

Outcome of the FOCUS SW Repair Stage 2 Testing

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Introduction

FOCUS SW Repair Stage 2 testing was designed for:

- A systematic evaluation of FOCUS SW Repair package across a range of substances, crops and application patterns
- A documentation of exposure outputs under revised modelling concepts
- A transparent comparison with the legacy FOCUS framework

This presentation:

- Key outcomes of Stage 2 testing
- Practical implications and proposed improvements

FOCUS SW Repair Stage 2 testing was performed under the auspices of the FOCUS Version Control Group, with endorsement from EFSA.

Materials and Methods

Test design

- Representative hypothetical test compounds (incl. metabolites), covering a systematic range of fate properties (from low to very high sorption and rapid to persistent degradation)
- Combined with seven crop groups with application patterns reflecting typical regulatory use scenarios
- Application timings were designed to cover diverse handling options (e.g. end-of-year applications)
- All substance–crop combinations were calculated using a predefined test matrix allowing for a thorough and reproducible comparison across scenarios.

Comparison metric

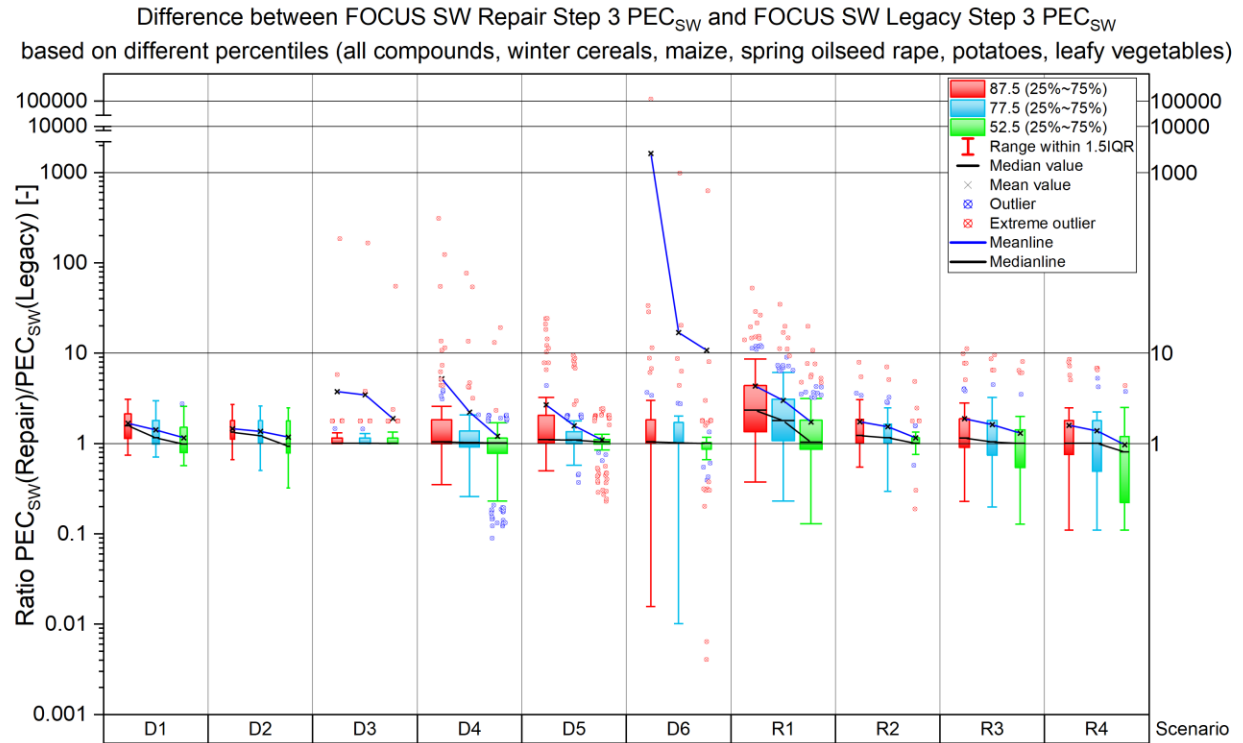
- 52.5th, 77.5th and 87.5th percentiles of annual maximum PEC_{SW} over 20 years
- Consistent with the percentile range discussed in the EFSA Scientific Report on FOCUS SW Repair

Percentiles are presented for illustrative comparison only; no judgement is made on regulatory relevance or appropriateness.

Results - Overall comparison across scenarios and crops

Central result, figure shows PEC ratios, FOCUS Repair divided by FOCUS Legacy across all scenarios, for the three percentiles

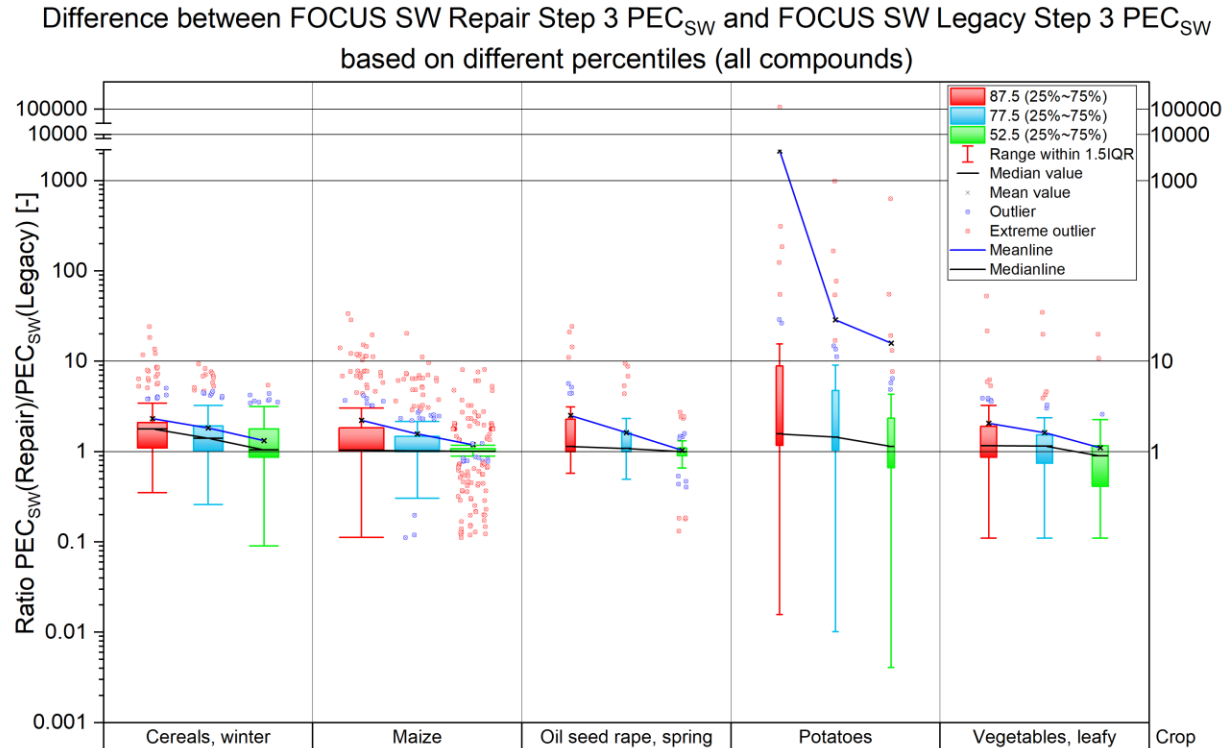
- Repair framework produces higher PEC_{SW} values than Legacy in most scenarios
- Differences increase towards higher percentiles
- Variability is scenario-dependent, spanning multiple orders of magnitude
- Extreme outliers → Extreme responses remain under investigation



Take home: FOCUS Repair is generally more conservative, but the magnitude varies substantially across scenarios

Results - Crop-group comparison (pooled across scenarios)

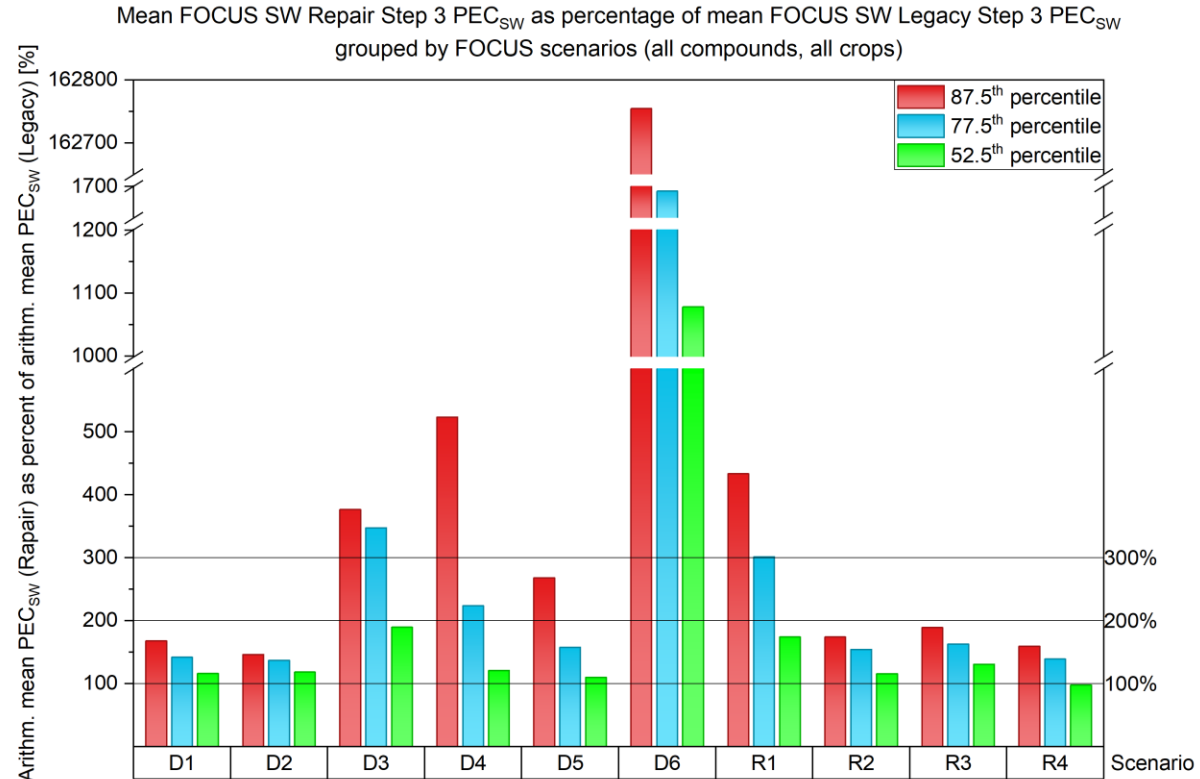
- Higher PEC_{SW} values under Repair observed across all crop groups
- Strong variability for arable crops, especially potatoes
- Drift-dominated crops (pome fruit, vines) show lower variability (additional follow-up work, including Step 4 evaluations, is intended)



Results - Summary metrics across scenarios

The figure shows mean PEC_{SW} Repair as a percentage of mean PEC_{SW} Legacy, by scenario and percentile

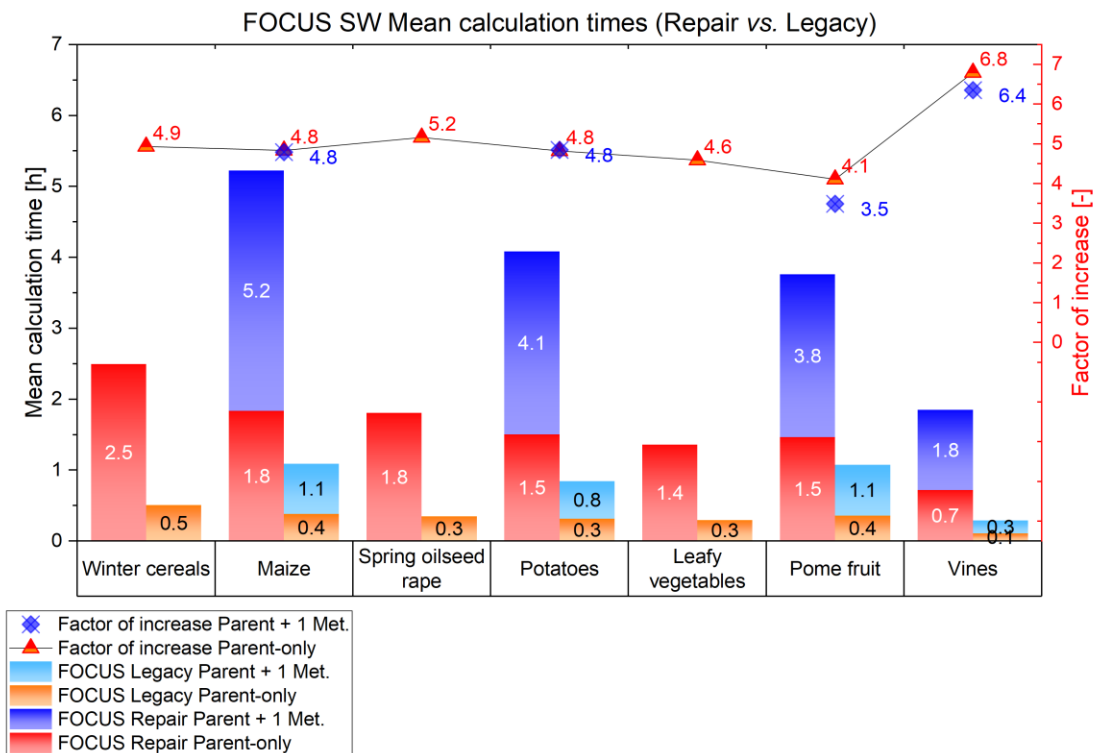
- Key message: no uniform scaling factor.
- The differences are both scenario- and percentile-dependent.



Results - Comparison of calculation times

Figure shows mean calculation times for MACRO + TOXSWA* per crop

- Key result: **~5 ×** increase of calculation time was observed for FOCUS Repair compared to FOCUS Legacy.
- Additional metabolites substantially increase calculation time
- Metabolite evaluations under the Repair framework require significantly more computational resources.



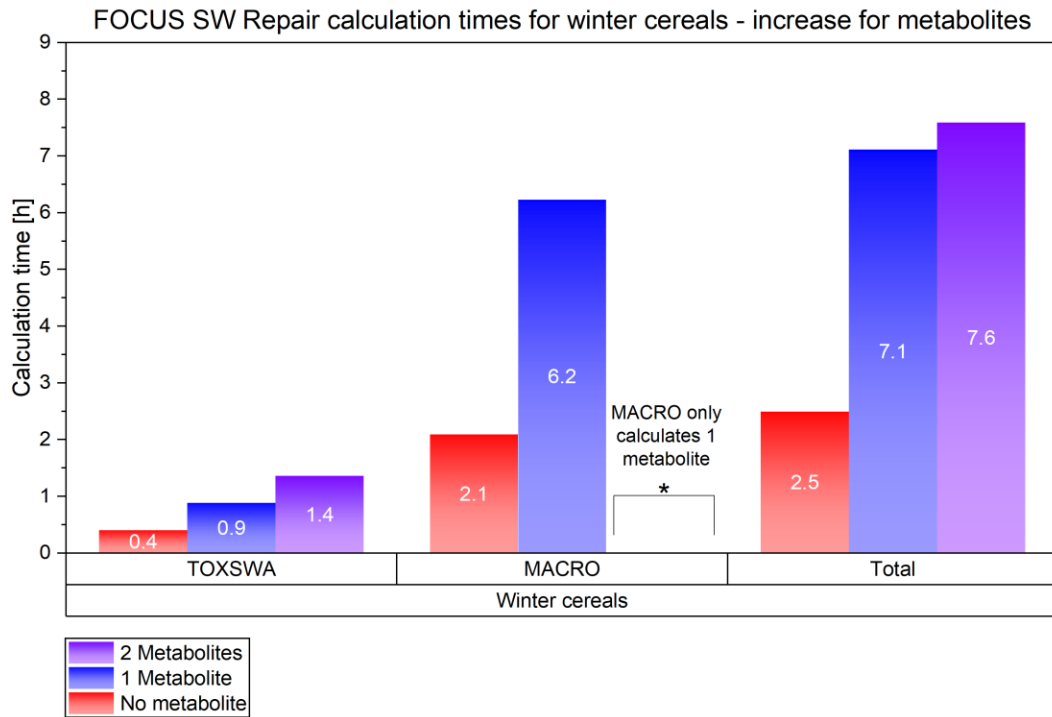
*PRZM not considered, as calculation times were comparatively short

Results - Impact of increasing number of metabolites

Additional analysis for winter cereals shows metabolite effect in more detail

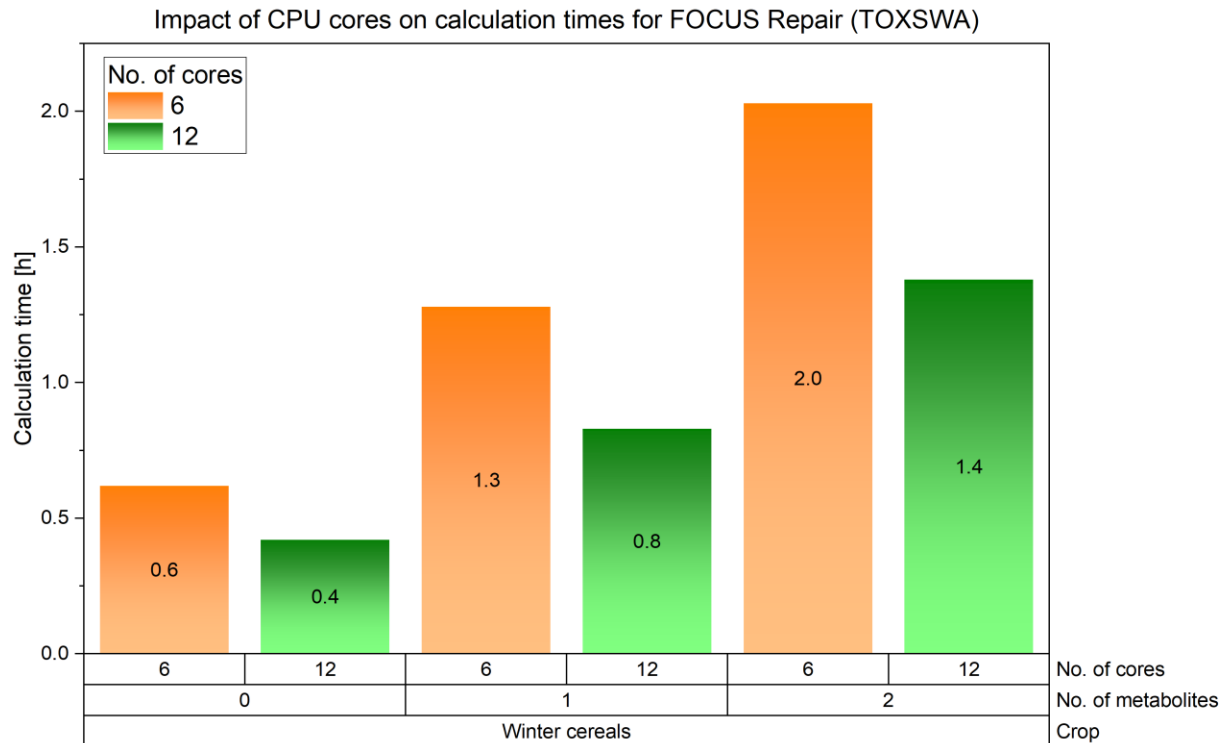
- Inclusion of metabolites leads to a significant increase in calculation time.
- The largest increase occurs when moving from parent-only to one metabolite, driven primarily by MACRO.
- Adding a second metabolite results in a further increase in total runtime via TOXSWA, while MACRO runtime remains unchanged due to the one-metabolite limitation.

Please note: High-end computer hardware was used for the calculations. Reduced hardware specifications may result in significantly higher calculation times!



Results - Impact of CPU cores on calculations

- Increasing number of parallel runs leads to a consistent reduction in total calculation time
- Absolute time savings become more pronounced with increasing metabolite complexity
- Largest reduction observed for one- and two-metabolite scenarios compared to parent-only cases



Please note: High-end computer hardware was used for the calculations. Reduced hardware specifications may result in significantly higher calculation times!

Conclusions

1. FOCUS SW Repair frequently results in higher PECsw values than the legacy framework
2. Differences are scenario-, crop- and percentile-dependent, with no uniform scaling
3. Metabolite behavior broadly mirrors parent compounds
4. Calculation times and project sizes increase substantially. Large project folders create practical constraints for storage, transfer and archiving
5. A limited number of unresolved software issues were identified and require follow-up before confirmatory reruns
6. Step 4 calculations were outside the Stage 2 testing scope
7. Results provide a transparent technical basis for further investigations
8. Regulatory interpretation is outside the scope

Proposed future improvements

Performance improvement

- Enabling parallel execution for MACRO (multi-threading)

Implementation concept

- Proven approach from existing workflows (UK drainage assessment workflow, UK CRD/HSE, EMMA — made available *free of charge*)
- Concept already implemented for the current FOCUS SW Legacy framework (internal use)
- Could be made available under a similar *non-commercial* approach for FOCUS SW Legacy and FOCUS SW Repair

Data handling

- Optional TOXSWA output profiles (full → minimal)
- To be aligned with future authority expectations

This concept is presented as a technical option for future implementations; no regulatory recommendation is made

FOCUS MACRO 5.5.4 SW / GW – Multi-threading Illustration

The illustrated automation concept is not specific to FOCUS SW Repair and is presented as a non-commercial, freely available approach that could be adapted to reduce runtimes in future workflows.

This short clip illustrates the practical concept.

MAMA v0.9

- MACRO Multithreading Automation -

Technical demonstration

Thank you for your patience!

Test compounds and parameterization

Parameter Test compounds	TC1a	TC1b with met.	TC1c	TC2a	TC2b	TC2c with met.	TC X	TC Y
Molar mass [g/mol]	300	300	300	300	300	300	300	300
Vapor pressure [Pa at 20°C]	1.0×10 ⁻⁷	1.0×10 ⁻⁷	1.0×10 ⁻⁷	1.0×10 ⁻⁷	1.0×10 ⁻⁷	1.0×10 ⁻⁷	1.0×10 ⁻⁷	0.1
Water solubility [mg/L at 20°C]	1	1	1	1	1	1	1	0.1
DT ₅₀ soil [d]	10	10	10	100	100	100	1000	1
K _{Foc} [L/kg]	100	1000	10000	100	1000	10000	1000000	10
Freundlich 1/n [-]	1 / 0.7***	1 / 0.7***	1 / 0.7***	1 / 0.7***	1 / 0.7***	1 / 0.7***	1 / 0.7***	1 / 0.7***
DT ₅₀ water [d]	1000	1000	1000	10	10	10	1000	1
DT ₅₀ sediment [d]	10	10	10	10000	10000	10000	1000	1
TSCF / PUF [-]	0	0	0	0	0	0	0	0
Remarks	Parent / Met	ff 1 to TC2b form. from all compartments			Parent / Met	ff 1 to TC1a form. from all compartments		Extreme compound
Compound properties								
Soil persistence	not persistent	not persistent	not persistent	moderately persistent	moderately persistent	moderately persistent	persistent	not persistent
Water phase persistence	persistent	persistent	persistent	not persistent	not persistent	not persistent	persistent	not persistent
Sediment phase persistence	not persistent	not persistent	not persistent	persistent	persistent	persistent	persistent	not persistent
Sorption	low	moderate	high	low	moderate	high	very high	very low
Rationale	rapid deg. in soil/sediment with increasing sorption			moderate deg. in soil with increasing sorption			slow/no deg./high sorption	rapid deg./low sorption
Test GAP Compound	TC1a	TC1b	TC1c	TC2a	TC2b	TC2c	TC X	TC Y
GAP 2 (maize)	Y	Y	Y	Y	Y	Y	Y	Y
GAP 1 (potatoes)	Y	Y	Y	Y	Y	Y	Y**	-
GAP 5 (vines)	Y	Y	Y	Y	Y	Y	Y**	Y*
GAP 4 (apples)	Y	Y	-	-	Y	Y	Y**	Y*
GAP 6 (spring OSR)	Y	-	-	-	Y	-	Y**	-
GAP 3 (winter wheat)	Y	-	-	-	Y	-	Y**/ Y*	-
GAP 7 (leafy veg.)	Y	-	-	-	Y	-	Y**	-

**additionally tested (included in current testing)*

***additional test GAP, not included in current testing*

****first tier 1/n = 1; second tier 1/n = 0.7; decision for tier 2 will be made at later stage (not included in current testing)*

Example test compound series properties

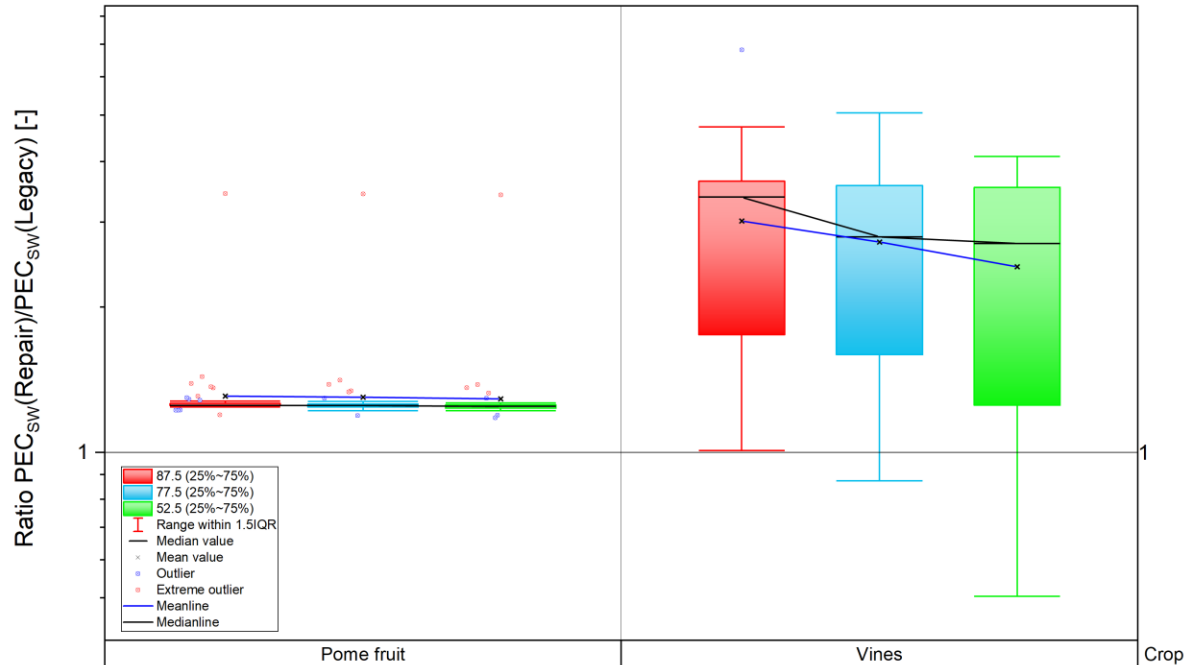
- TC1 series: rapid degradation in soil (DT_{50} in soil = 10 d) and sediment (DT_{50} in sediment = 10 d) while varying sorption from low to high.
- Key parameters were held constant (e.g. molar mass, vapor pressure, water solubility) while the K_{FOC} was increased stepwise (100 $\rightarrow$ 1,000 $\rightarrow$ 10,000 L/kg) to evaluate the sensitivity of predicted PEC_{SW} to sorption under otherwise comparable conditions.
- Water-phase persistence was set to a regulatory default (DT_{50} water = 1000 d), ensuring that differences in PEC_{SW} are not driven primarily by rapid aqueous degradation. Two TC1 variants were included to assess the correct implementation of parent–metabolite handling (formation fractions from compartments)

Computer Hardware used for testing

Category	Parameter	Specification
Manufacturer	DELL ALIENWARE	ALIENWARE X16
Operating system	OS name	Microsoft Windows 10/11 Pro
	OS version	25H2 (64-bit)
Hardware	CPU	Intel(R) Core(TM) Ultra 9 185H (2.30 GHz)
	Cores / threads	16 / 32 (22 logical processors)
	Installed RAM	32 GB
GPU	Graphic card	NVIDIA GeForce RTX 4080
Storage / Size	Storage type	SSD, 8 TB

Drift-dominated crops

Difference between FOCUS SW Repair Step 3 PEC_{SW} and FOCUS SW Legacy Step 3 PEC_{SW}
based on different percentiles (all compounds, pome fruit and vines)



Project file sizes

