

Evaluating Groundwater Exposure Concentration for Precision Application in Europe: A Robust Methodology

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Syngenta, 4 September 2026

XVIII SYMPOSIUM ON PESTICIDE CHEMISTRY



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Precision Application (PA)

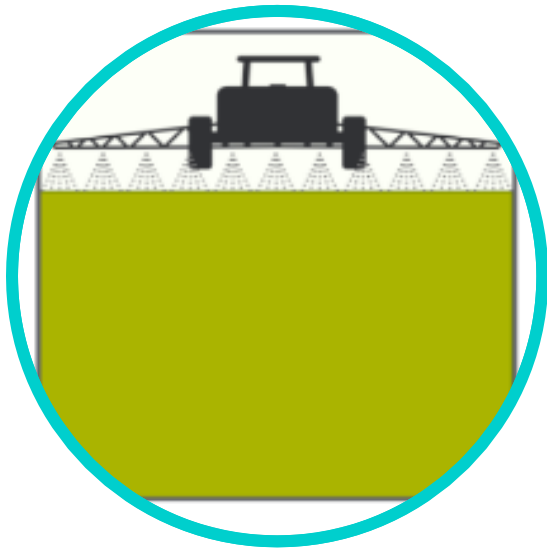
Key Principle:

- The application rate in the treated area (g/unit area treated) remains unchanged; only the treated fraction of the field is reduced (less than 1.0).
- Total mass loading across the entire field decreases proportionally.



Example:

- Broadcast GAP: Broadcast application rate 1×1000 g/ha
- PA GAP: PA application in rows 1×1000 g/ha, 0.5 Treated field fraction (0.5ha)
- Total applied amount within 1ha field: Broadcast 1000g, PA 500g
- Treatment rate in treated areas is the same: 1×0.1 g/m² (1ha = 10,000 m²)



Implication for Groundwater Exposure:

- EUPAF recommended*:
 - apply % treated field to the broadcast PEC_{gw} → direct scaling of $PEC_{gw,0}$
- Question: Is the EUPAF approach appropriate for all FOCUS GW scenarios?

The Conversion factor (= % treated field), throughout this presentation, ' % treated field' is used

Non-linear Sorption in EU FOCUS framework

In all regulatory leaching models, the partitioning between solid and liquid phases is described by the Freundlich sorption equation

The freundlich equation for sorption in the equilibrium domain*:

$$X_{eq} = K_{F,eq} c_{L,r} \left(\frac{c_L}{c_{L,r}} \right)^{1/n}$$

X_{eq} = pesticide content sorbed in the equilibrium domain, kg/kg

$K_{F,eq}$ = Freundlich sorption coefficient for the equilibrium domain, m²/kg

$c_{L,r}$ = reference concentration in the liquid phase, kg/m³

1/n = Freundlich exponent

Key Points:

- The partition coefficient depends on the liquid-phase concentration (C_L).
- The Freundlich exponent (1/n) determines the non-linearity of the sorption isotherm.
- Stronger sorption (lower 1/n) results in lower leaching concentrations.

Most pesticides have 1/n between 0.7 and 1.1 in regulatory assessments².

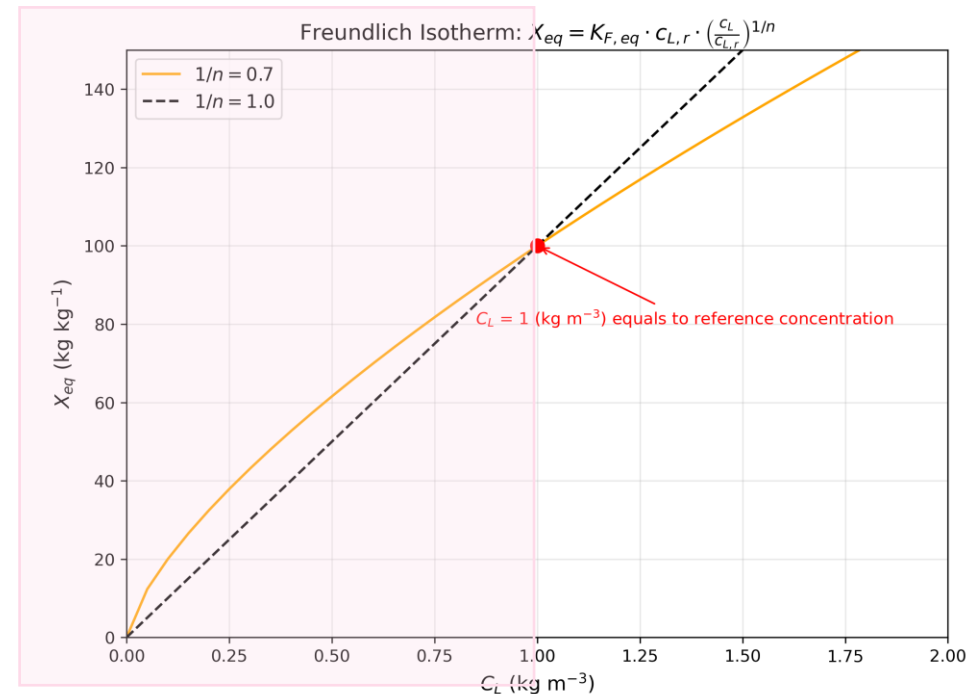
* Leistra, M, 2001. et al

¹ SANTE/12586/2020 – REV 1. 2021.October. Guidance on how aged sorption studies for pesticides should be conducted, analysed and used in regulatory assessments

² Nearly all measured 1/n values are between 0.7 and 1.1 although sometimes values as low as 0.6 or as high as 1.2 have been measured” (Boesten et al., 2015)

For $C_L < 1 \text{ kg} \cdot \text{m}^{-3}$:

- With $1/n < 1$, sorption increases and leaching decreases
- With $1/n \approx 1$, approximates linear relationship
- With $1/n > 1$, reduced sorption, more leaching (physically unrealistic for the soil matrix¹, is outside the scope of this study)



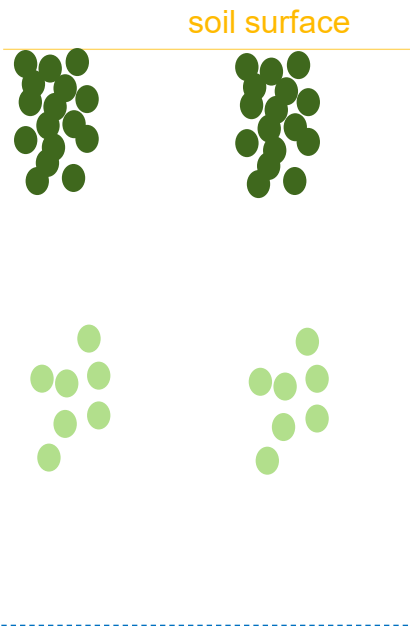
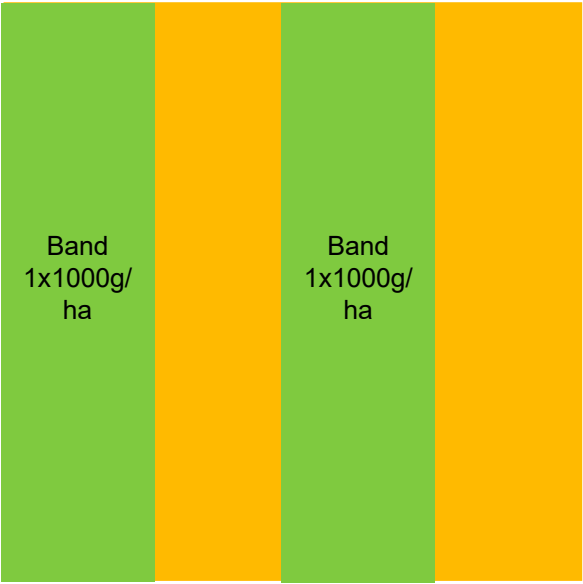
Non-linear Sorption Implications for PA



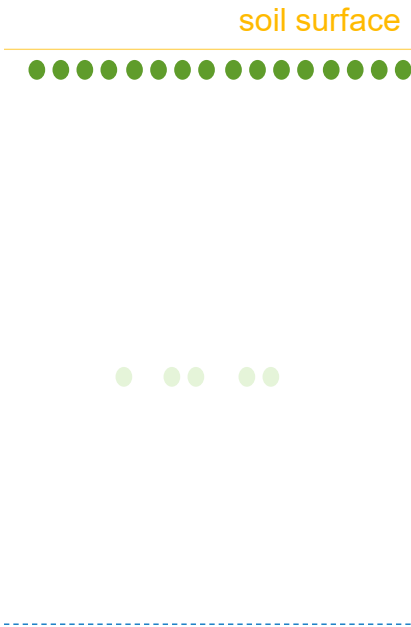
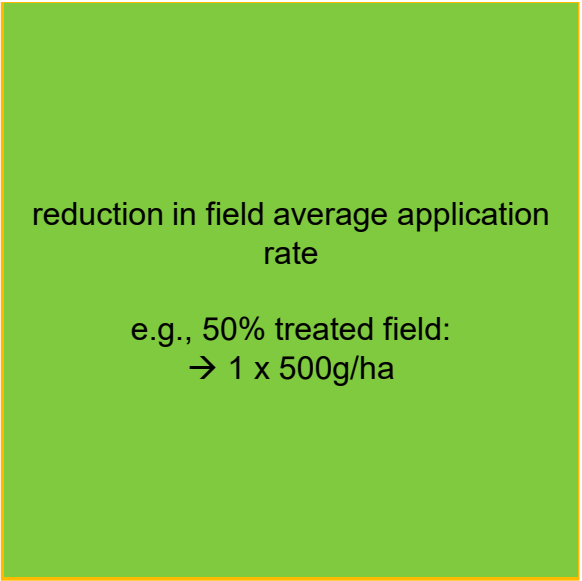
Relevance to Precision Application:

- PA results in a reduction in field average application rate
 - However, applied rate in PA treated areas is the same as broadcast
 - Due to non-linear sorption, the relationship between mass loading per treated area and mass leached is not necessarily linear.
- The partition coefficient depends on the liquid-phase concentration (C_L).
 - The ratio for the solid/liquid partitioning often increases as the concentration decreases

Direct scaling of $PEC_{gw,0}$



Field averaged application rate



Reference Case: Example GAP: 1x 1000g/ha, PA impact: 50% treated field

Methodology: Comparing Two Approaches for Estimating PA PEC_{gw}

Reference Case:

Example GAP: 1x 1000g/ha, no crop simulated, 1 application date

PA impact: 50% treated field

→ FOCUS $PEC_{gw,0}$ = modelled concentration at 100% treated field

Method 1- Direct Scaling of $PEC_{gw,0}$

(EUPAF recommendation)

- $PEC_{gw,1} = PEC_{gw,0} \times 50\%$ treated field
- Simple post-processing; no re-run of leaching model required.

Method 2- Field-averaged Application Rate*

- Field-averaged rate= broadcast application rate $\times$ 50% treated field
- $PEC_{gw,2}$ = modelled concentration using the reduced (field-averaged) rate
- Requires a new model run at the lower application rate.

1. Which method is conservative when considering all different Freundlich non-linearity for both parent and metabolite?
2. Does the method apply to all FOCUS GW scenarios including both chromatographic flow and preferential flow?

“Concluding, using a reduced dose for a particular PPP as result of precision application techniques in the leaching assessment for regulatory purposes is defensible for substances with linear sorption or weak non-linearity of sorption”. (Ter Horst, M.M.S., E.L. Wipfler, K. van Boheemen, J.F.M. Huijsmans, 2023. Impact of precision application of herbicides on leaching to groundwater. Wageningen, Wageningen Environmental Research, Report 3293. 46 pp.; 11 fig.; 9 tab.; 17 ref.)

Simulation Parameters

A comprehensive 3 million parent – metabolite simulations set was evaluated to ensure robustness of the conclusions.

Application Scenario:

Rate: 1 x 1000g/ha, 1 application date, no crop (FOCUS-PEARL v5.5.5), winter cereal¹ (FOCUS-MACRO v5.2)

Parameters - Parent / Metabolites	Values in PEARL/MACRO
Degradation (DegT50) (days)	10, 25, 50, 100, 200, 400, 800*, 1000 days
Sorption (Koc) (mL/g)	2 – 40,000
Freundlich exponent (1/n)	0.6 (parent only)*, 0.7 (parent only)*, 0.8*, 0.92, 1.0
% treated field	10% – 100%
Total No. of unique substance properties	17,530 in PEARL, 5,300 in MACRO (including non-leaching and persistent substances)
Per scenario No. of simulations	105,180 in PEARL, 31,800 in MACRO

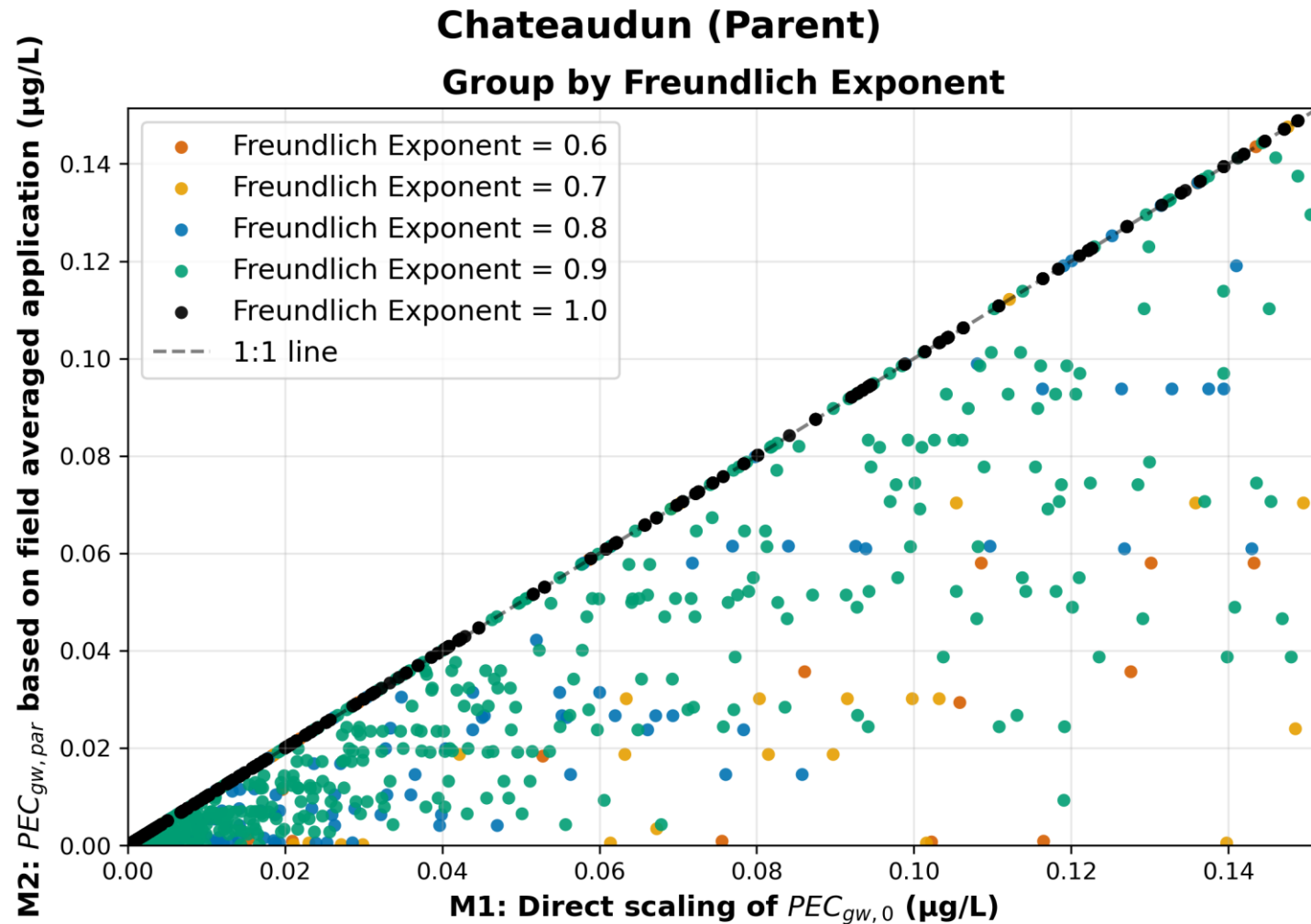
*not assessed for metabolites in MACRO due to computational time

PEARL (per FOCUS scenario) : 350,600 unique combinations

MACRO: 106,000 unique combinations

¹ No 'bare soil' option in FOCUS MACRO, possible to simulate via changing plant parameters.

Results: Parents, FOCUS-PEARL v5.5.5 Châteaudun Scenario



- ❑ Method 1 (direct scaling) consistently yields equal or higher PEC_{gw} than Method 2 across all tested $1/n$ values ($1/n \leq 1$).
- ❑ The difference between methods increases as $1/n$ decreases (stronger non-linearity).
- ❑ At $1/n = 1.0$ (linear sorption), both methods produce identical results.

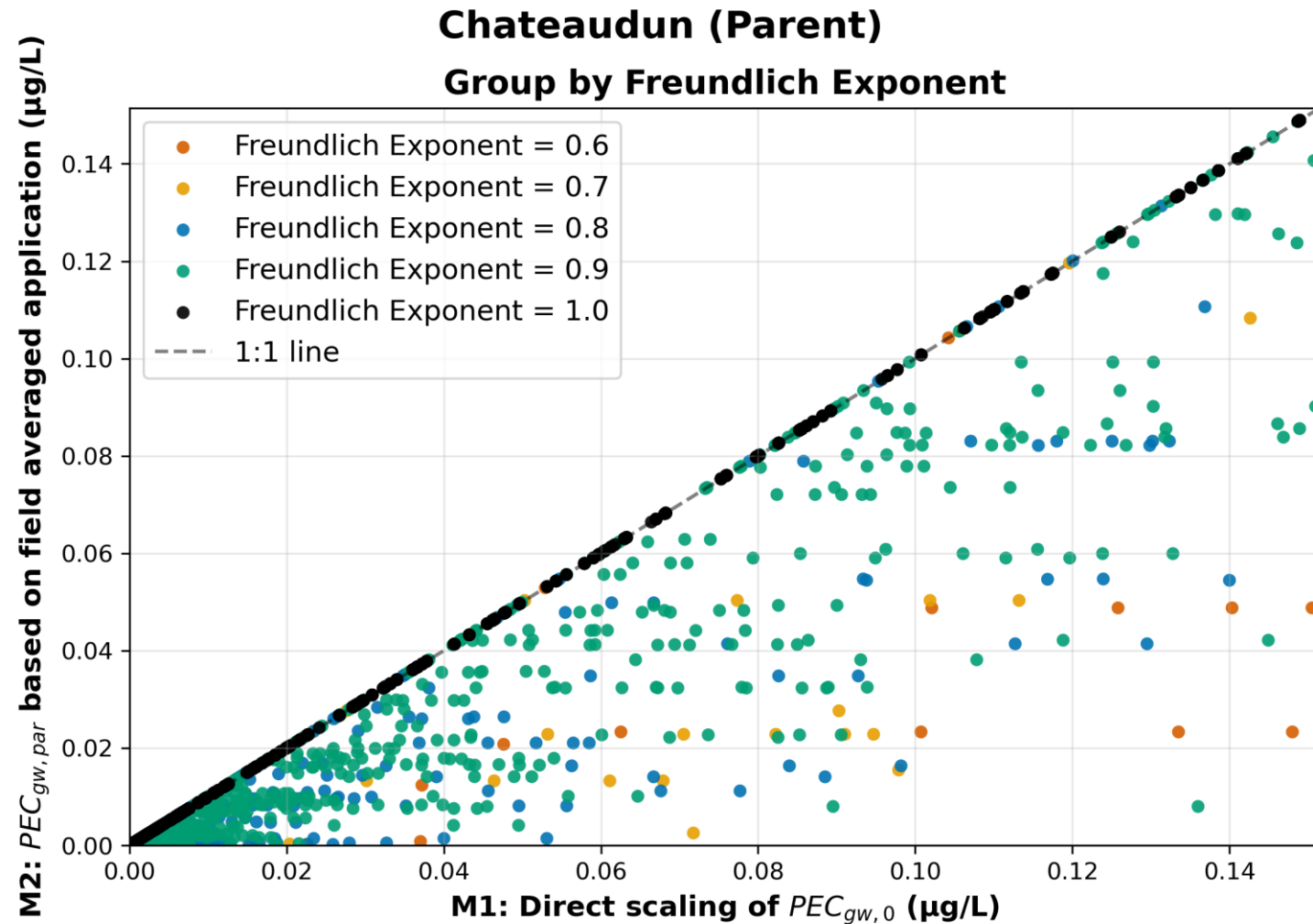
**The ratio (Method 2 / Method 1) is almost always ≤ 1 .
The non-linearity of Freundlich sorption is the key driver.**

Results are filtered for substances yielding PEC_{gw} concentrations near the 0.1 $\mu\text{g/L}$ regulatory threshold

Full PEC ranges are in the supplementary slide.

Method 1 = Direct scaling $PEC_{gw,0}$
Method 2 = Field-averaged application rate

Results: Parents, FOCUS-MACRO v5.2 Châteaudun Scenario



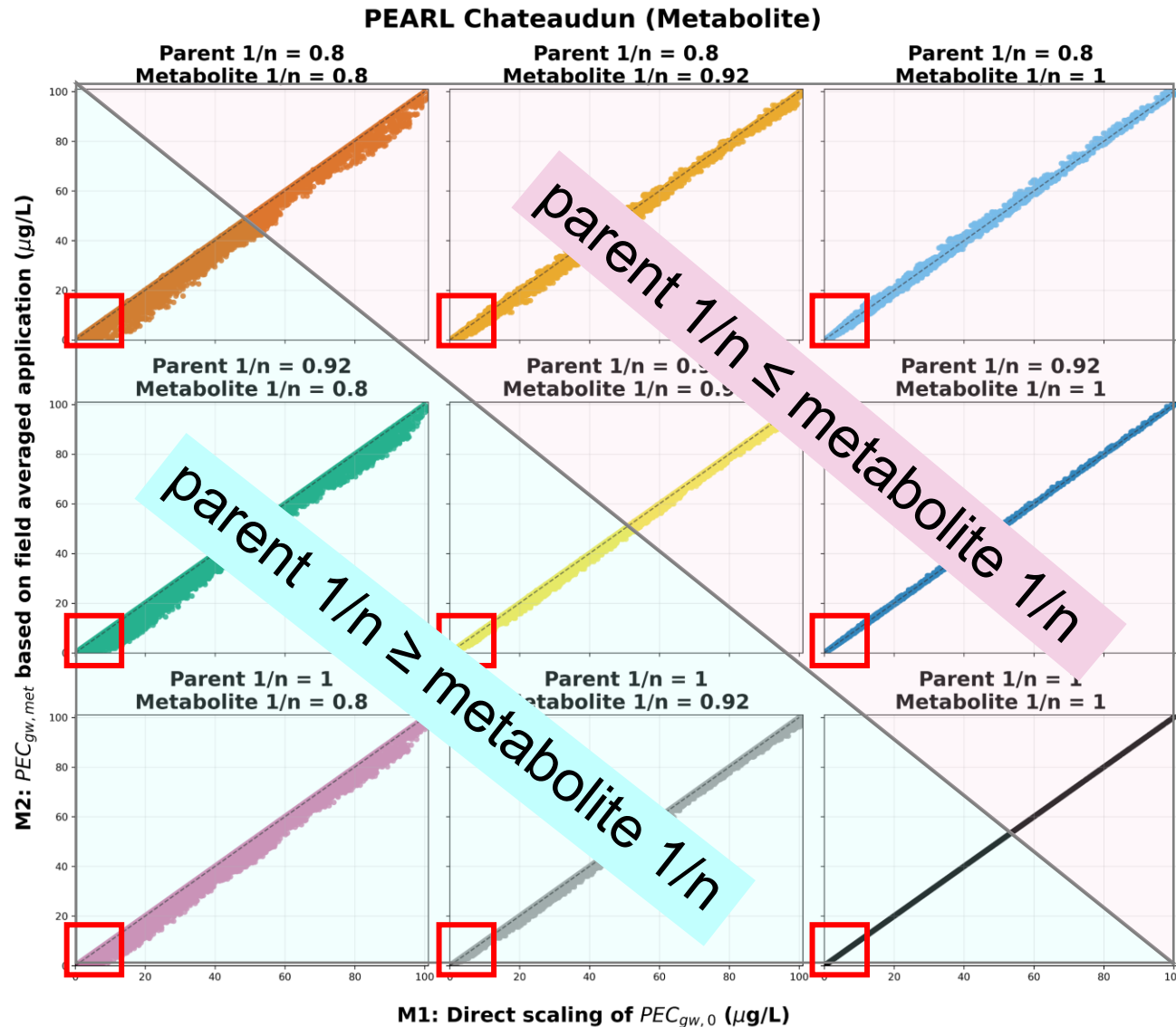
- ❑ The same pattern is observed: Method 1 (direct scaling) consistently yields equal or higher PEC_{gw} than Method 2 across all tested $1/n$ values ($1/n \leq 1$).
- ❑ Preferential flow (macropore transport) in MACRO does not alter the conclusion.
- ❑ The direct scaling approach remains protective under preferential flow conditions.

Results are filtered for substances yielding PEC_{gw} concentrations near the 0.1 $\mu\text{g/L}$ regulatory threshold

Full PEC ranges are in the supplementary slide.

Method 1 = Direct scaling $PEC_{gw,0}$
Method 2 = Field-averaged application rate

Results: Metabolites, FOCUS-PEARL v5.5.5 Châteaudun Scenario

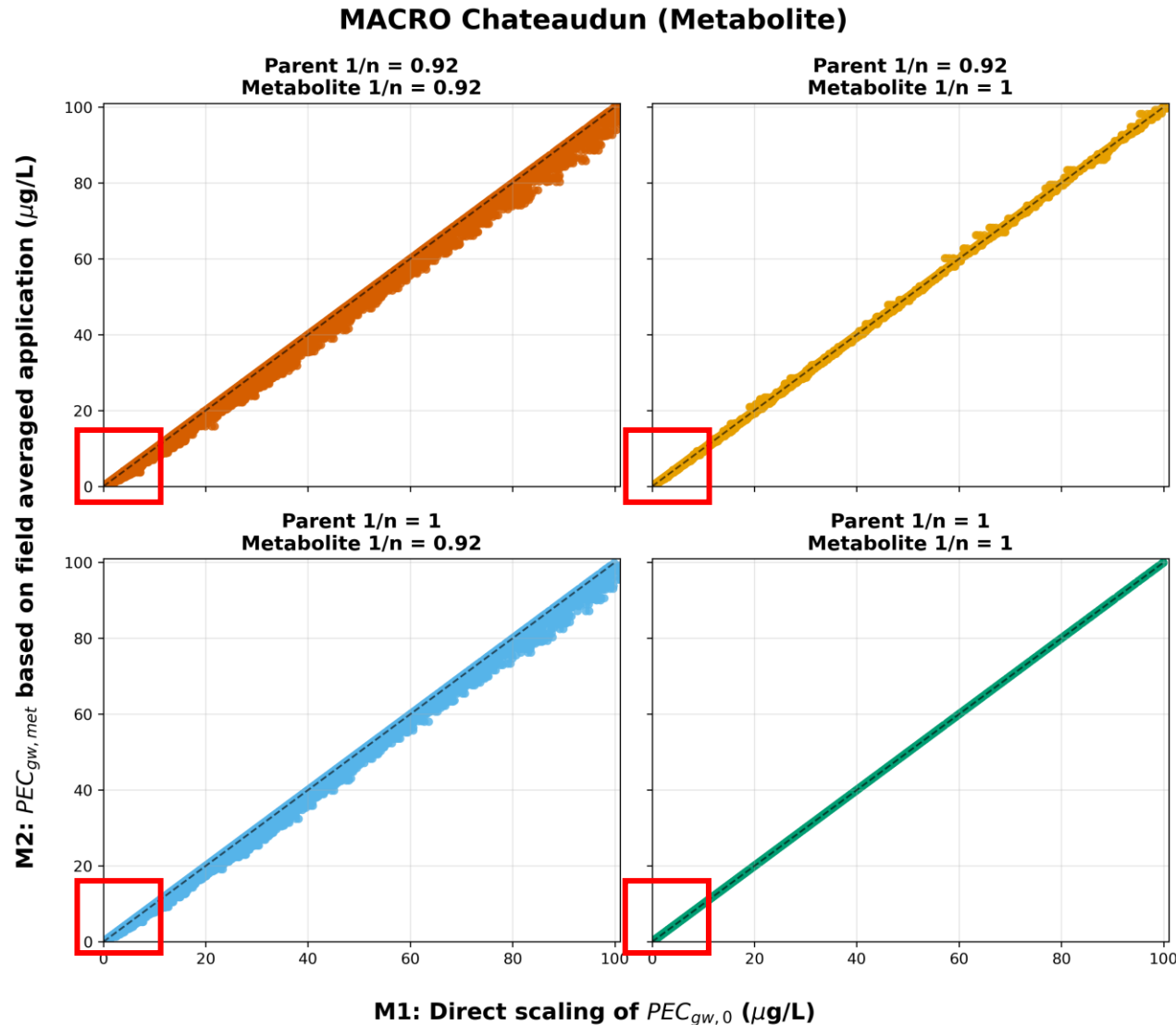


The Freundlich exponents of the parent and metabolite are the key driver of the result.

1. When the parent exponent is greater than or equal to the metabolite exponent, $PEC_{gw,met}$ from Method 1 is generally greater than or equal to $PEC_{gw,met}$ from Method 2.
2. When the Freundlich exponent of the parent is lower than the one of the metabolite, then in some cases Method 1 provides smaller $PEC_{gw,met}$ compared to Method 2.
3. At $1/n = 1.0$ (linear sorption), both methods produce identical results.

Method 1 = Direct scaling $PEC_{gw,0}$
Method 2 = Field-averaged application rate

Results: Metabolites, FOCUS-MACRO v5.2 Châteaudun Scenario



Similar to that observed in PEARL. The Freundlich exponents of the parent and metabolite are the key driver of the result.

1. When the parent exponent is greater than or equal to the metabolite exponent, $PEC_{gw,met}$ from Method 1 is generally greater than or equal to $PEC_{gw,met}$ from Method 2.
2. When the Freundlich exponent of the parent is lower than the one of the metabolite, then a few isolated cases Method 1 provides smaller $PEC_{gw,met}$ compared to Method 2.
3. At $1/n = 1.0$ (linear sorption), both methods produce identical results.

Method 1 = Direct scaling $PEC_{gw,0}$
Method 2 = Field-averaged application rate

Full PEC ranges are in the supplementary slide.

Discussion

- Non-linear sorption of parent and metabolite is the key driver of the differences in the results
 - In **over 97%** (> 3 million) the $PEC_{gw,met}$ derived from Method 1 are greater or equal to those derived from Method 2
 - There are few cases where $PEC_{gw,met}$ calculated with Method 1 are smaller than with Method 2 (only when parent $1/n <$ metabolite $1/n$).
 - The metabolite concentration is impacted by both parent and its own nonlinear sorption. When parent have strong non-linear sorption while metabolite have weak linear sorption, Method 1 (direct scaling the PEC_{gw}) did not scale linearly and could result in slightly lower values than Method 2.
 - Not all scoped chemical substances exist on the market... ...there are some quite extreme parameter combinations!
- When looking only at a subset of the data, where parent $PEC_{gw,par} \leq 0.5 \mu\text{g/L}$, metabolite $PEC_{gw,met}$ values derived from method 1 is greater than or equal to Method 2 in 99.94% of cases.

Method 1 = Direct scaling $PEC_{gw,0}$
Method 2 = Field-averaged application rate

Conclusion

Direct scaling of $PEC_{gw,0}$ is conservative for parent compounds in all tested simulations, and for metabolites in 97.07% of cases in over 3 million parent – metabolite simulations. Exceptions (<3%) occurred almost exclusively when the parent Freundlich exponent was lower than that of the metabolite.

- For Parent:
 - 100% valid (based on 180,000 runs), Method 1 (EUPAF recommendation, direct scaling: $PEC_{gw} \times \% \text{ treated field}$) results in consistently equal or higher concentration than Method 2 (field-averaged rate) across all tested Freundlich exponent values ($1/n = 0.6$ to 1.0), and this pattern applies overall to all FOCUS chromatographic flow scenarios and FOCUS-MACRO preferential flow Châteaudun.
- For metabolite:
 - 97.07% of cases (based on 3,261,400 runs) across all FOCUS GW scenarios, where Method 1 (EUPAF recommendation, direct scaling: $PEC_{gw} \times \% \text{ treated field}$) result in equal or higher concentration than Method 2 (field-averaged rate) across tested Freundlich exponent values.

Concluding: Direct scaling of $PEC_{gw,0}$ by the % treated field is appropriate and pragmatic for regulatory assessment of both parent and metabolites.

Special thanks for following colleagues:

Sevil Payvandi
Kerstin de Vries
Peter Rainbird
Helena Andrade
Edna Roedig
Michael Bird



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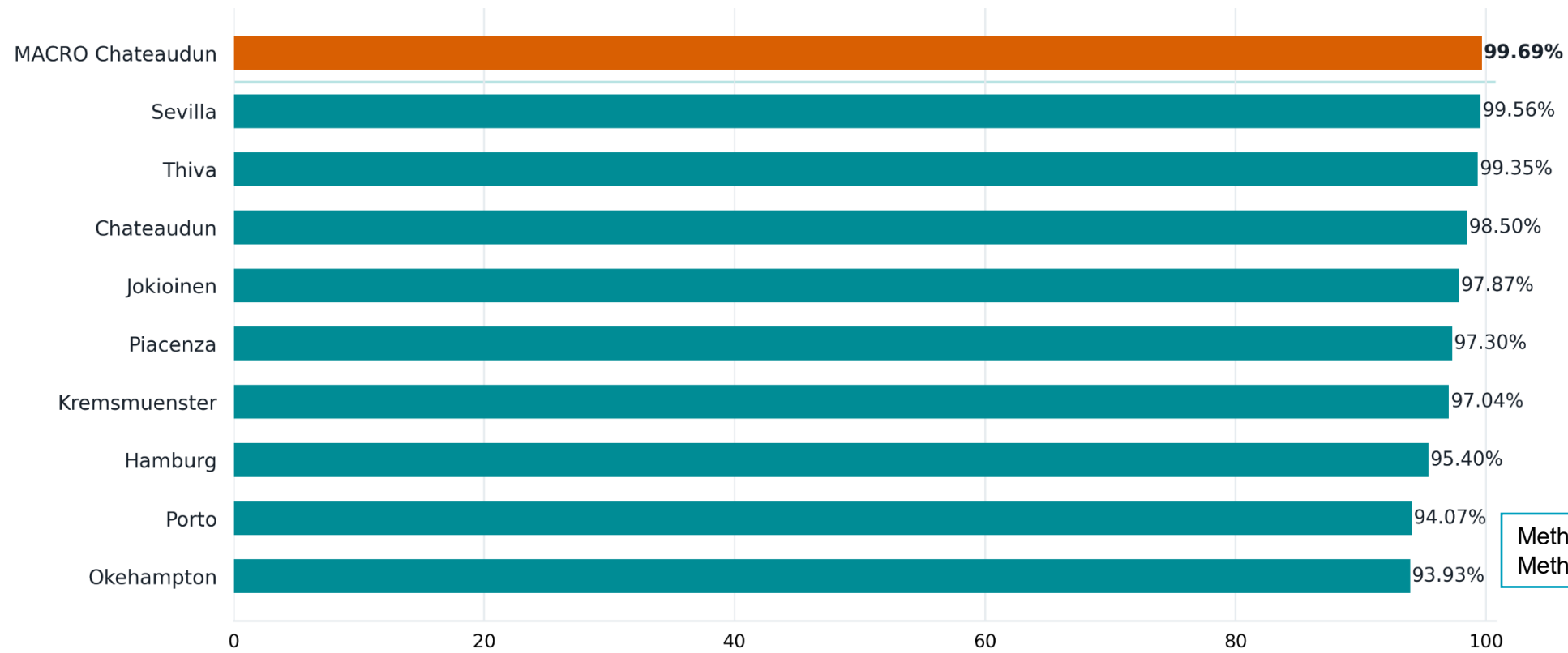
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Results: EUPAF-recommended approach (Method 1) applies for metabolites in nearly all cases

Share of cases in which direct scaling of $PEC_{gw,met}$ produced a value greater than or equal to the field-averaged application-rate approach ($M1 \geq M2$)

Overall result: 97.07% (n = 3,261,400)

FOCUS PEARL chromatographic flow FOCUS MACRO preferential flow



SUMMARY

FOCUS-PEARL scenarios
97.01% (n=3,155,400)

FOCUS MACRO scenario
99.69 % (n =106,000)

Method 1 = Direct scaling $PEC_{gw,0}$
Method 2 = Field-averaged application rate

KEY TAKEAWAY

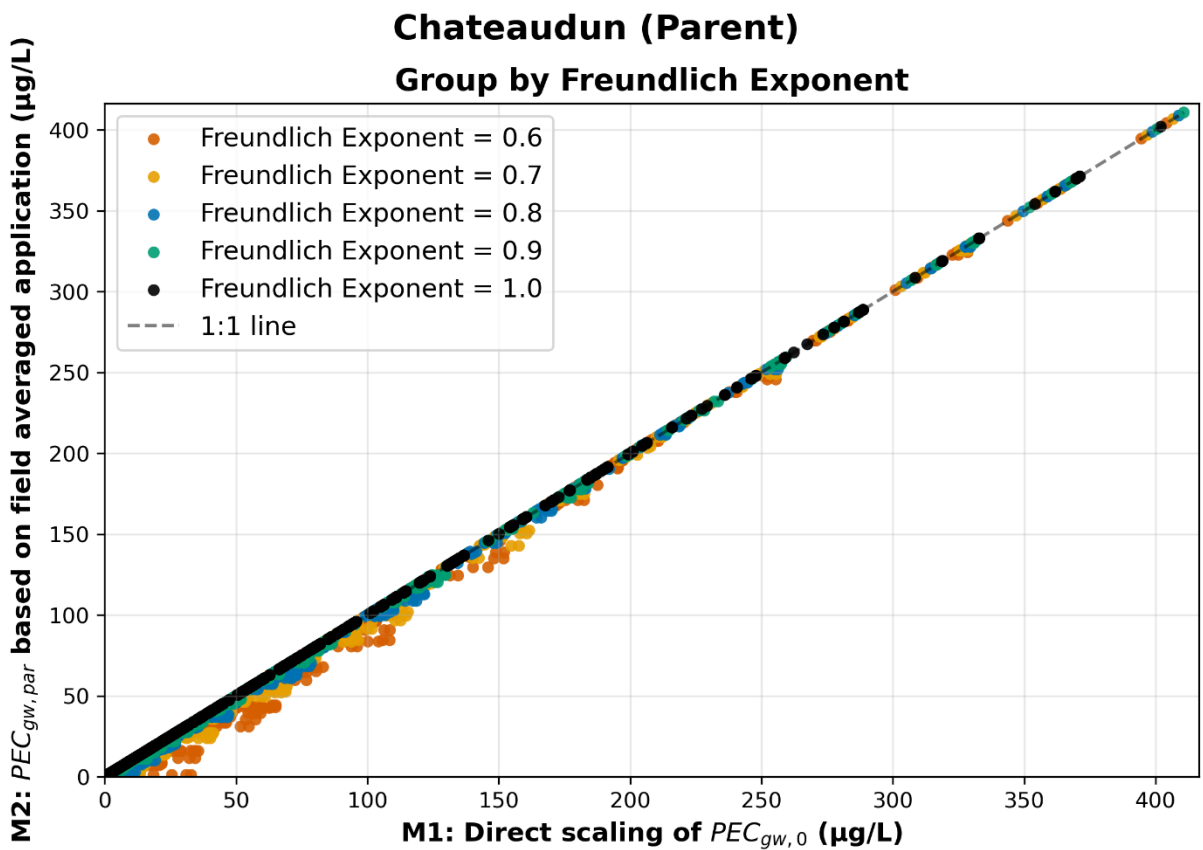
Across over 3 million evaluated cases, direct scaling produced $PEC_{gw,met}$ values greater than or equal to those obtained using the field-averaged application-rate approach in 97.07% of cases.

References:

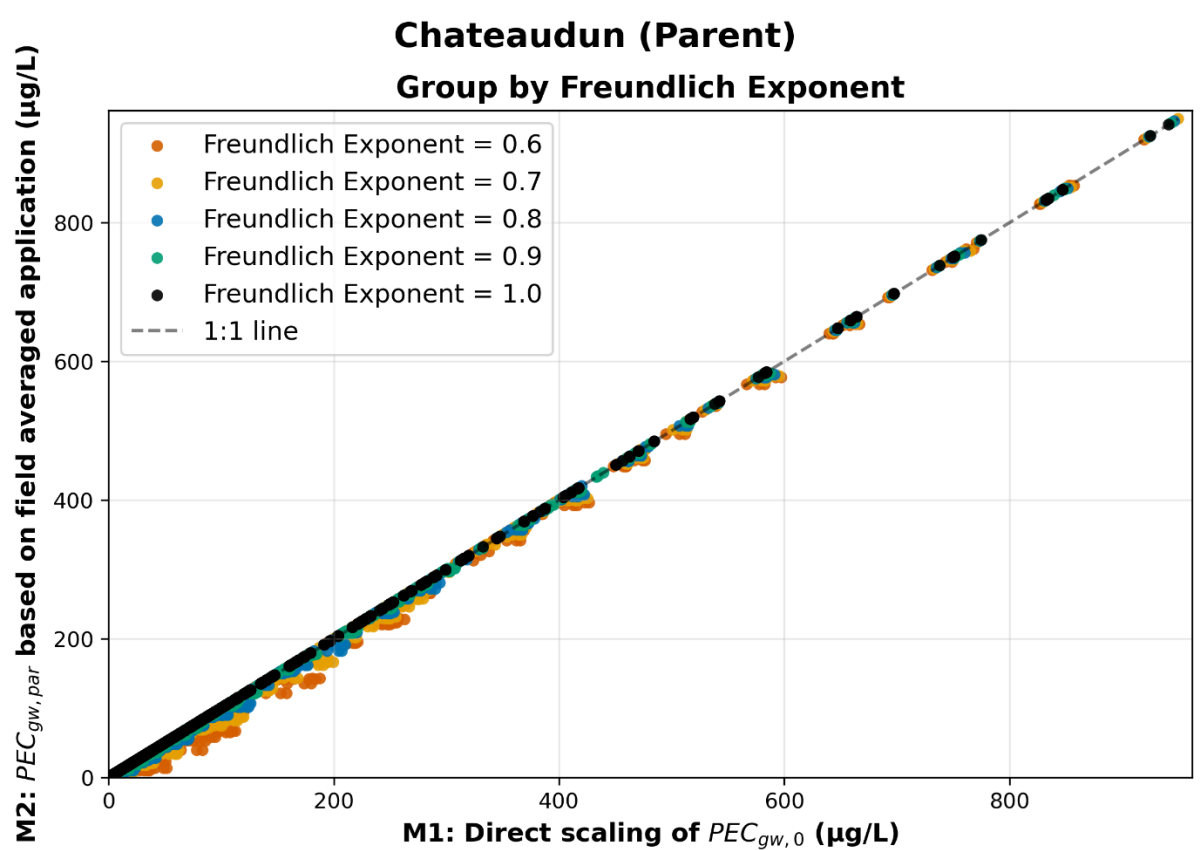
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2. Leistra, M., A.M.A. van der Linden, J.J.T.I. Boesten, A. Tiktak and F. van den Berg, 2001. PEARL model for pesticide behaviour and emissions in soil-plant system; Description of the processes in FOCUS PEARL v 1.1.1. Bilthoven, National Institute of Public Health and the Environment. Wageningen, Alterra, Green World Research. RIVM report 711401009/Alterra-rapport 013; 116 blz.; 9 fig.; 1 tab.; 42 ref.
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4. Boesten et al., 2015. Leaching of plant protection products and their transformation products : proposals for improving the assessment of leaching to groundwater in the Netherlands : version 2
5. Ter Horst, M.M.S., E.L. Wipfler, K. van Boheemen, J.F.M. Huijsmans, 2023. Impact of precision application of herbicides on leaching to groundwater. Wageningen, Wageningen Environmental Research, Report 3293. 46 pp.; 11 fig.; 9 tab.; 17 ref.
6. Ruiz, S., Payvandi, S., Sweeney. P., Roose. T., Analytical equation for rapid estimation of pesticide leaching risk accounting for nonlinear sorption with bulk soil biodegradation. Soil and Ecosystem Processe. DOI: 10.1002/saj2.7012

Full PEC ranges – Parent only

Chromatographic flow

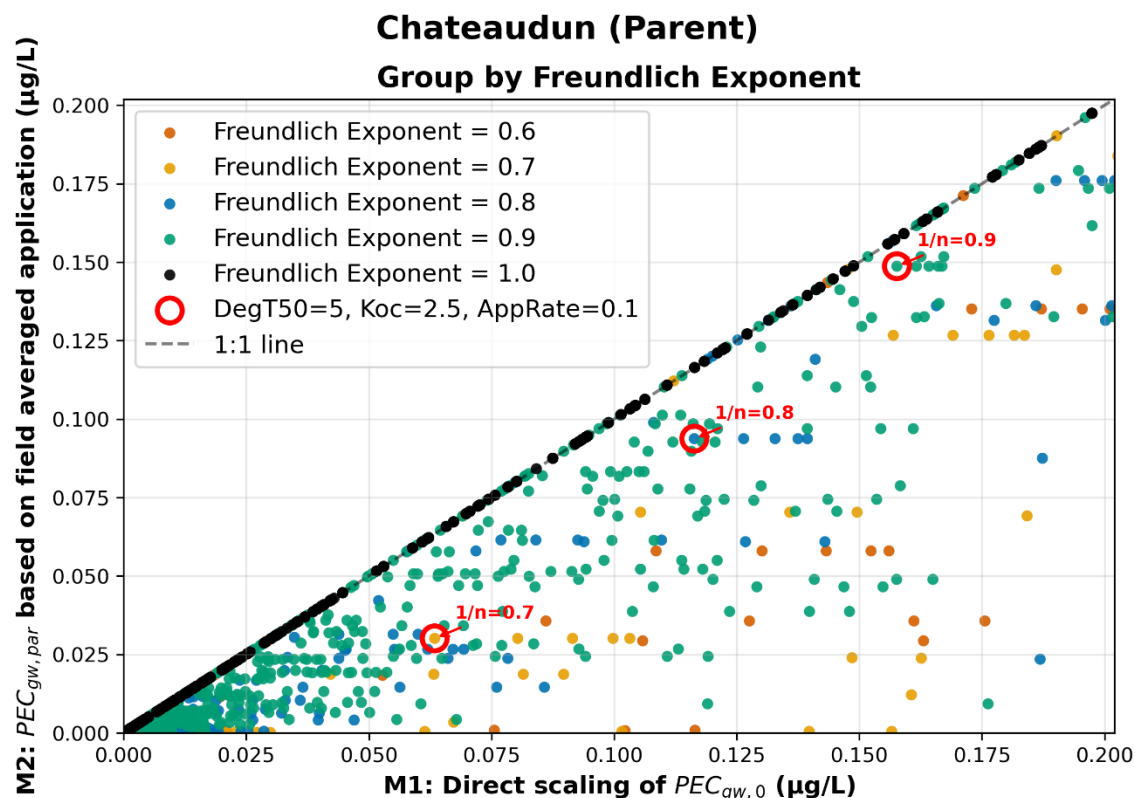


Preferential flow

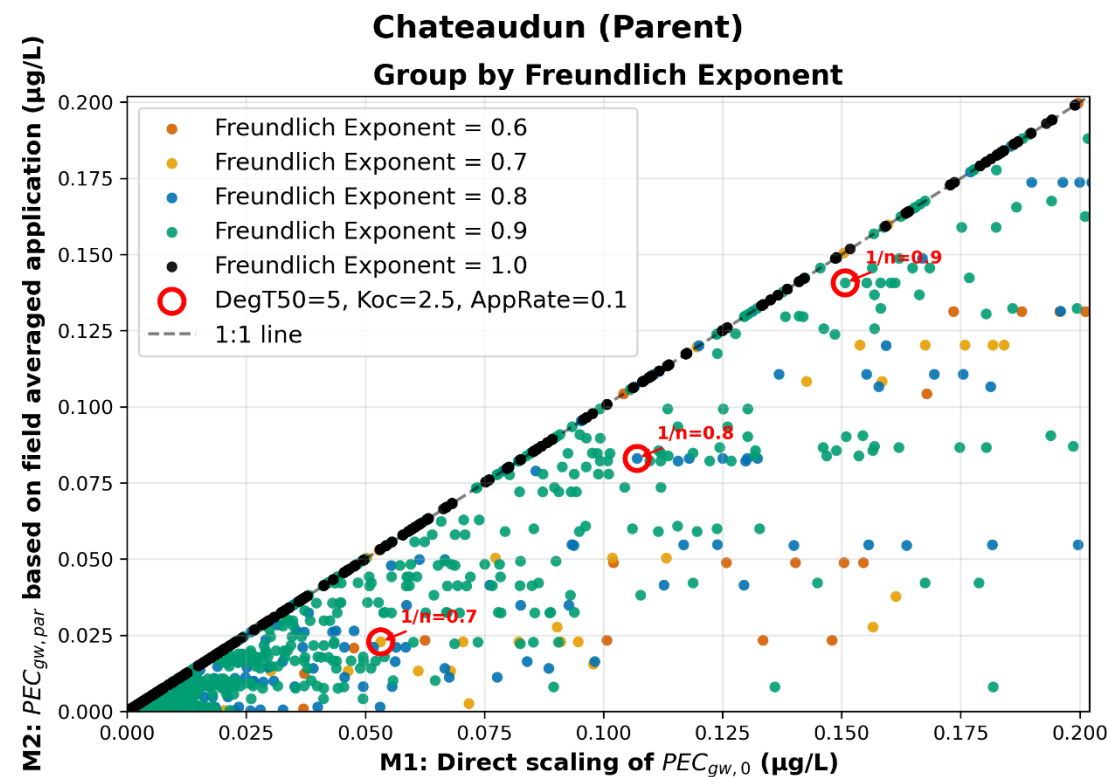


Example - Impact of Freundlich Exponent – Parent only

Chromatographic flow

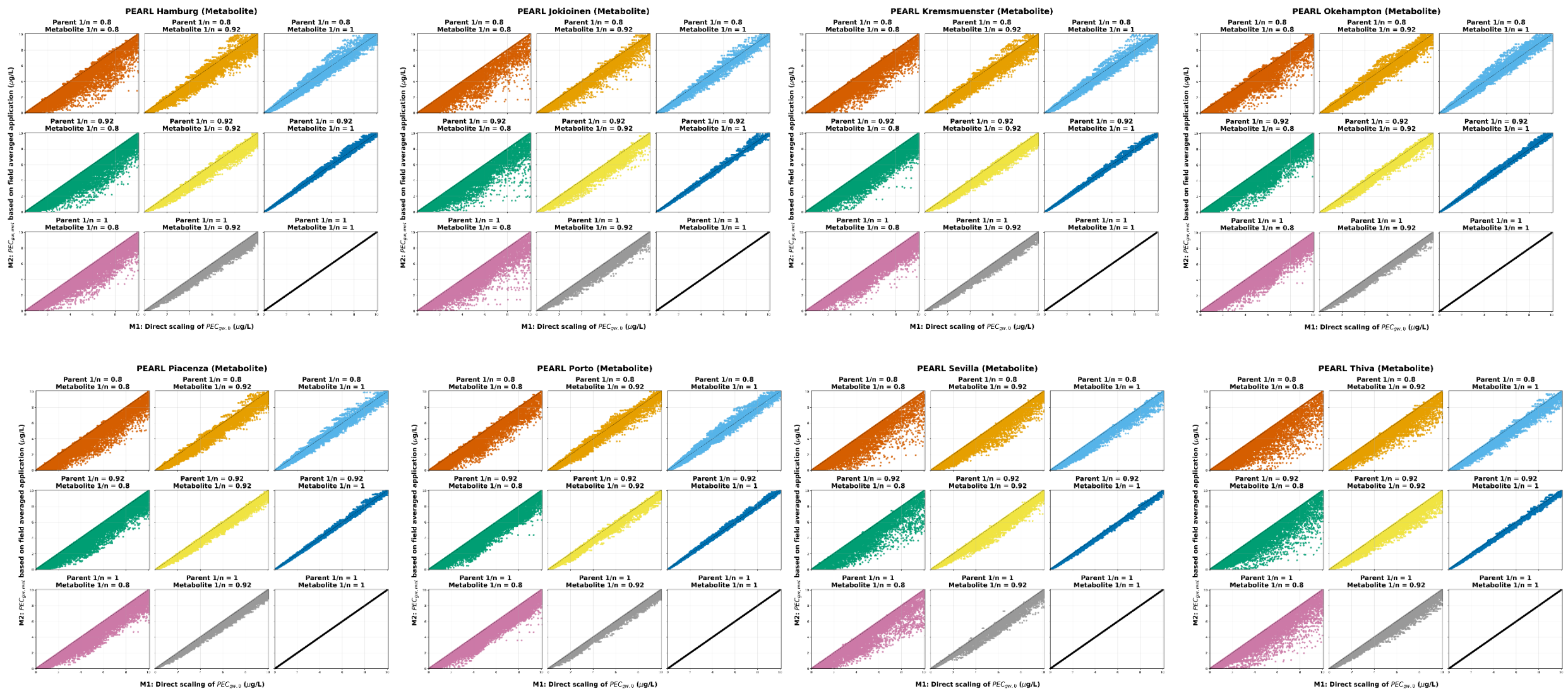


Preferential flow

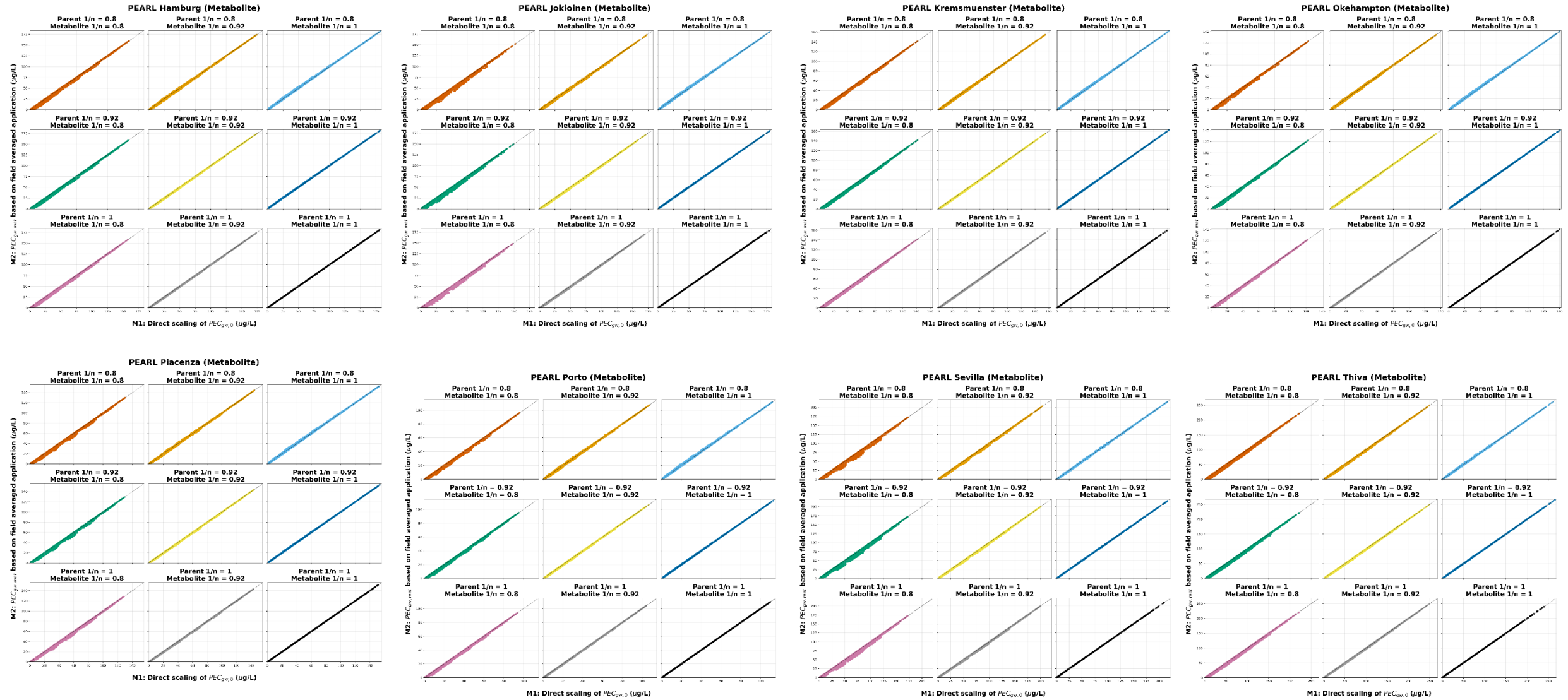


At $1/n = 1.0$ (linear sorption), both methods produce identical results. As $1/n$ decreases, the difference between the two methods increases.

FOCUS PEARL scenarios, metabolites (concentrations < 10 µg/L)



FOCUS PEARL scenarios, metabolites (all concentrations)



FOCUS MACRO scenario, metabolites (all concentrations)

