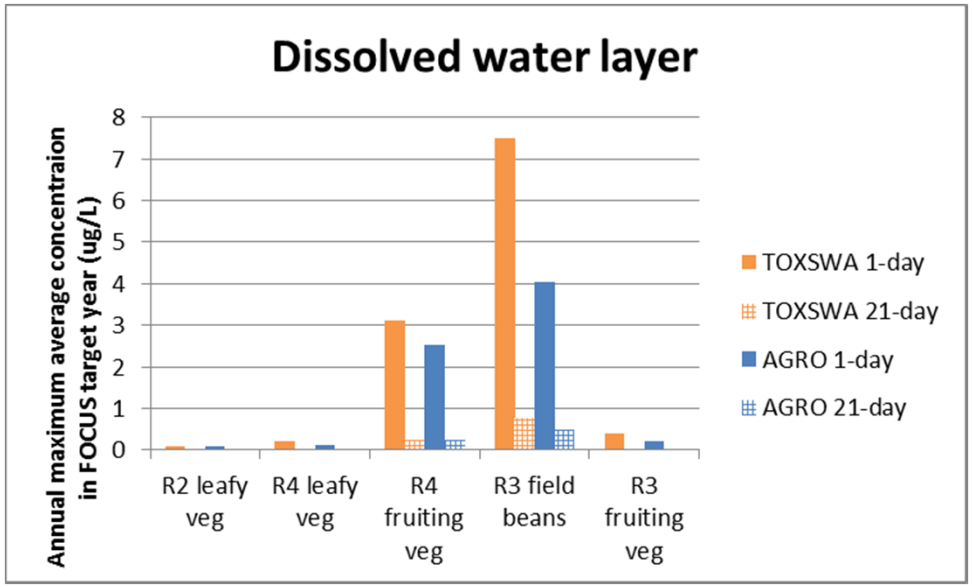
Slightly more pesticide stored in bulk bed sediment in TOXSWA

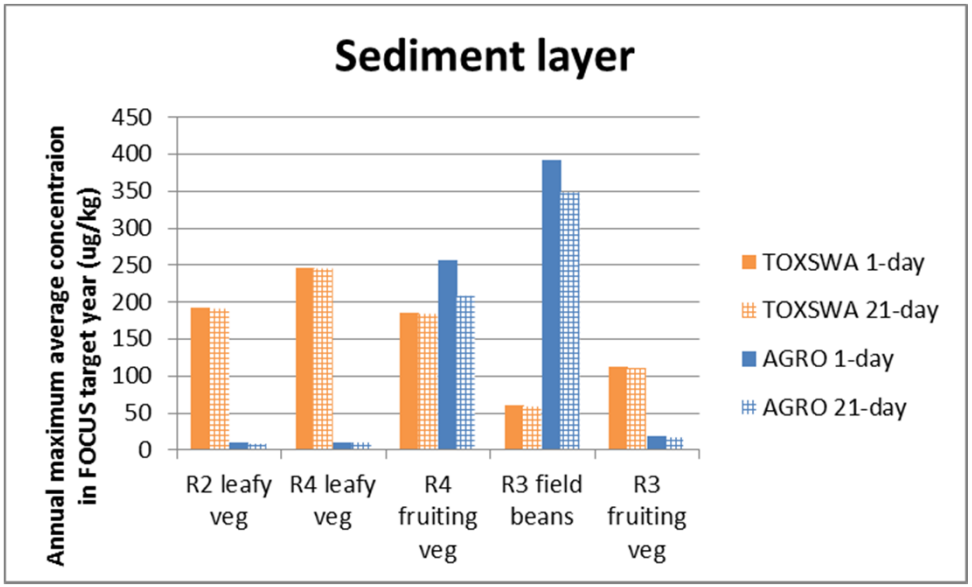


TOXSWA and AGRO stream concentrations – high Koc

In contrast to pond simulations, AGRO sediment concentrations were lower than TOXSWA for some scenarios

Model differences in factors determining pesticide distribution led to different amounts of pesticide leaving the water body by stream outflow





Scenario	R2 highest flow leafy veg	R4 moderate flow leafy veg	R4 moderate flow fruiting veg	R3 lowest flow field beans	R3 lowest flow fruiting veg
Spray drift/runoff total load	0.07g/1g	0.07g/3.25g	**1.4g/2.3g**	**1.42g/0.37g**	0.07g/0.8g

TOXSWA and AGRO stream concentrations – high Koc

TOXSWA eroded sediment loading deposited directly in sediment does not leave stream via outflow

- Sediment concentrations increase with increasing sediment loading

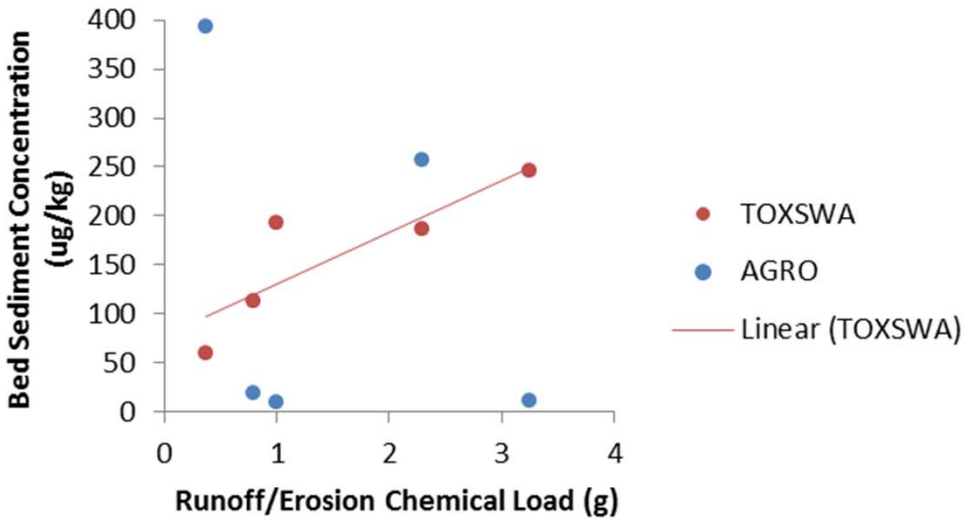
AGRO eroded sediment loading added to water layer largely leaves the stream via outflow

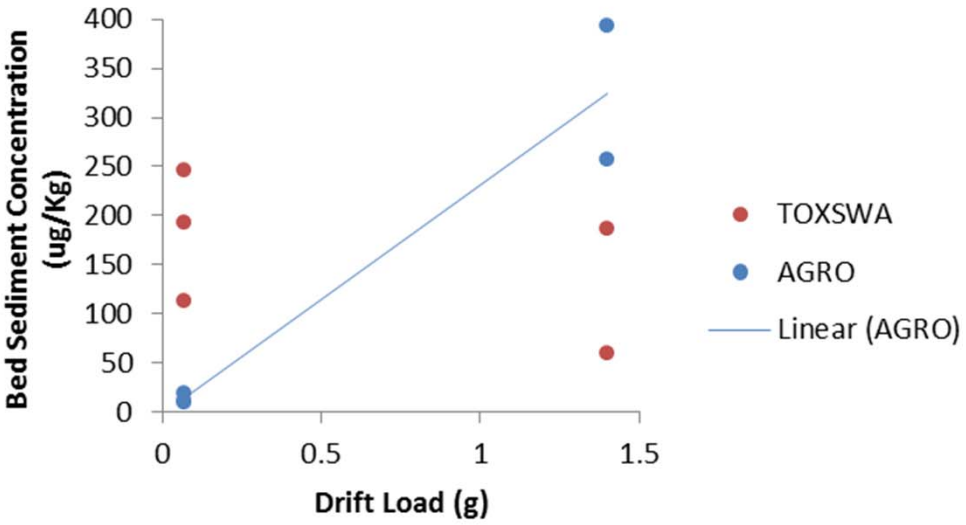
- Result is lower sediment concentrations

For spray drift loadings, AGRO pesticide mass mostly dissolved (no added eroded soil for sorption)

- Dissolved pesticide diffuses to sediment before it can leave stream via outflow
- Result is higher sediment concentrations

Maximum daily average concentration in FOCUS target year for each of the 5 stream simulations





Conclusions

TOXSWA and AGRO dissolved water concentrations were similar across a range of stream and pond water bodies, regions, and crops.

Differences between TOXSWA and AGRO were most obvious in their predictions of sediment concentrations due to different conceptual models for sediment processes

Sediment concentrations followed different patterns for the pond and stream water bodies due to the higher stream flow rates that increased lateral transport of pesticide in the water layer

The model differences were most important for compounds with high Koc like the pyrethroids that adsorb strongly to particulates

For compounds with low Koc, TOXSWA and AGRO predictions were almost identical

Future work

Comparison of AGRO and TOXSWA predictions to mesocosm observations for high Koc compounds to improve understanding of model advantages and limitations

Development of a potentially more physically realistic model that combines the AGRO sediment dynamics with the multilayer benthic sediment profile of TOXSWA

Thank you.

Contact / lpadilla@stone-env.com