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Leachability as a Measure for Substance Mobility in the PMT/vPvM Framework

Dimitrios Skodras, Judith Klein, Michael Klein

Mobility determined by adsorption or leaching

Focus on mobility while persistence and toxicity are set

Definitions

- **PMT / vPvM:** New hazard category amending CLP regulation (in force 20-04-2023)
 - P & T: Persistence & Toxicity. Defined in PBT classification (ECHA, R11)
 - M: Mobility
- **Mobility:** Potential of the substance to move in soil to the groundwater (GW) or to a distance from the site of release. (EC 2020/878)
 - adsorption: measure of affinity of substance in soil
 - leachability: calculated mobility through leaching models
- **Leachability:** Potential of chemical to reach GW

$$Leachability = \frac{M_{substance}(reaching\ GW)}{M_{substance}(applied|released)}$$

Adsorption constant as simple mobility criterion

Determine Koc thresholds based on monitor findings in drinking water (DW) sources

- 350 REACH registered + 191 not REACH registered substances monitored in DW and GW (Arp&Hale 2019)

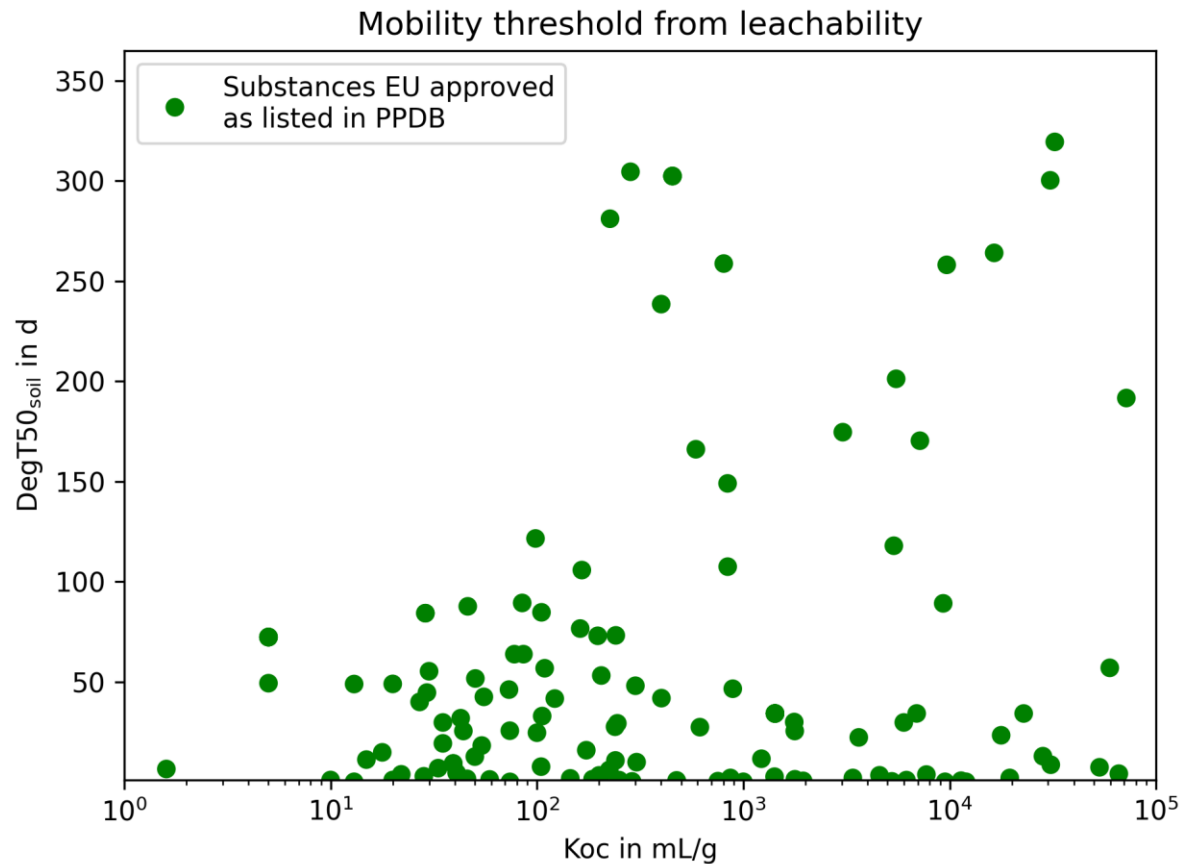
- Proposals for vM/M:

	M	vM
UBA (127/2019)	$3 < \log K_{oc} < 4$	$\log K_{oc} < 3$
COM Delegated Regulation (2023/707)	$2 < \log K_{oc} < 3$	$\log K_{oc} < 2$

- Issues with Koc as sole mobility criterion (ECETOC 139, 2021; Arp&Hale 2022, Collard et al 2023, Pawlowski et al 2021): Does not include
 - (local) environmental impacts on mobility (not only OC but pH, clay content etc.)
 - degradation within soil or sediment (sufficiently fast bio-degradation)
- Proposal:**
 - take $\log K_{oc}$ criterion as first approach
 - take leachability as higher tier

Leachability vs. Adsorption – PPP mobility correlates with persistence in soil

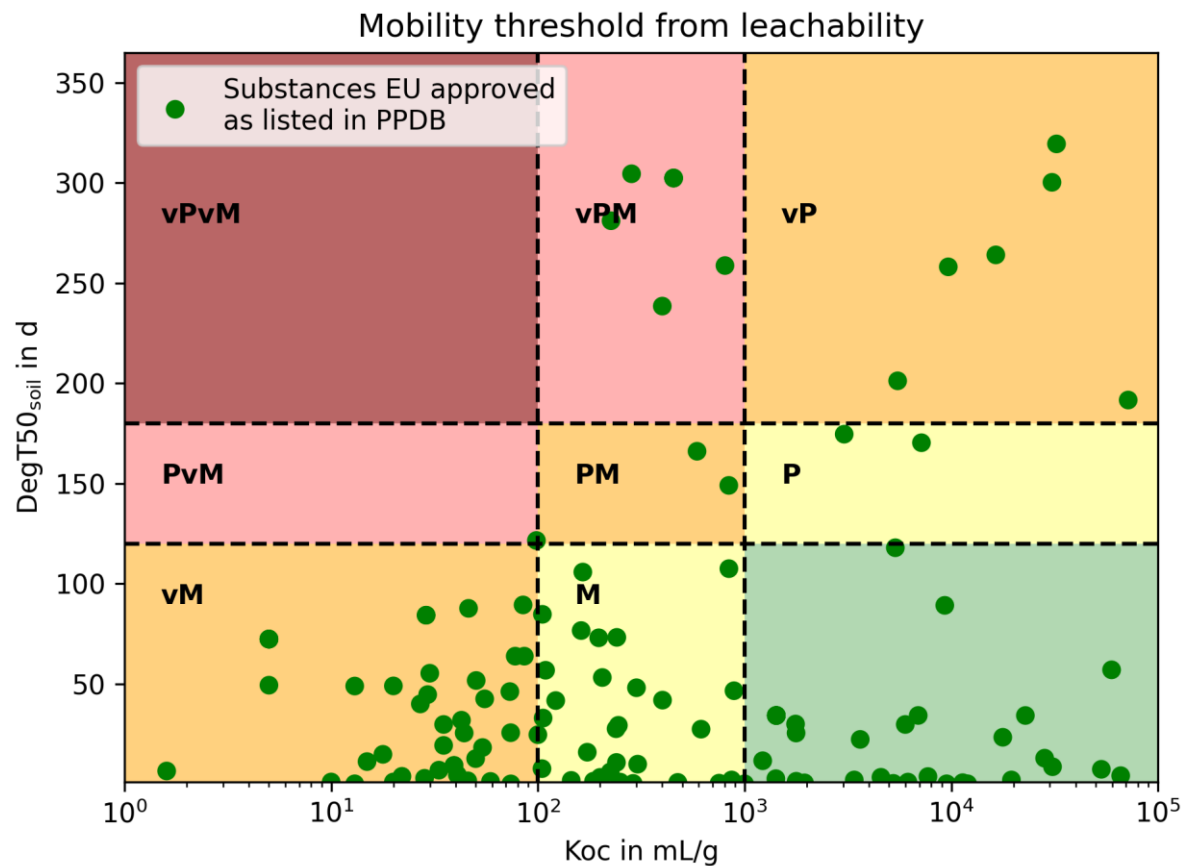
Plant Protection Products – Get overview on persistence and sorption



- Pull data from Pesticide Property DataBase
 - covers 1944 insecticides, biocides, fungicides
 - contains real and current data
 - easily accessible
- 655 substances with DegT50_{soil}/Koc pair and approval status (DegT50_{soil} @ 20 °C → 12 °C)
- 155 of which are approved under EC 1107/2009

Leachability vs. Adsorption – PPP mobility correlates with persistence in soil

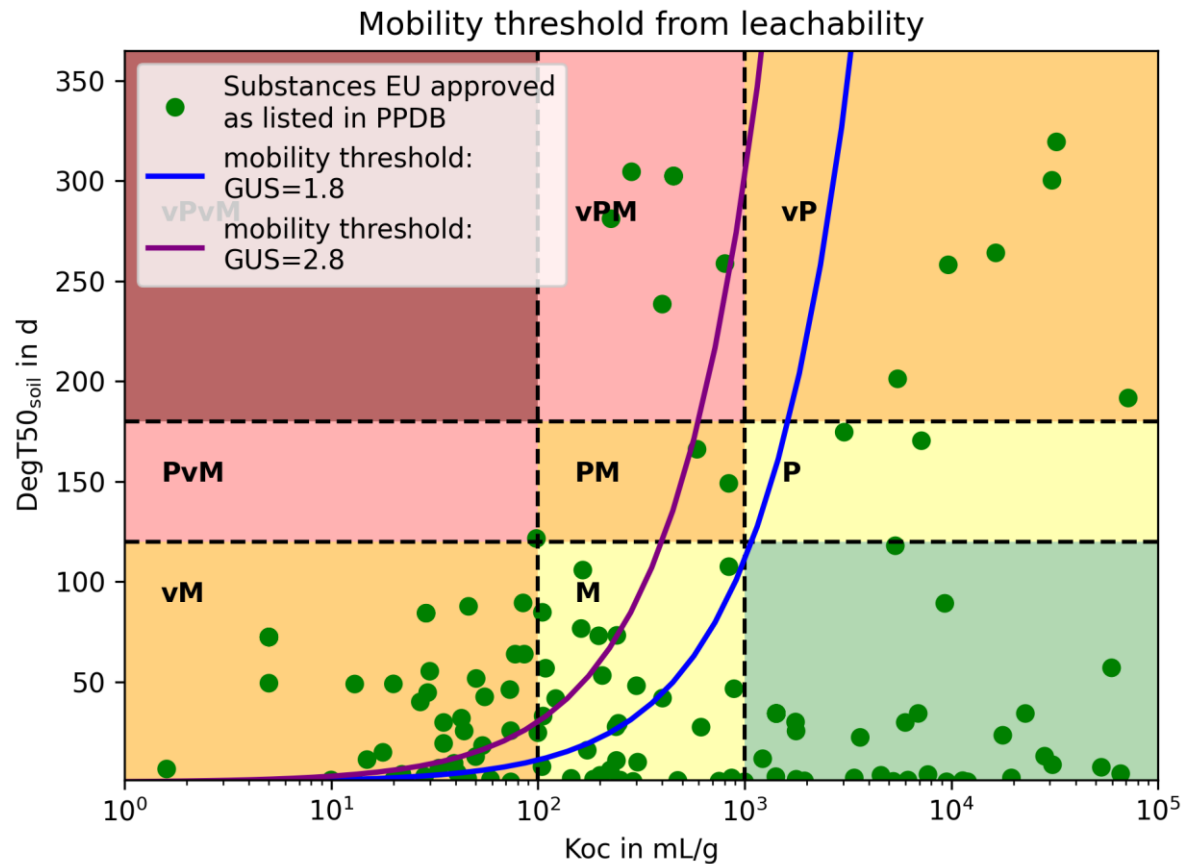
Plant Protection Products – many are not sorbing well but are also not persistent in soil



- Thresholds for P/vP and M/vM (COM Delegated Regulation 2023/707)
- Majority: DegT50_{soil} < 120 d but DegT50_{water} > 40 d
- Check with monitored substances (Arp&Hale 2019)
 - most found PPP not 1107-approved (PPDB)
 - however for 5: max. concentration > 0.1 µg/L
- Many PPP not well sorbing (logKoc < 3)
- Most approved substances not detected in SW and GW monitoring
- **All available information of data rich substances should be considered**

Leachability vs. Adsorption – PPP mobility correlates with persistence

Combine K_{oc} and $DegT50_{soil}$ to a leachability index



Groundwater ubiquity score (Gustafson, 1989)

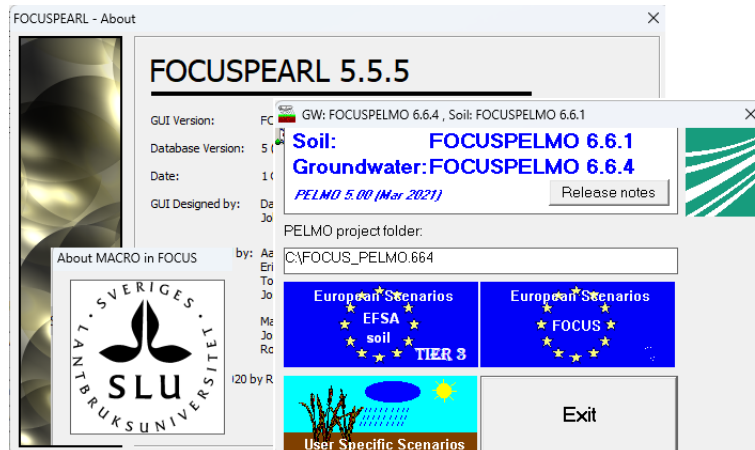
$$GUS = \log DegT50_{soil} (4 - \log K_{oc})$$

	Non-Leacher	Leacher
GUS	$GUS > 2.8$	$GUS < 1.8$

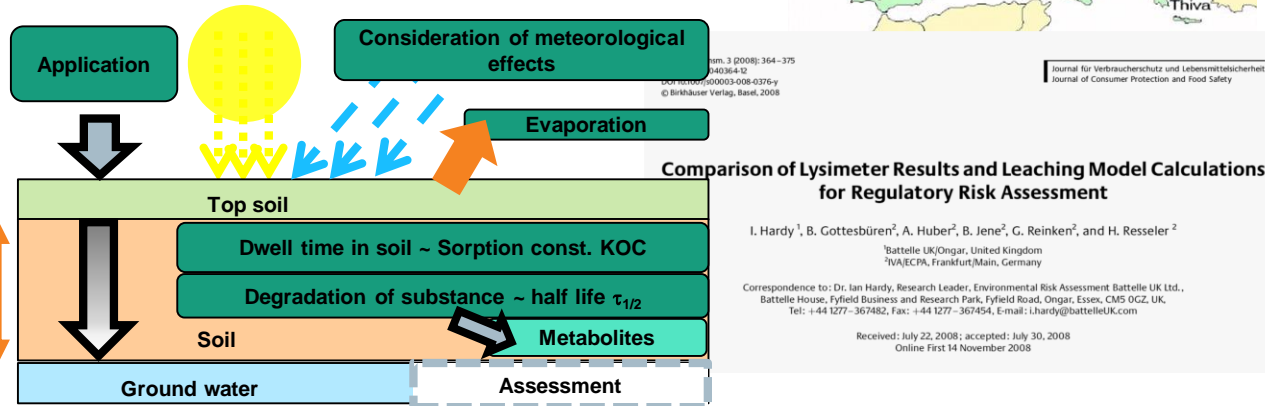
- Not an intrinsic substance property (exposure dependent)
- **But:** GUS lacks environmental effects

FOCUS Models – Assess pesticide fate in GW

Calculate statistically conservative Predicted Environmental Concentration in GW (PEC_{gw})



- FOCUS GW (SANCO/13144/2010).
 - PEC in groundwater calculated with leaching simulation
 - 4 Models (PEARL, **PELMO**, MACRO, PRZM)
 - 9 realistic worst-case scenarios covering European pedo-climatic conditions
- FOCUS PELMO (esdac.jrc.ec.europa.eu/projects/pelmo)
 - used for PPP registration in EU
 - validated concerning its conservatism (Hardy et al 2008, UBA 2014)
 - calculates leaching with mechanistic processes



Modelling Leachability – use FOCUS PELMO for environmental influences

Calculate leachability matrix with varying Koc and DegT50_{soil}

Koc\DegT50	1	2	...
0			
1			
⋮			

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SIMULATION OF PESTICIDE AND METABOLITE TRANSPORT WITH
PELMO 5.0 (VERSION DEC 2020)

Compound: (0 ) Pesticide D, 1 kg/ha 1 day before emergence
Soil:      Ver 4 Porto
Crop:     Ver 4 Porto, winter cereals
Climate:  Ver 4 Porto scenario (41.23 N, 8.68 W)   Year:01

SIMULATION TIME: 26 YEARS ( 1. 1. -- 31.12.)

FOCUS PELMO 6. 6. 4
CURRENT SIMULATION MONTH:  YEAR 17 SEP. |
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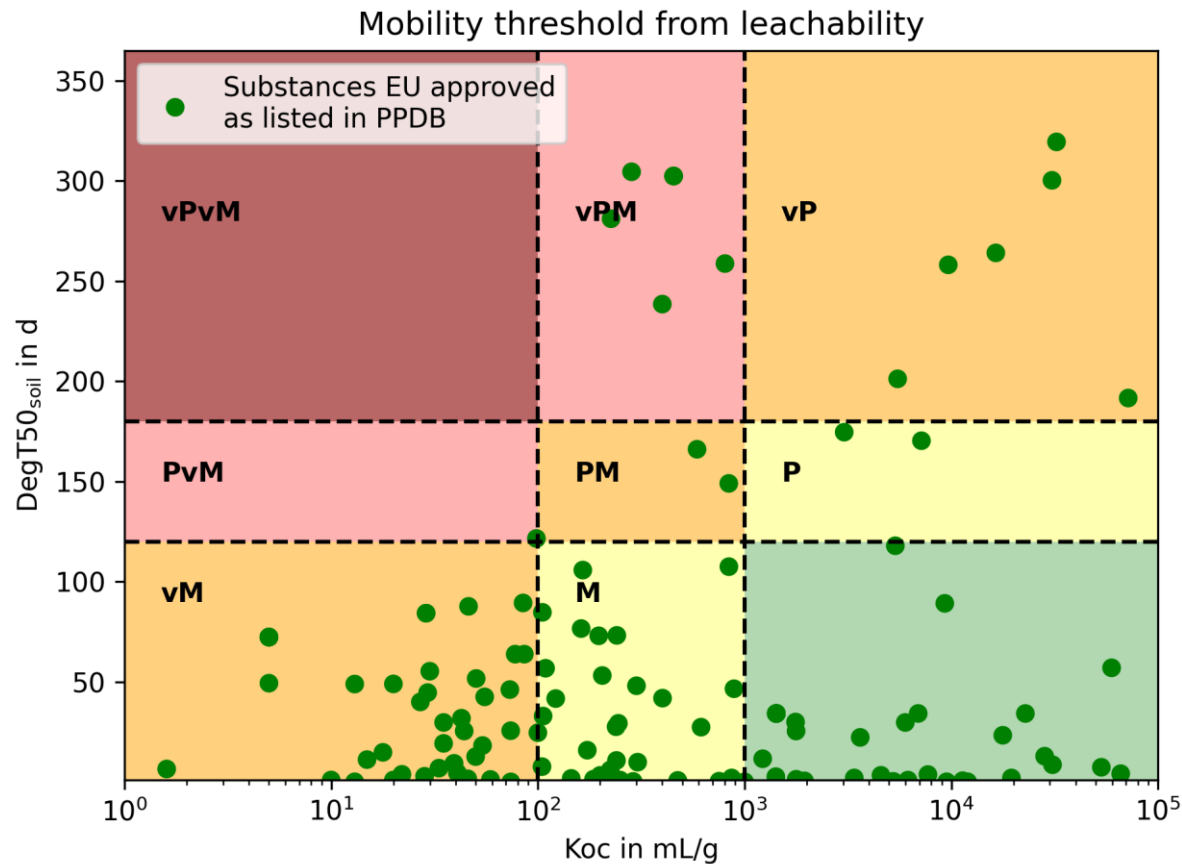
42 Koc x 21 DegT50_{soil} x 9 locations = 7938 simulations

Koc\DegT50	1	2	...
0	#	#	#
1	#	#	#
⋮	#	#	#

1. Vary Koc and DegT50_{soil} while all other substance properties set to defaults (S_w , P_{vap} , M_{mol} , etc.)
2. Monthly application for 120 simulation years at 9 locations
3. Worst-Case assumptions:
 - Linear sorption (rate independence)
 - No plant interception/uptake
 - No volatilization or photodegradation
4. Obtain 90th percentile worst-case annual **leachability matrix**

Mobility thresholds – First choice: 1% and 10% leachability

Somewhat arbitrary bounds assess most approved PPP as not mobile



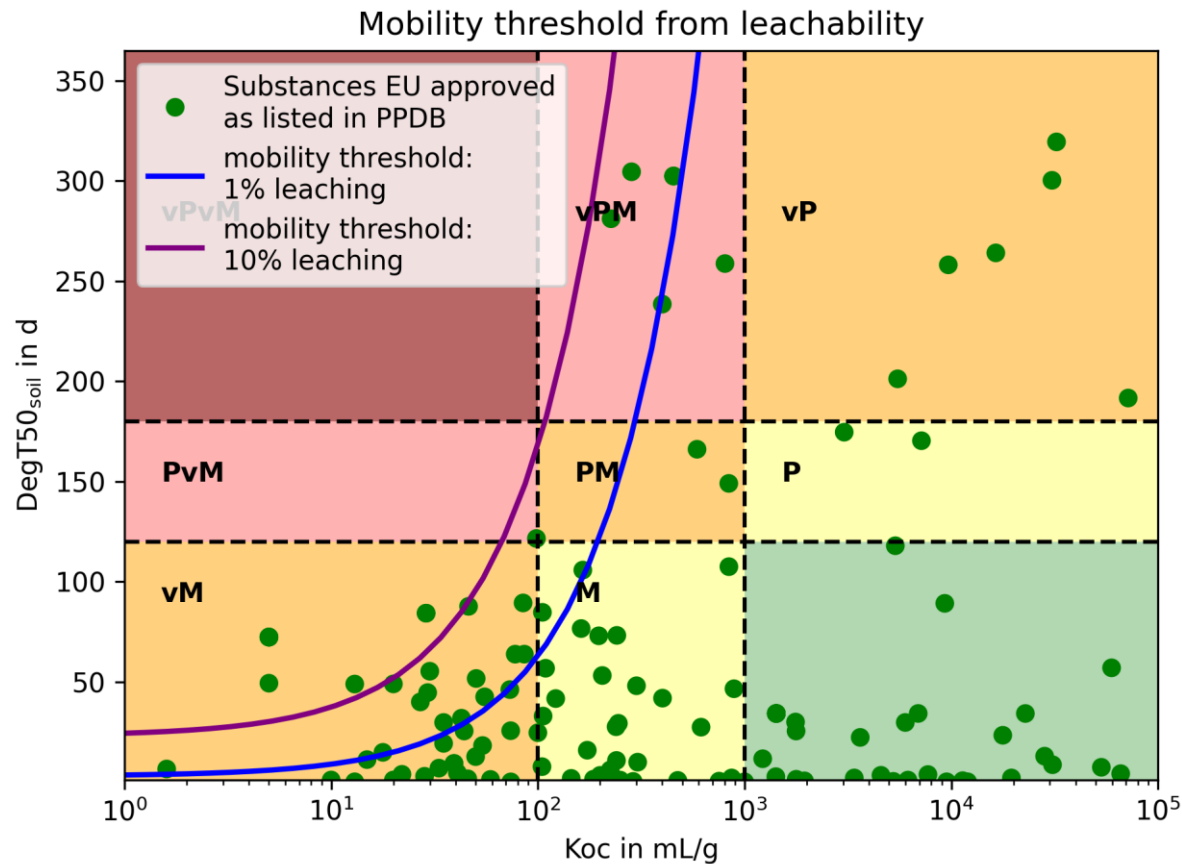
Question remains: what is (very) mobile?

Proposed choice:

	M	vM
LeachCalc (2023)	1% < Leachability < 10%	Leachability > 10%

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Question remains: what is (very) mobile?

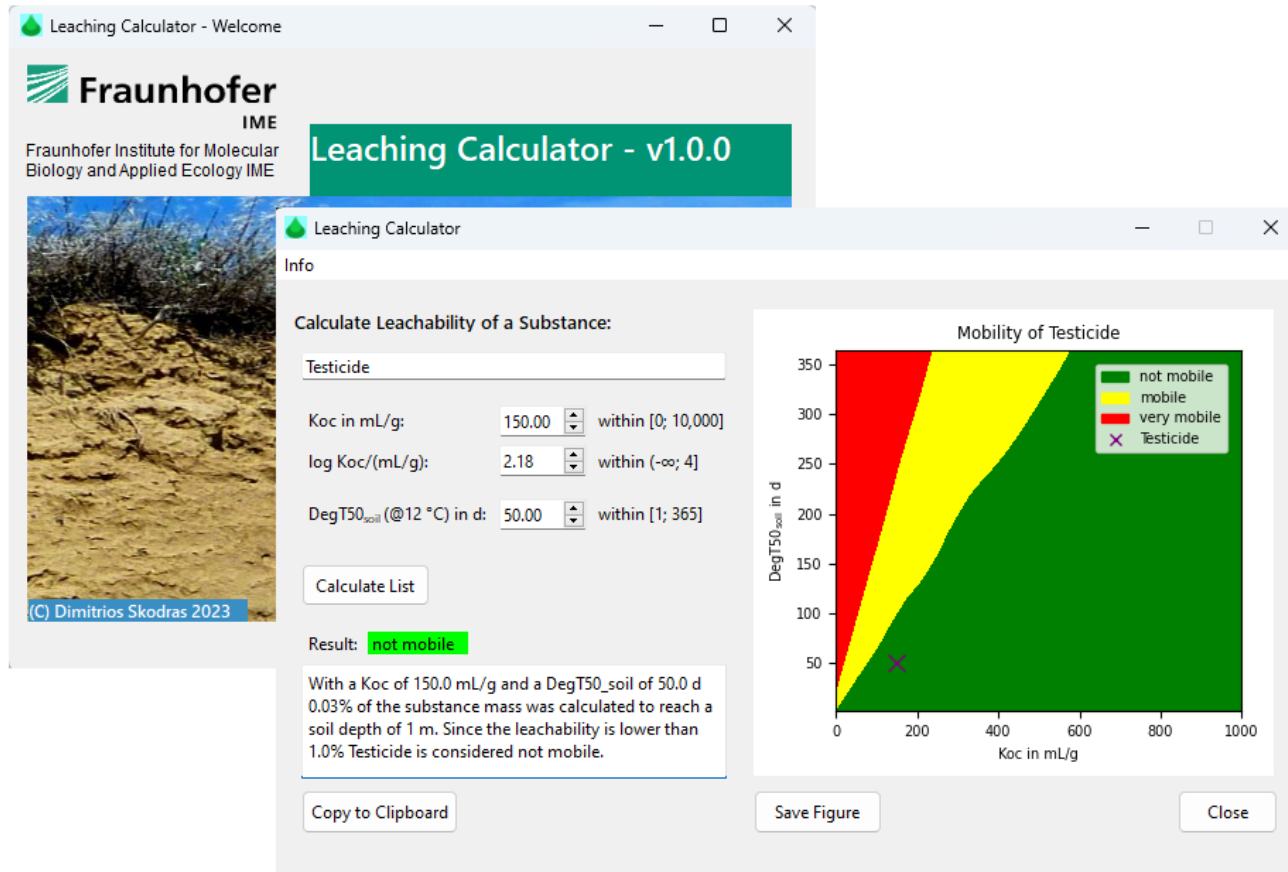
- Proposed choice:

	M	vM
LeachCalc (2023)	1% < Leachability < 10%	Leachability > 10%

- Assesses most currently approved PPP as not mobile
- Conservative character shown with a number of substances shown as mobile despite exposure assessment and monitoring
- Threshold choices can be discussed

Leaching Calculator – User friendly tool to calculate leachability

Assess mobility in the demonstrated leachability approach with proposed thresholds

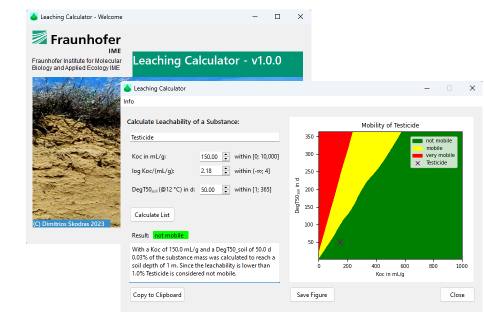
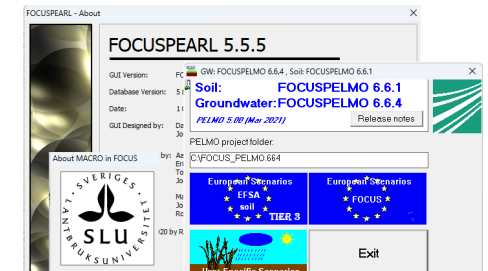


- Freely accessible under <https://www.software.ime.fraunhofer.de/>
- No installation required! Standalone executable. Source code on GitHub.
- Insertion of substance name, $\text{DegT50}_{\text{soil}}$ and Koc
- Can also calculate list of substances
- Uses spline-interpolation on leachability matrix
- Creates short report text and plot updated on every change
- Available as Command-Line Interface too

Conclusion: Leachability serves as higher tier assessment for mobility

- Koc** as a measure for mobility
 - simple and serves as a good screening method
 - assesses many PPP as M/vM even though experiments and model simulations do not show leaching
 - does not consider soil degradation or environmental effects
- Leachability** as a measure for mobility
 - does consider soil degradation and environmental effects; hence more realistic
 - more complicated to calculate
 - can easily be computed with pesticide leaching model
- LeachCalc** as a program to calculate leachability
 - uses results from FOCUS PELMO with representative scenarios and conservative assumptions
 - yields leachability for $Koc/DegT50_{soil}$ data pairs
 - comes as user-friendly GUI (and CLI), as open source and stand-alone programs

	M	vM
UBA (127/2019)	$3 < \log Koc < 4$	$\log Koc < 3$
EC (CA/03/2021)	$2 < \log Koc < 3$	$\log Koc < 2$



Thank you for your attention

Contact

Dr. Judith Klein
Modelling & Bioinformatics
Tel. +49 2972 302 256
judith.klein@ime.fraunhofer.de
www.ime.fraunhofer.de



Contact

Dimitrios Skodras
Modelling & Bioinformatics
Tel. +49 2972 302 282
dimitrios.skodras@ime.fraunhofer.de
www.ime.fraunhofer.de

