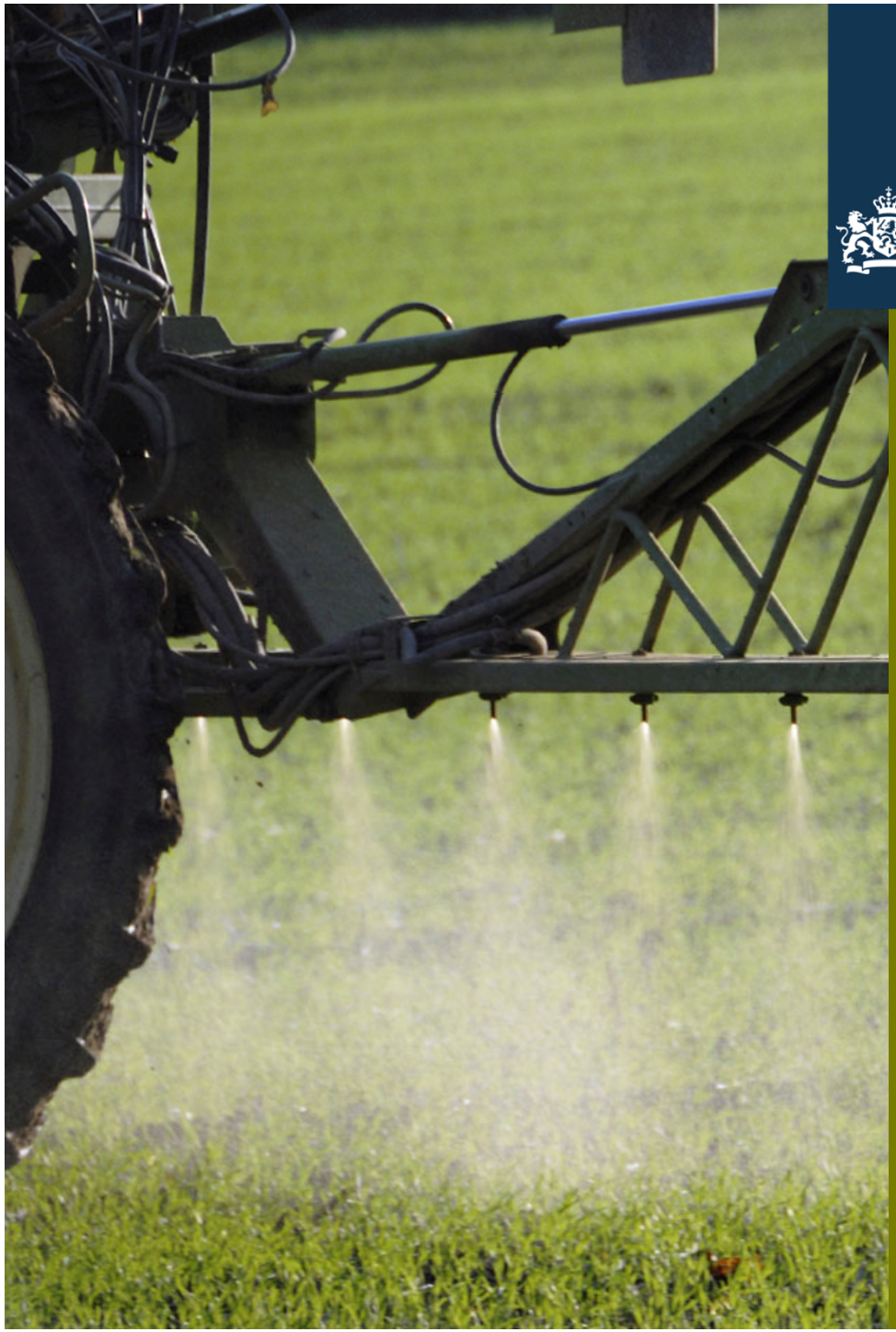


Planbureau voor de Leefomgeving

The EFSA PPR Opinion on the UK Aged Sorption Guidance

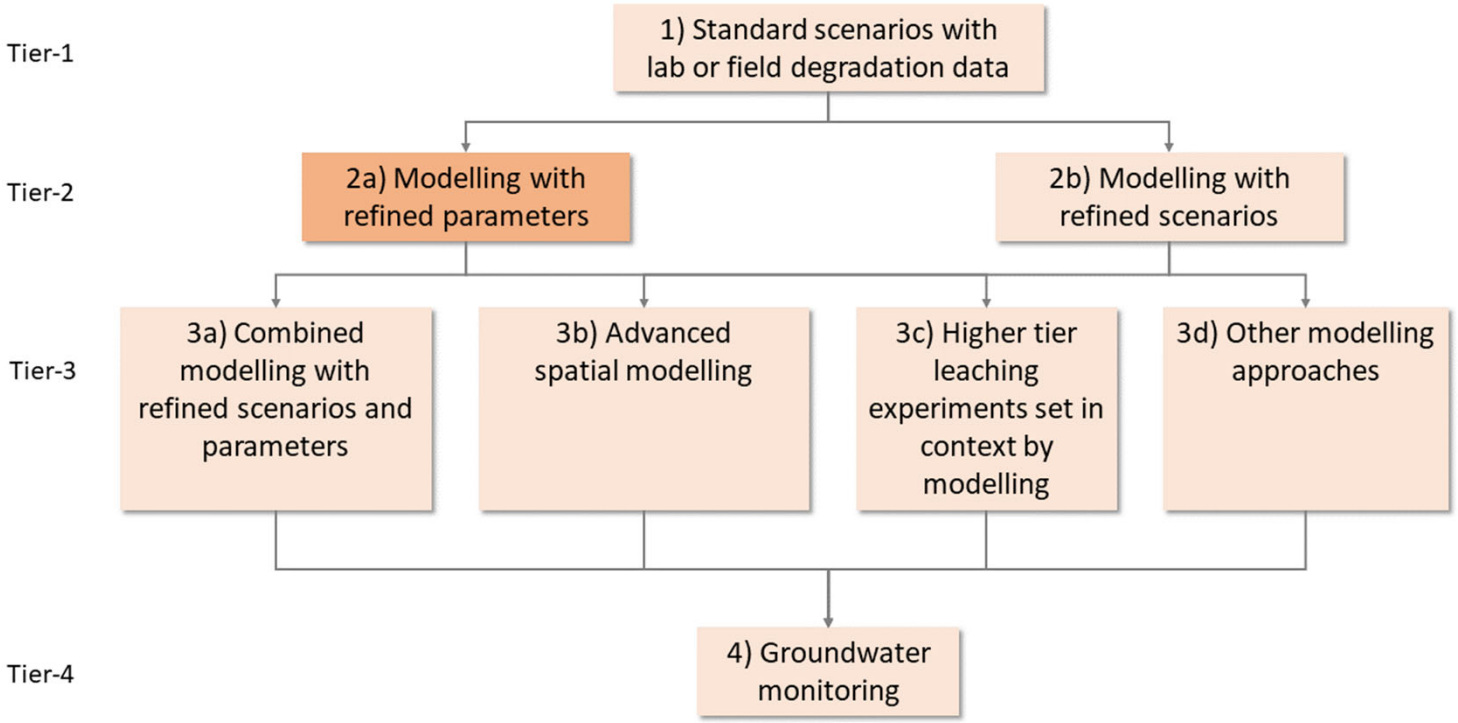
Aaldrik Tiktak

October 2018
European Modelling Workshop
Copenhagen

Outline of presentation

- Introduction
- Issues already covered in the statement
- Case studies
- Combining first tier and higher tier data
- Handling of metabolites
- Deriving aged sorption parameters in field studies
- Conclusions and recommendations

Aged sorption is a higher tier approach



- Lower tier data cannot be ignored in higher tiers of the risk assessment

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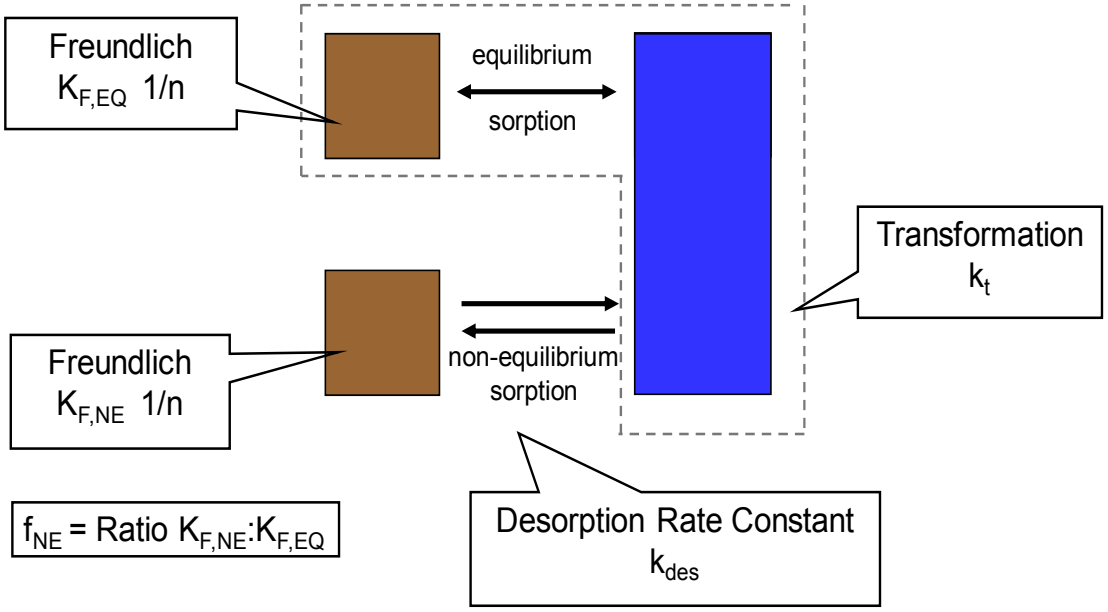
The two-site model is a reasonable compromise

- The guidance uses the **PEARLNEQ-model**, which uses a two side model for sorption
- The two-site model is a reasonable compromise between
  - the ability of the model to describe aged sorption under a range of situations
  - the possibility to determine reliable model parameters from experiments with reasonable effort
  - comparable models are acceptable as well



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Cases studies: the core of the opinion

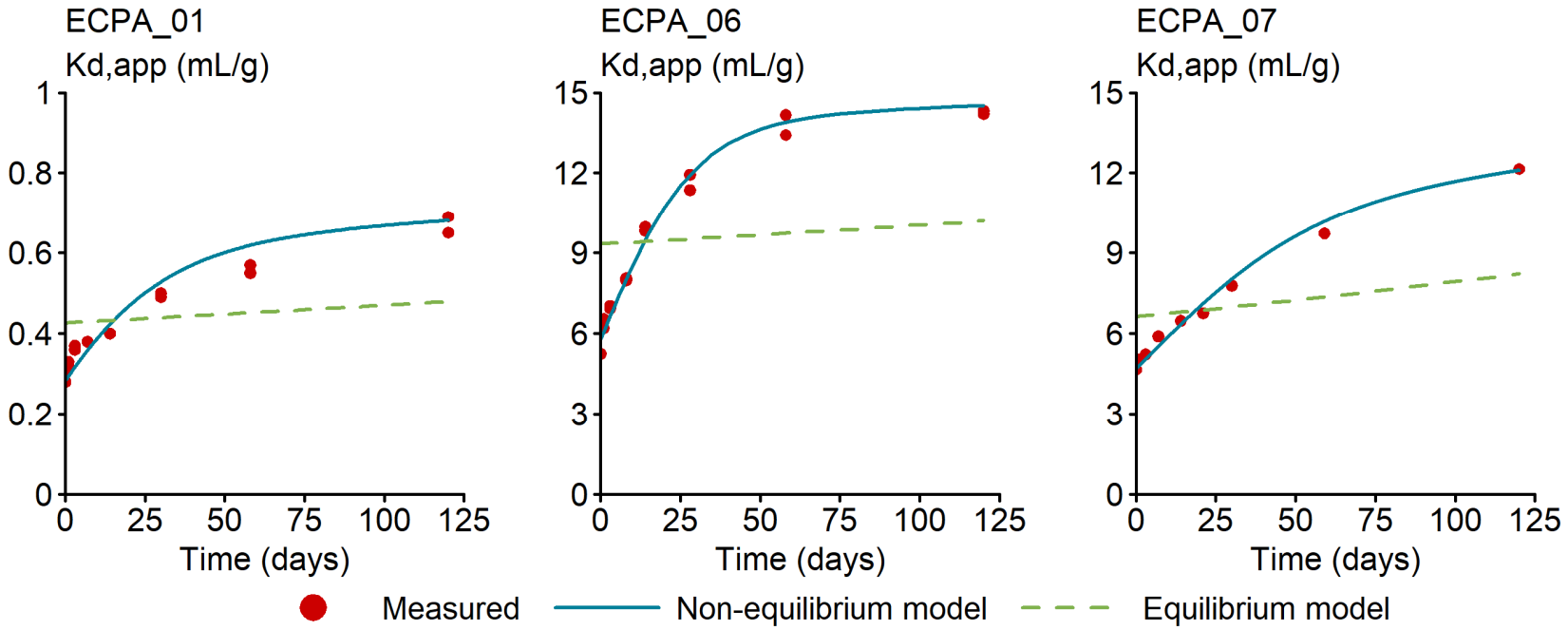
- ECPA provided data on roughly 50 substances
- The WG chose three substances for testing the guidance
  - Contrasting properties: ECPA-01 low sorption, ECPA-07/06: intermediate and high sorption
  - Both lower-tier and higher tier data available

Table 1: Overview of datasets provided by ECPA used for testing the guidance document

Substance name	ECPA-01	ECPA-06	ECPA-07
	Lower-tier data		
Full study reports	No	Yes	Yes
DegT50 lab (d)	Data not evaluated	115 – 318	50 - 173
DegT50 field (d)	No data	68 – 224	No data
K_{om} (L kg^{-1})	2 – 28	122 – 238	43 - 77
1/*n* (-)	0.86 - 0.95	0.87 - 0.97	0.84 - 0.90
	Data on time-dependent sorption		
Full study reports	No	Yes	Yes
Number of studies	4	4	4
f_{NE} (-)	0.43 - 0.49	0.63 - 0.79	0.35 - 0.76
k_{des} (d-1)	0.042 - 0.058	0.027 - 0.047	0.028 - 0.039
$DegT50_{eq}$ (d)	62 -144	78 - 177	45 - 80

Aged sorption was relevant in all cases

- The GD asks for a visual and statistical check of the fit
  - Both passed the pre-set quality criteria
- Example: increase of the sorption coefficient with time

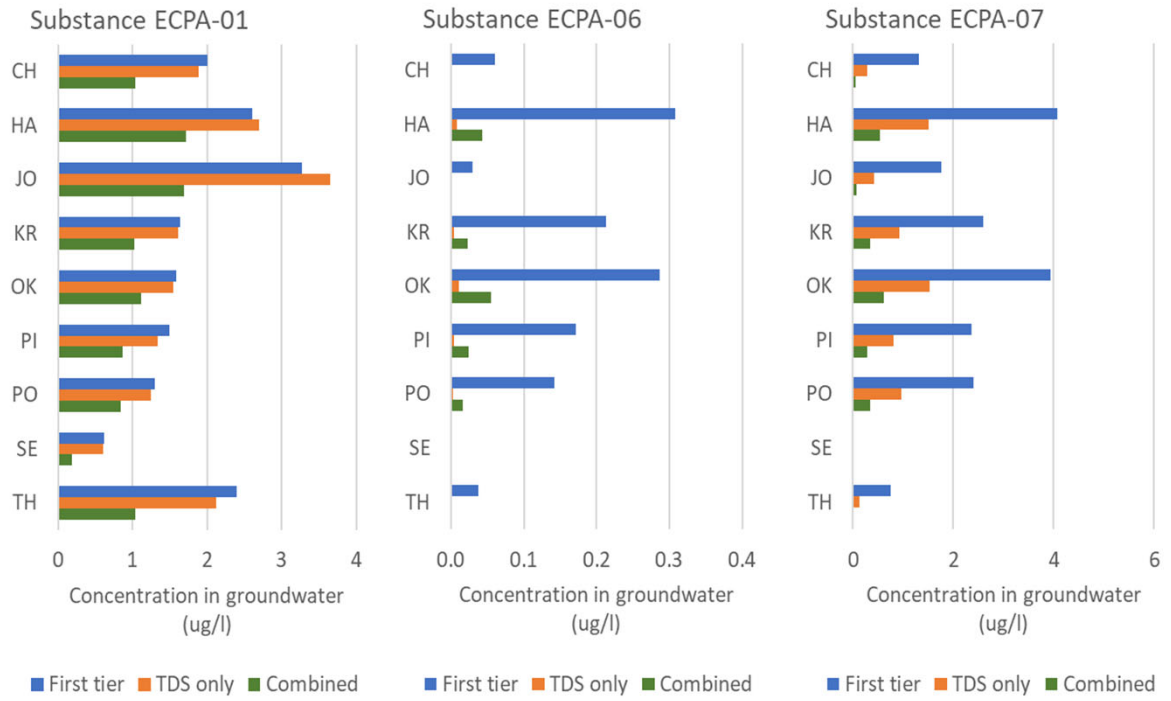


Applicability of the GD is complicated for non-experts

- A **user-friendly software tool** that support the entire workflow was missing
  - Recommendation: develop such a tool after consultation of stakeholders
- The GD suggested **refinement options** for model fitting that may give ambiguous results
  - The WG recommends a simplified procedure using $K_{om,eq}$ as a fitting parameter only
- A **flowchart** describing how to combine lower and higher tier studies is missing

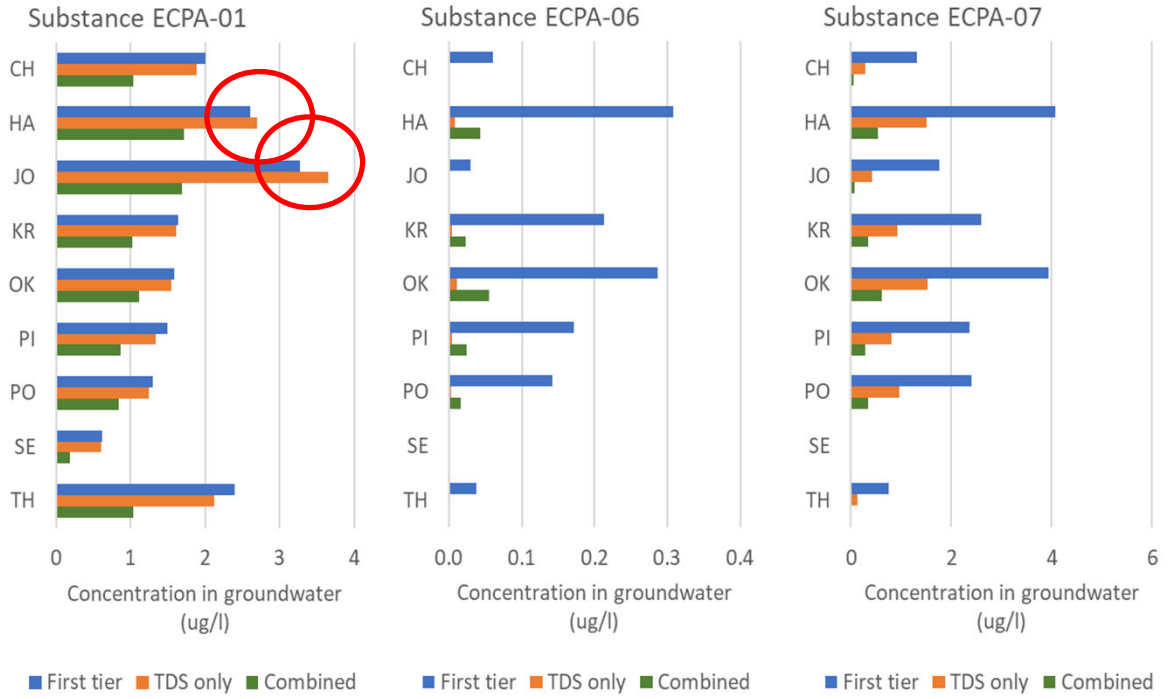
Results

- Aged sorption always **reduces leaching** for a specific soil
  - Effect larger for substances with a high K_{om}



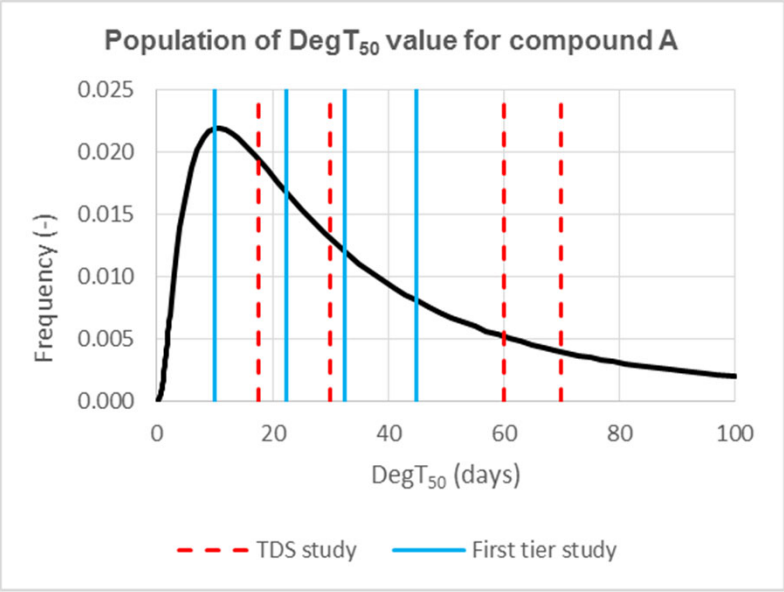
Results

- Aged sorption generally **reduces leaching**
  - Effect larger for substances with a high K_{om}
  - Samples from different subsets of soils may complicate this finding



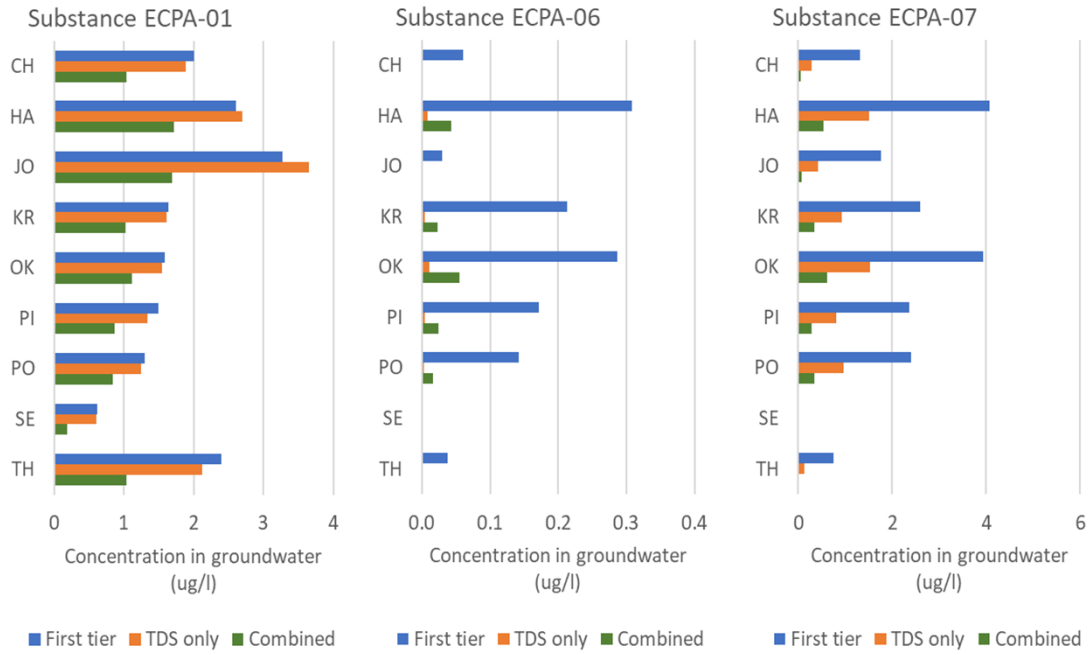
Handling variability of half-lives in soil

- Four samples not enough to provide a robust estimate of properties in all soils
  - Coefficient of Variation of half-lives >25%
  - So if different soils are taken for Tier-1 than for Tier-2a, **a higher geomean** half-live can be obtained with higher leaching



Use all half-live values

- Given this large variability, the WG recommends using half-lives **from all soils** (Tier-1 and Tier-2a combined)
  - This may lead to higher leaching at Tier-2a but was never been the case in our examples



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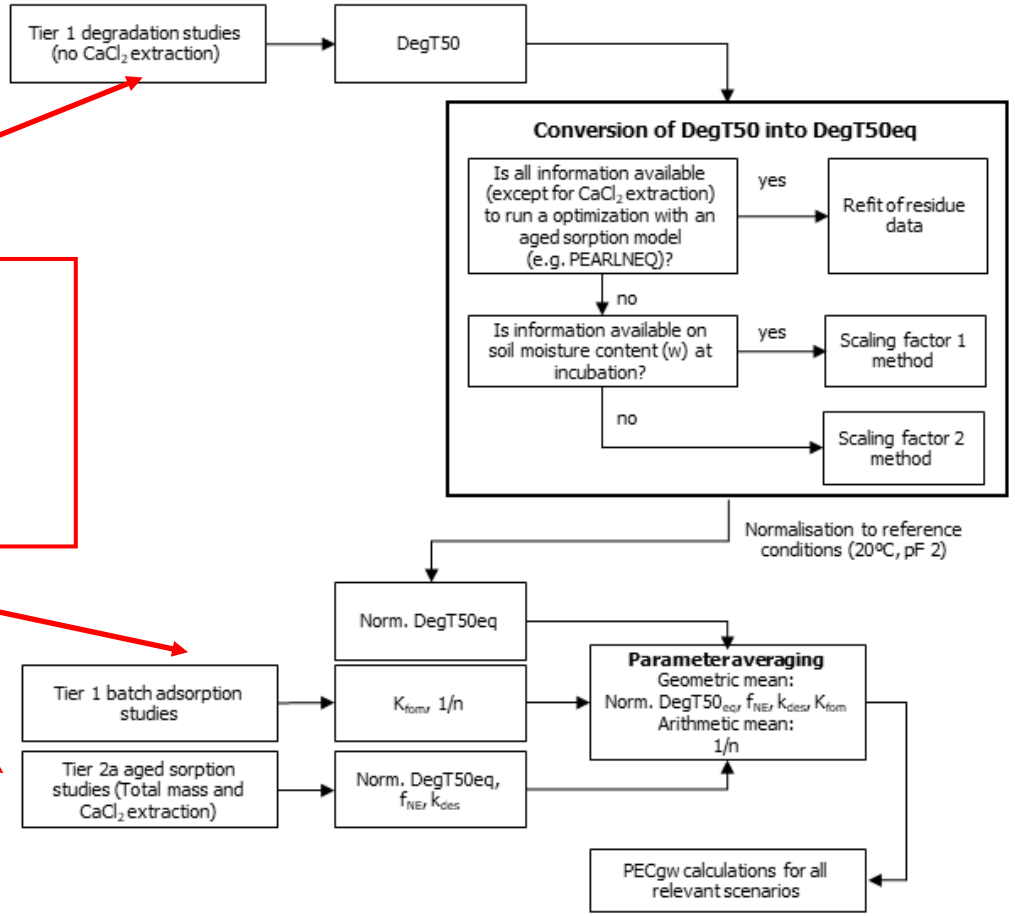
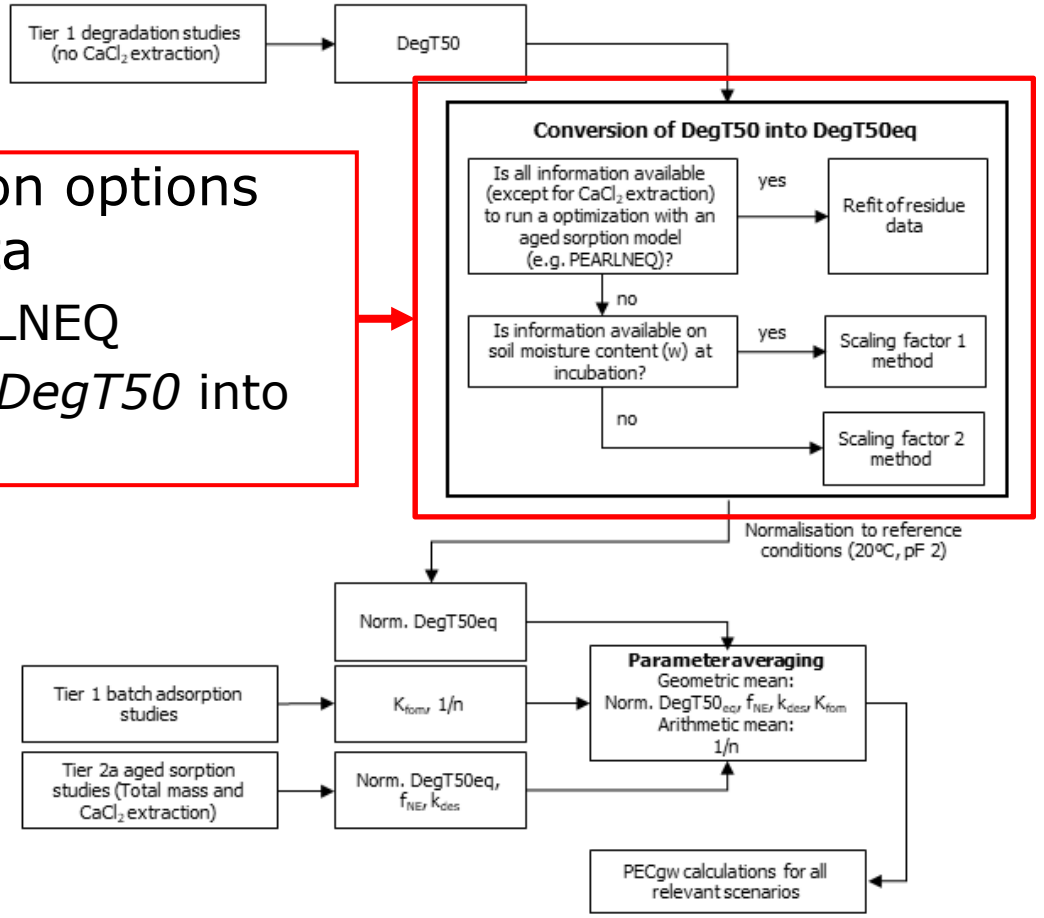
Flowchart for combining the tiers

- Three study inputs:
  - Tier-1 degradation
  - Tier-1 adsorption
  - Tier-2a aged sorption



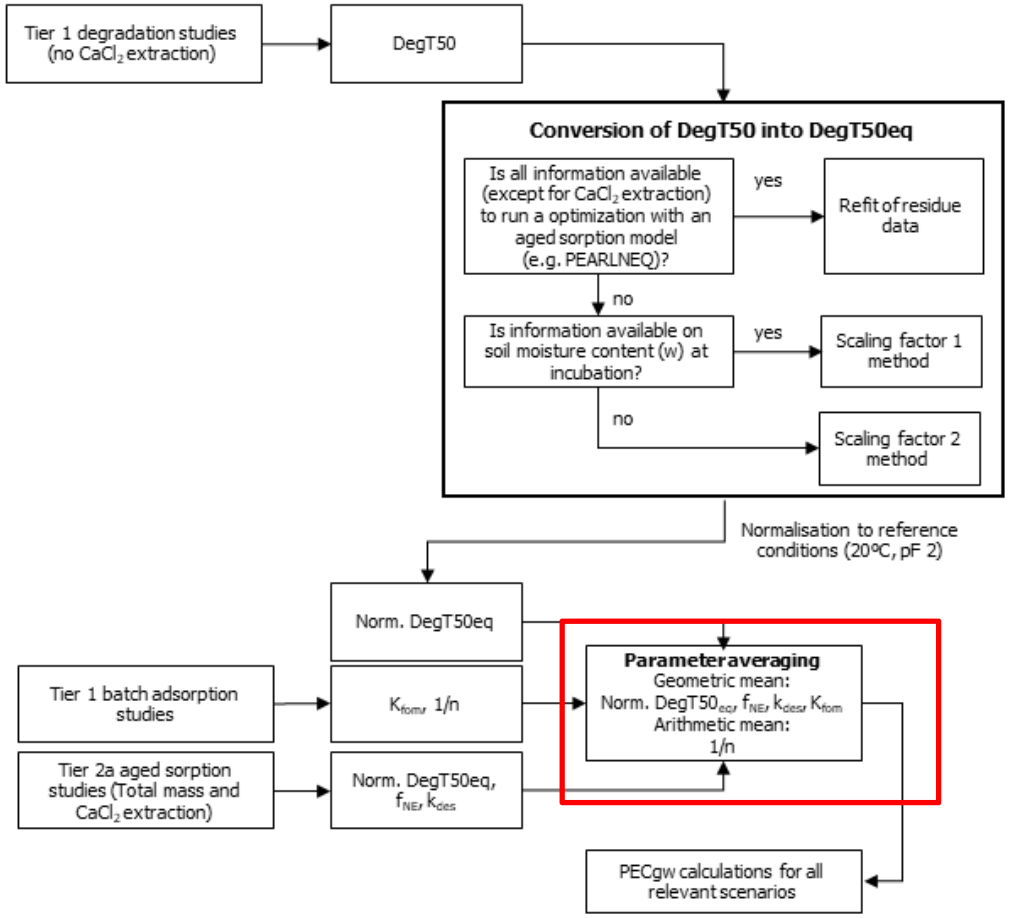
Flowchart for combining the tiers

- *DegT50* conversion options depending on data
  - Refit using PEARLNEQ
  - Options to scale *DegT50* into *DegT50eq*



Flowchart for combining the tiers

- Averaging procedures



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- **Deriving aged sorption parameters in field studies**
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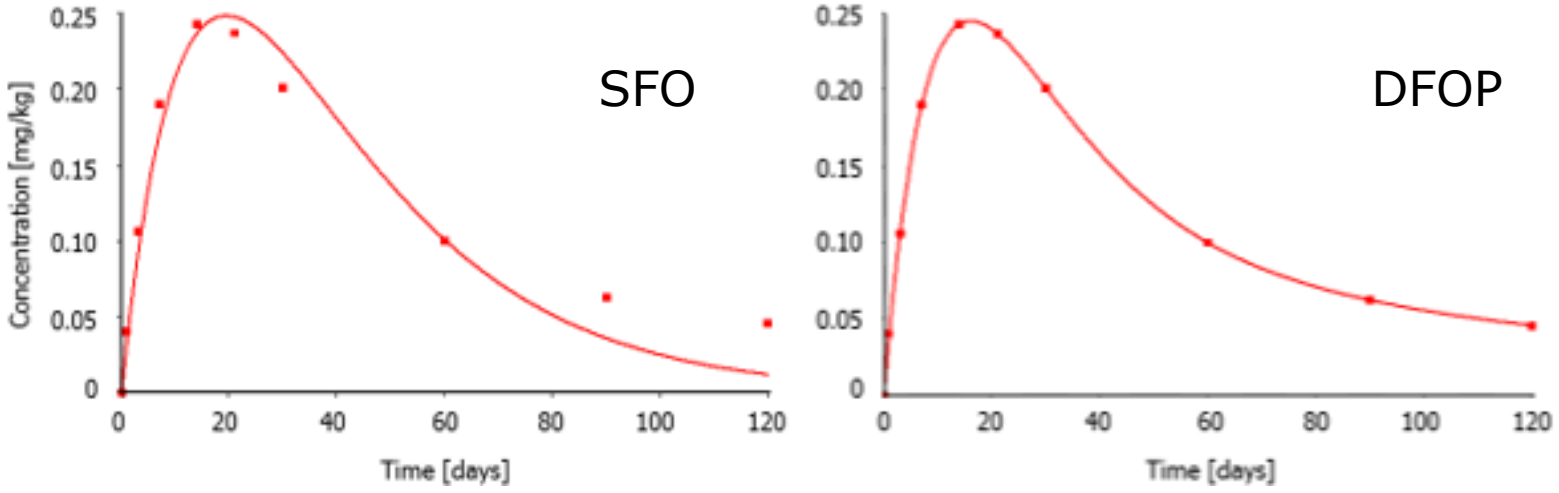
Aged sorption and metabolites

- GD was not conclusive, so the WG provided recommendations based on simulations with artificial compounds:
  - Derive aged sorption from **metabolite-dosed** studies
  - Derive the formation fractions from parallel **parent-dosed studies**, provided that the parent and the metabolites are fitted with the best model, i.e. the DFOP model

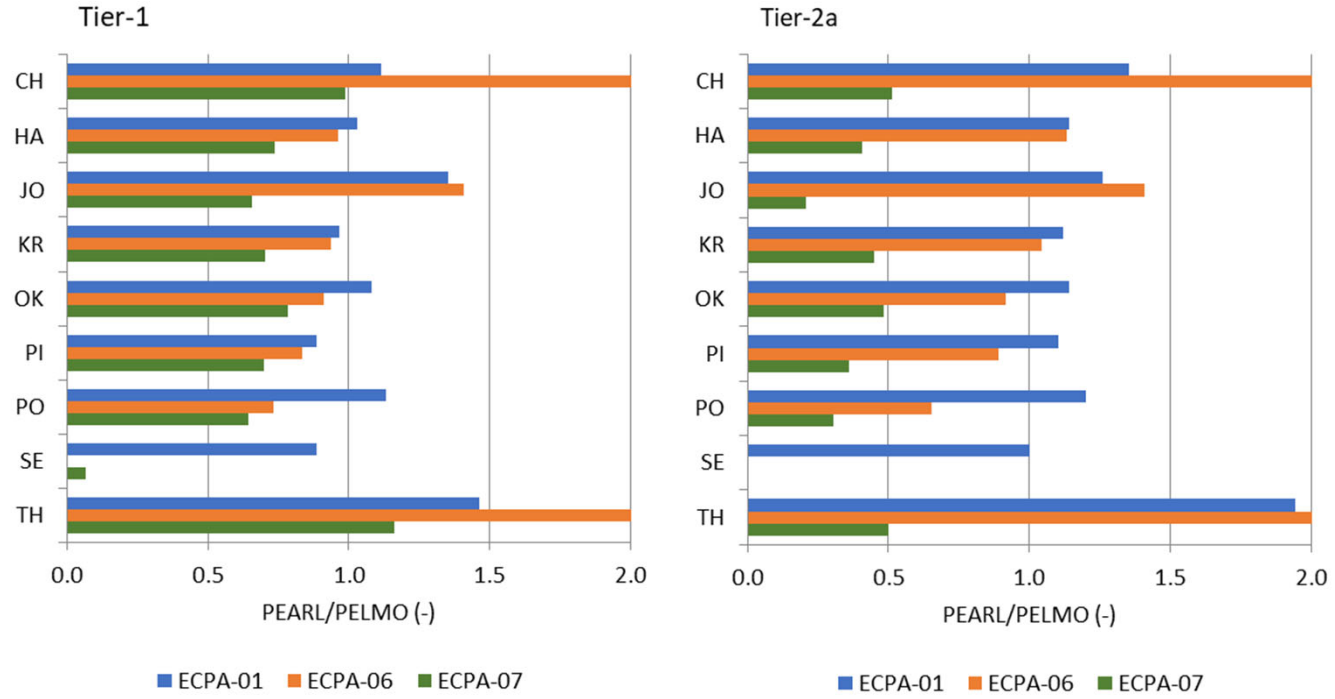


Aged sorption and field studies

- Deriving aged sorption parameters from field studies requires **inverse modelling** with numerical models such as PEARL or PELMO
- The GD does not contain fully worked out guidance to parameterize such models and a dataset to test this was not available
- For these two reasons, the WG recommends further development and testing of the guidance for field studies before it is used in regulatory practice

Two models will still be needed

- Differences between PEARL and PELMO increase slightly
- Usually within a factor of two, which is very small given the overall uncertainty



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- Deriving aged sorption parameters in field studies
- **Regulatory Relevant Conclusions**

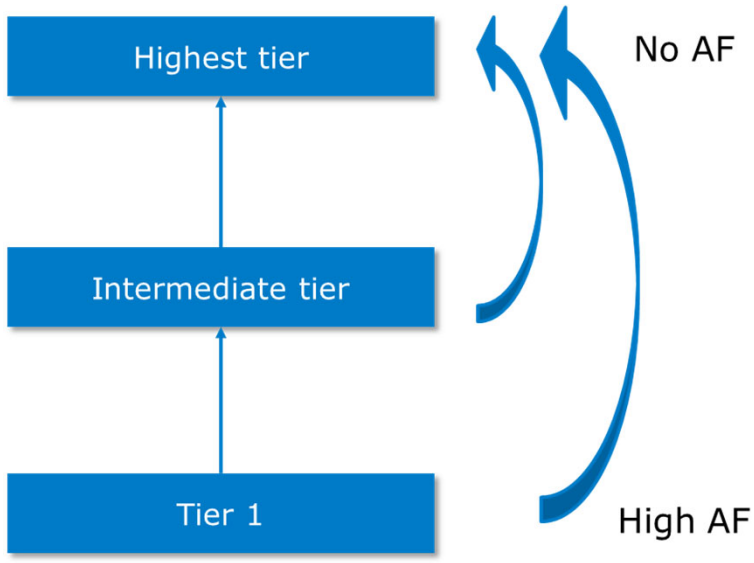
Regulatory Relevant Conclusion - 1

- General impression:
  - Authors of the revised GD have followed most of the recommendations in the statement
  - A very well worked-out GD
  - Some recommendations left

- The Panel considers the guidance **suitable for use in the regulatory process** after the recommendations in this scientific opinion have been implemented
  - With the exception of the guidance for field studies

Regulatory Relevant Conclusion - 2

- The FOCUS GW Tiered-Approach needs revision
  - **Calibration** of lower tiers against higher tiers necessary to avoid that regulators ask for lower-tier assessments
  - To avoid inconsistency it is recommended to always carry out a **$CaCl_2$ extraction**, even for Tier-1 assessments
  - For calibration an **agreed version of a spatial model** (e.g. GeoPEARL) is absolutely necessary
  - Guidance for dealing with **monitoring data** is needed as well



Regulatory Relevant Conclusion - 3

- Given the potential large effect of including aged sorption, the GD is too optimistic about the contribution of various sources of **uncertainty** to the leaching assessment
- **Variability of degradation and sorption** coefficients should be dealt with in the leaching assessment
  - Variability of these parameters is considerable (>50%)
  - Ignoring this variability leads to an underestimation of the leaching concentration (refer to EFSA GD on PECs in soil)

Acknowledgements

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  - Aaldrik Tiktak (Netherlands)
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  - Michael Stemmer (Austria)
  - Ton van der Linden (Netherlands)

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Disclaimer - the views expressed in this presentation are those of the author, and not those of EFSA.

In memoriam Ton van der linden

- During the development of the opinion, we lost an outstanding scientist and a loyal and friendly working group member