Für Mensch & Umwelt

Umwelt Bundesamt

Pesticide Behaviour in Soils, Water and Air, 31 Aug. 2017, York

How protective is FOCUS groundwater modelling on sandy soils? – A comparison of simulated and measured leachate concentrations

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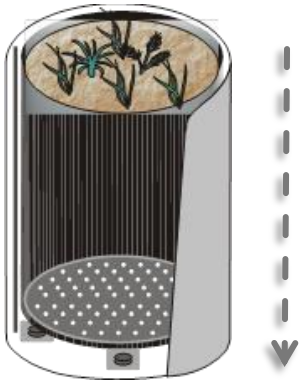
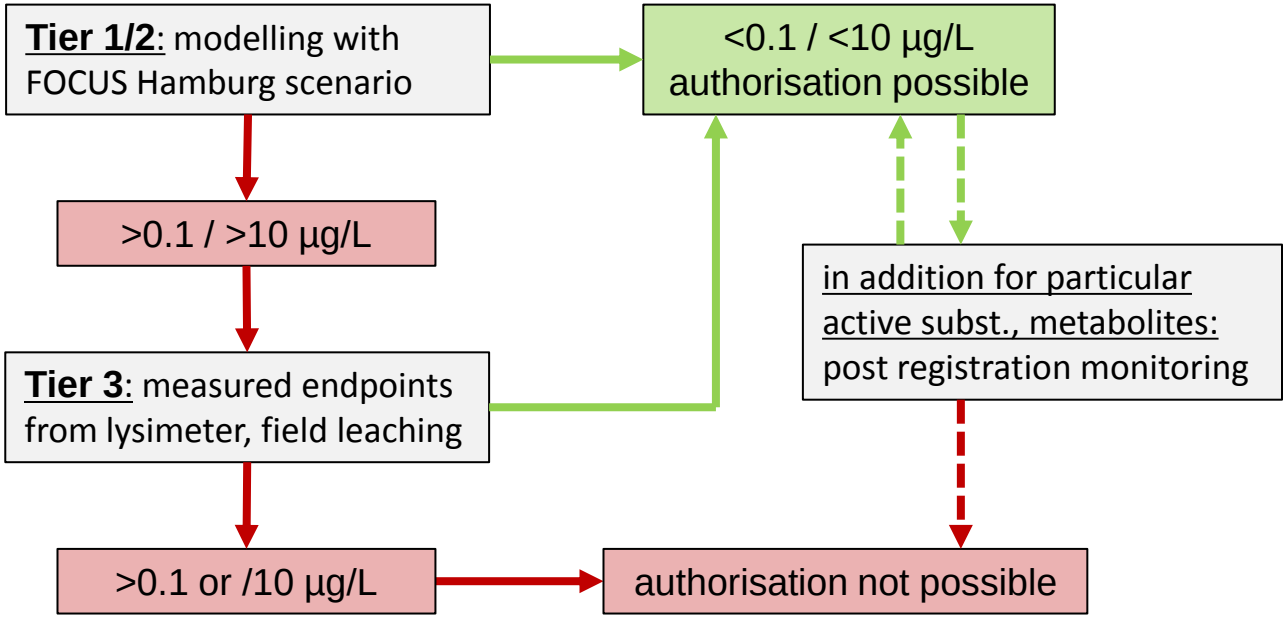
Outline

- National Groundwater Risk Assessment in Germany
- Regulatory Questions
- Objectives of the Lysimeter Comparison Study
- Data Collection, Preparation & Evaluations
- Results of Comparison Analysis
- Summary of Results
- Regulatory Conclusions

National Groundwater Risk Assessment in Germany

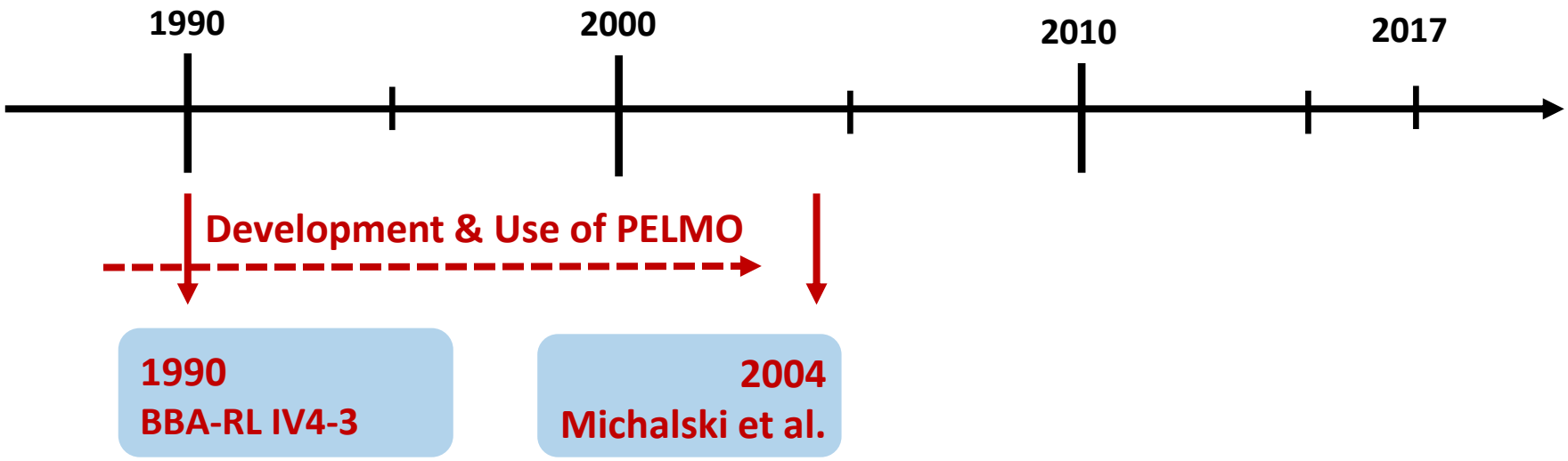


leachate concentration in 1 m soil depth



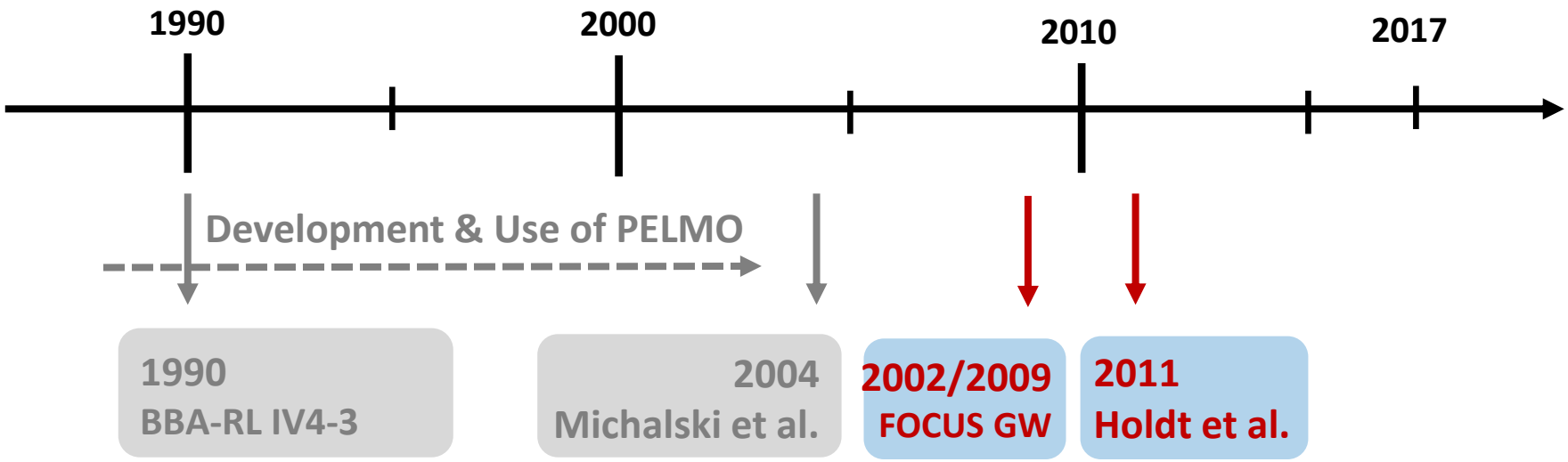
- FOCUS Hamburg modelling + national inputs used in lower tier assessments
- Lysimeter studies are accepted as higher tier studies, measured maximum annual averages concentrations can overwrite modelled concentrations from FOCUS “Hamburg”
- Post registration monitoring studies can be additionally required in exceptional cases

National Groundwater Risk Assessment in Germany



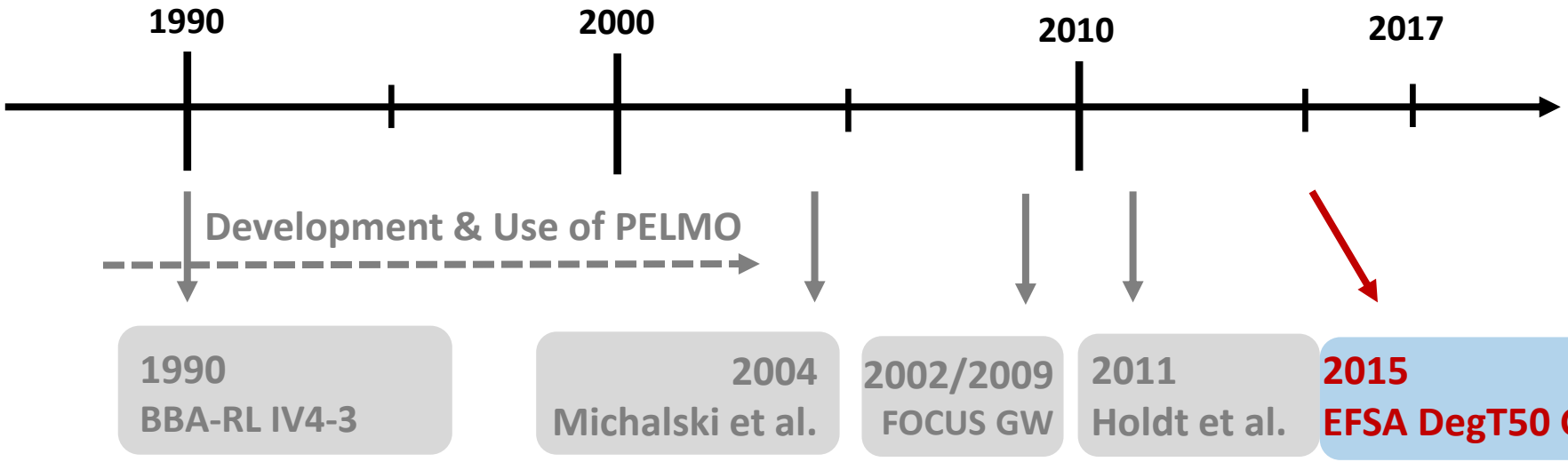
- Conditions for national lysimeter studies defined since 1990
- PELMO + national input parameter developed in parallel, published 2004
- The national „Hamburg“ scenario represents comparable soil, climate conditions
- Thoughts behind: *Sandy soils with low organic carbon content and atlantic climate conditions cover nationwide environmental conditions for PPP leaching*

National Groundwater Risk Assessment in Germany



- Change from national PELMO 3.0 to FOCUS PELMO for harmonisation reason
  - It means also changes in the “Hamburg” scenario
- EU endpoint selection by averaging has been partly accepted, different national endpoints are required for some compounds
- FOCUS critique: Lysimeters are, as endpoint studies, not protective enough due to single applications and short study durations

National Groundwater Risk Assessment in Germany



- New degradation and adsorption endpoints for modelling required for EU risk assessment
- will impact product registration in future

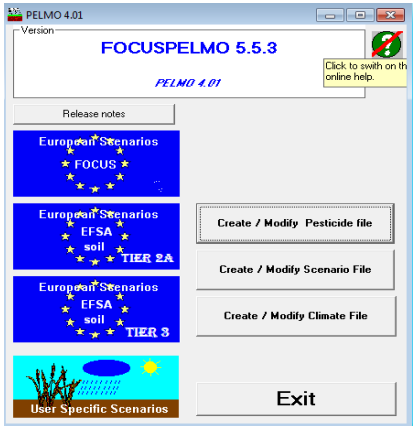
Regulatory Questions

- *Is FOCUS Hamburg modelling protective enough?*
  - *Do FOCUS "Hamburg" conditions represent national realistic worst case conditions?*
  - *Are FOCUS Hamburg results still more conservative than lysimeter results?*
- *How do the different endpoint selection procedures (national, previous EU, new EU) influence the modelling results? Is further harmonization possible?*
- *Can inverse modeling be used as standard tool to overcome uncertainties in lysimeter measurements due to single applications and short study durations?*

Study Objectives

RLP Agroscience Institute for Agroecology

Fraunhofer IME

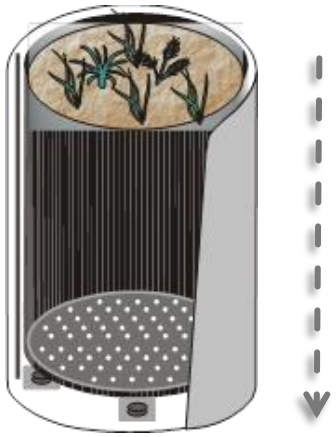


1st step analysis:

To compare FOCUS Hamburg modelling results with lysimeter measurements

2nd step analysis:

To evaluate the influence of single/double applications and study durations in lysimeter experiments by inverse modelling (FOCUS PELMO)



Advisory opinion 77639 (on behalf of the Umweltbundesamt, will be published as UBA Texte):
Klein, M. (2017): *Comparison of different methodologies for selecting PELMO input parameters for groundwater modelling of plant protection products including current EU guidance (SANCO/12117/2014 - final, 2014).*

Study Report (on behalf of the Umweltbundesamt, unpublished):
Klein, M., Thomas, K., Trapp, M., Gueriche, D. (2016): *Protection of the groundwater against loads of plant protection products: validation of the new EU-simulation model FOCUS PELMO 4 for a reliable prediction of the leaching potential of PPP into groundwater. Part AI/AII.*

Data Collection, Preparation & Evaluations

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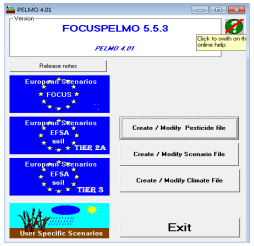

- ✓ 33 lysimeter studies selected for **1st step analysis** according to German Guidance (1990)
  - ✓ which shall ensure comparable soil and climate conditions to the „Hamburg“ scenario
- ✓ 33 registered (2012) active substances & 71 metabolites chosen for investigations
  - ✓ Leachate concentration > LOD, as far as possible
- ✓ Degradation & adsorption endpoints derived according to previous, new EU and national approach (LoEP or all available studies)
- ✓ Lysimeter crop & application conditions used for FOCUS modelling
- ✓ 80th percentile from 20 years modelling compared with max average annual from lysimeters

- ✓ Subset of 15 lysimeter cores selected for **2nd step analysis** by data quality
  - ✓ 8 active substances, 6 metabolites selected for inverse modelling
  - ✓ Inverse modelling to derive DT_{50} , k_{foc} values from field lysimeter results
  - ✓ Extended simulations for 20 years and yearly applications under lysimeter conditions

Data Collection, Preparation & Evaluations

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Modelling endpoint selection procedure	Previous EU practice	New EU guidance (EFSA 2014)	National guidance (Holdt et al. 2011)
DT_{50}	Geometric mean, (Maximum) (take field instead of lab. data, if available)	New evaluation of lab. & field $DegT_{50}$ values - cannot be considered, take previous EU value	Geometric mean, (Maximum) (take field instead of lab. data, if avail.) 10./90. percentile, if variation is high (> 100 %)
kfoc	Arithmetic mean	Geometric mean	Arithmetic mean, if correlation exists between kf & oc-content or variation of kfoc is low (≤ 60 %), otherwise use kf values
kf	-/-	-/-	Arithmetic mean, if no correlation exists between kf & oc-content or other soil properties (pH, clay, CEC) & variation of kf is low (≤ 100 %) Otherwise use of the 10.percentile

Results of Comparison Analysis – Active substances

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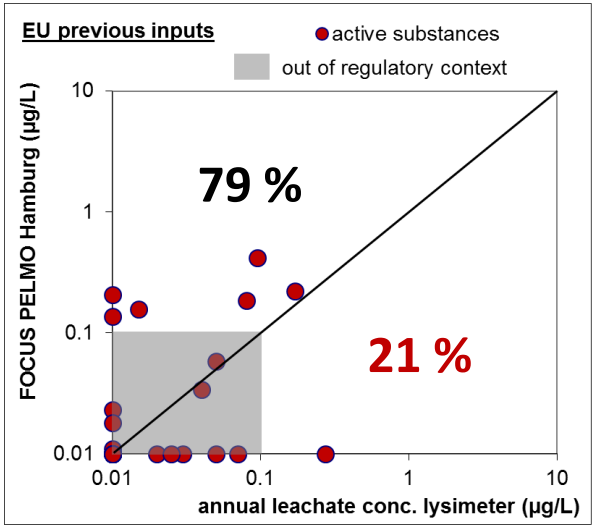
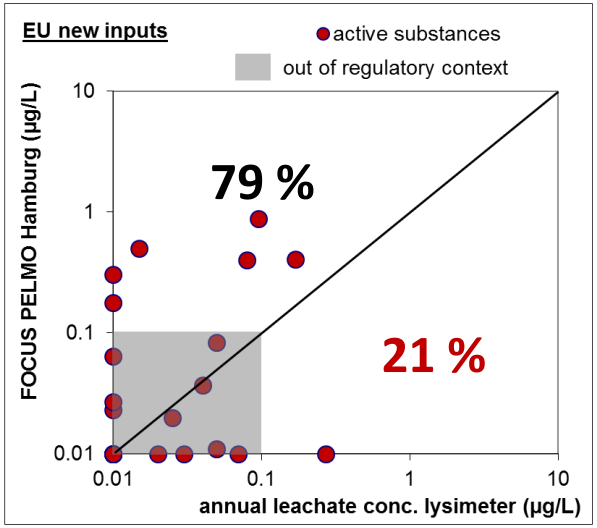
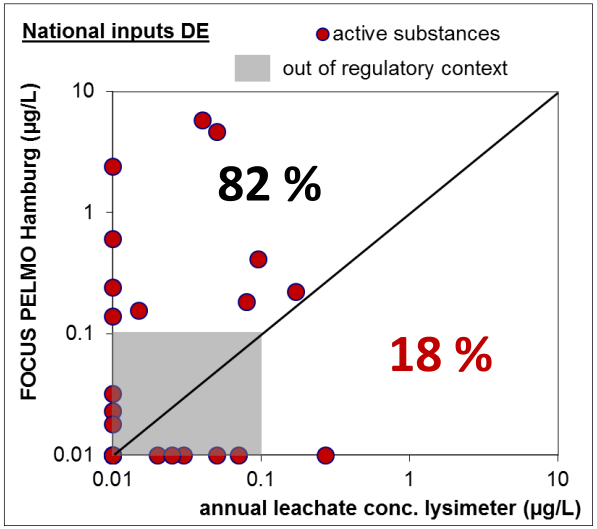
33 Active substances	Direct comparison of absolute values	
	FOCUS Hamburg ≥ Lysimeter	FOCUS Hamburg < Lysimeter
Previous/New EU	**79 %** (26)	**21 %** (7)
National DE	**82 %** (27)	**18 %** (6)



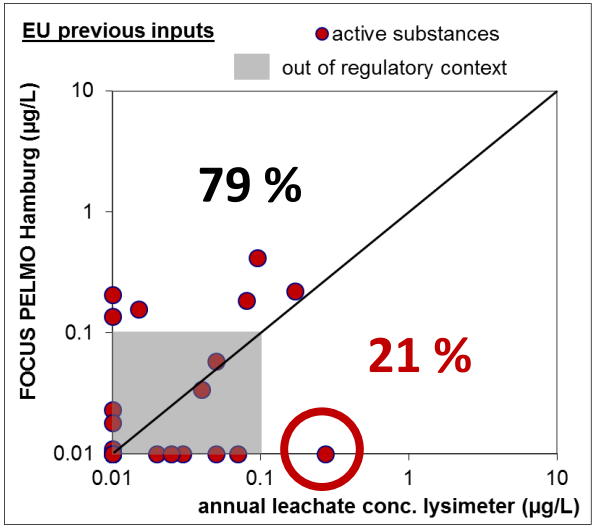


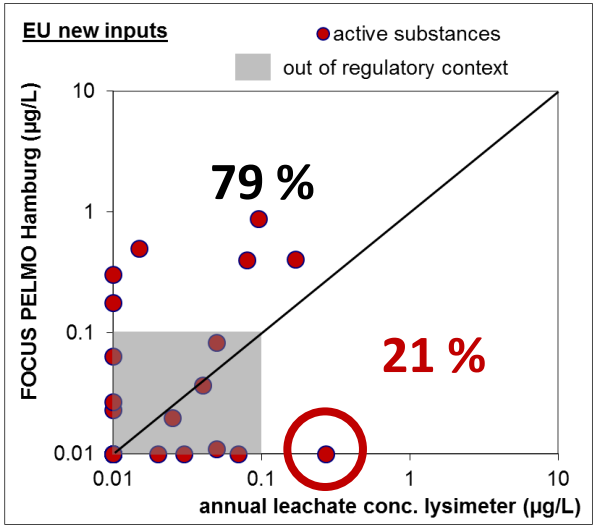


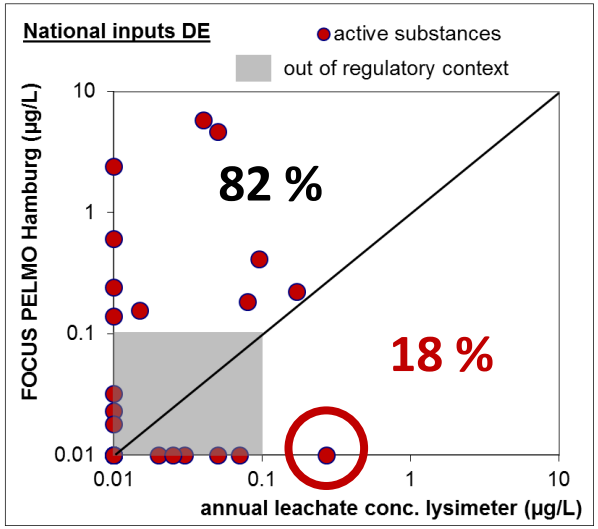
- Almost for the same number of active substances (**80 %**) PECs from modelling were higher than lysimeter measurements, marginal effects from different mod. endpoints.
- For about **20 %** of active substances lysimeter show higher results (> 0.01 µg/L).

Results of Comparison Analysis – Active substances

33 Active substances	Direct comparison of absolute values		Regulatory relevant
	FOCUS Hamburg ≥ Lysimeter	FOCUS Hamburg < Lysimeter	FOCUS Hamburg < 0.1µg/L Lysimeter ≥ 0.1µg/L
Previous/New EU	**79 %** (26)	**21 %** (7)	**3 % (1)**
National DE	**82 %** (27)	**18 %** (6)	







- Only for 1 a.s. FOCUS modelling did not estimate any leaching, but the lysimeter shows concentrations > 0.1 µg/L. (The lysimeter has been already discussed as not useful for regulatory purposes: oc-content < 1%, occurence of preferential flow)
- The regulatory impact is negligible. Acceptable predictions were reached for almost all a.s.

Results of Comparison Analysis – Active substances

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8 Active substances	Direct comparison		Regulatory relevant
	FOCUS H ≥ Lys.	FOCUS H < Lys.	FOCUS H < 0.1µg/L Lysimeter ≥ 0.1µg/L
Previous EU	**6**	**2**	**0**
New EU	**6**	**2**	**0**
National DE	**7**	**1**	**0**

- National modelling endpoints deviated from EU endpoints for 8 active substances:
  - Measured lysimeter concentrations are in 1 case higher than FOCUS Hamburg results (national inputs), in 2 cases using EU endpoints.
  - However, for non of those two parent compounds a regulatory relevant under-estimation was observed by using the three endpoint selection procedures.
- The analysis for active substances again confirms, that the national endpoint selection does not lead to very different results.

Results of Comparison Analysis - Metabolites

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71 Metabolites	Direct comparison of absolute values	
	FOCUS H ≥ Lysimeter	FOCUS H < Lysimeter
Previous EU	**72 %** (51)	**28 %** (20)
New EU	**79 %** (56)	**21 %** (15)
National DE	**82 %** (58)	**18 %** (13)

- Similar percentages as for active substances are found for metabolites:
  - For 72-82 % of the metabolites a conservative and safe prediction by modelling was reached in the direct comparison of absolute values.
  - **18-28 %** of the metabolites have been measured in higher concentrations (> 0.01 µg/L) in lysimeter experiments.
- The national approach leads to safest predictions (82 %).
- Similar results (safe predictions of 79 %) were conducted for calculations with geometric mean adsorption values (new EU approach).
- The previous EU modelling approach leads to less conservative results (28 %).

Results of Comparison Analysis - Metabolites

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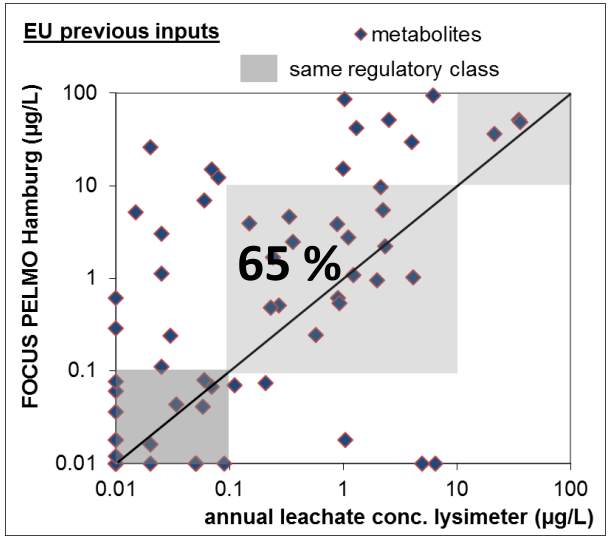
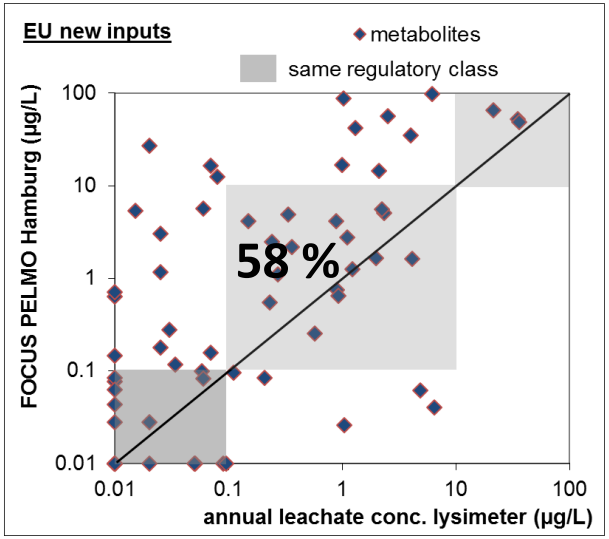
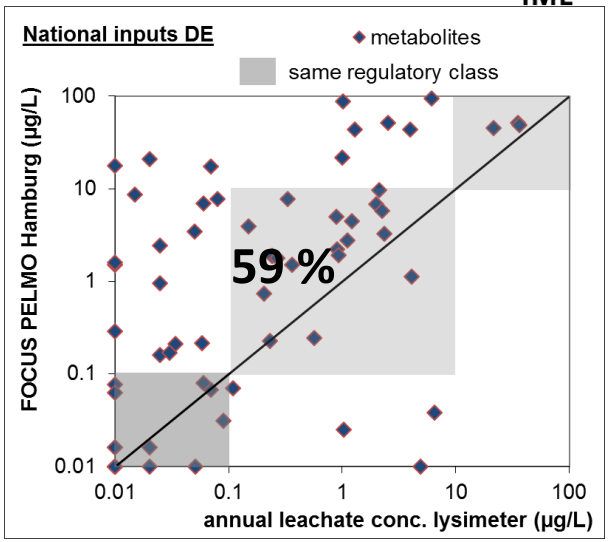


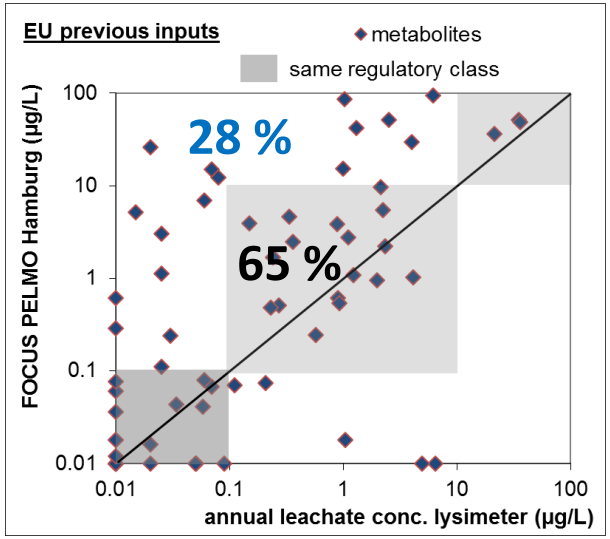


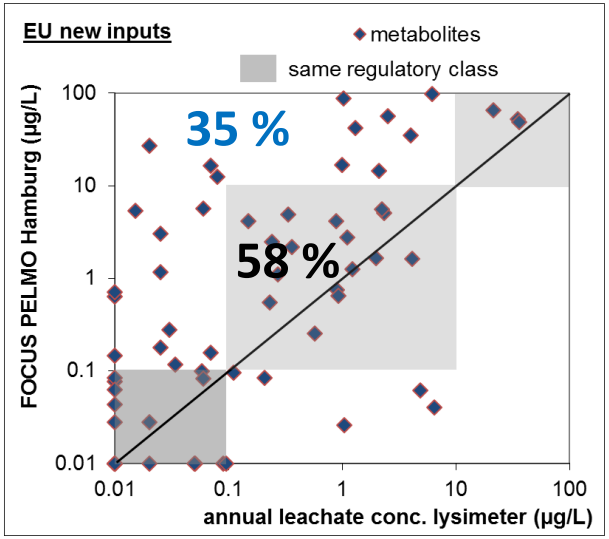


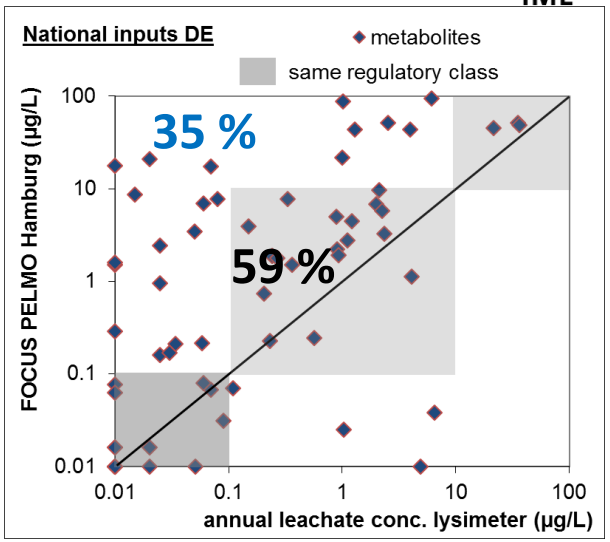
- Considering regulatory relevant classes: **<0.1 µg/L / >0.1-10 µg/L / >10 µg/L**, modelling and measurements results in the same class are found for the majority of metabolites (**59-65 %**): Best agreement was reached with previous EU endpoints.

Results of Comparison Analysis - Metabolites

Fraunhofer IME



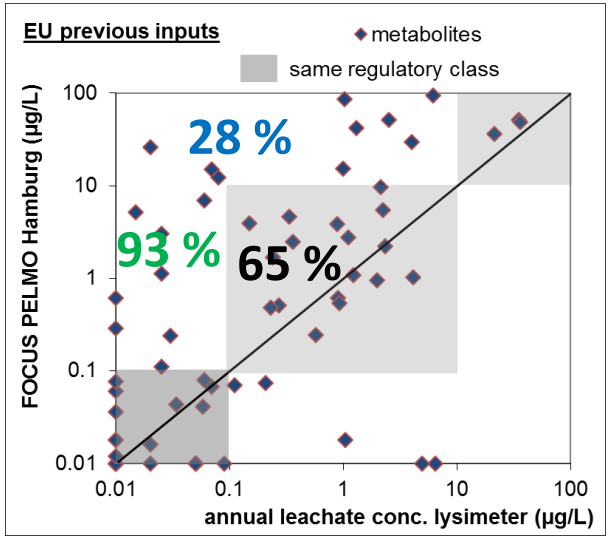


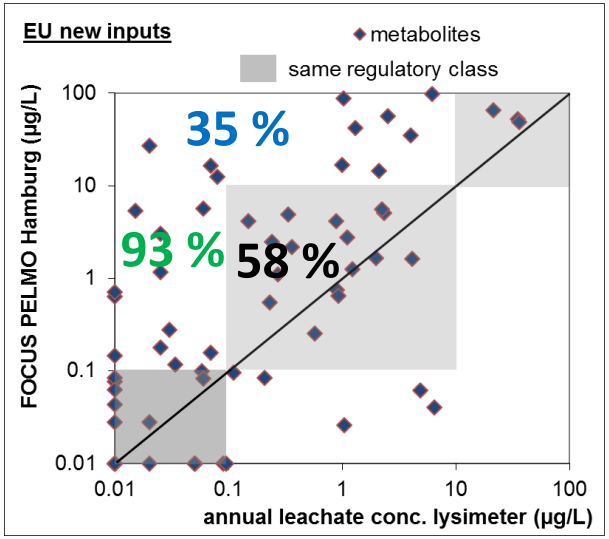


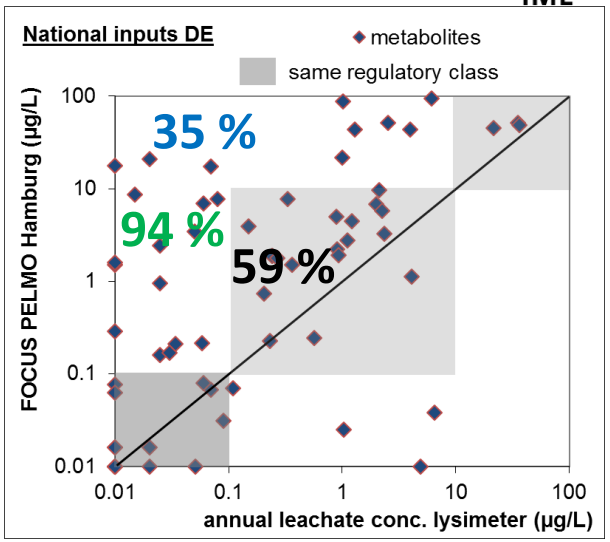
- Considering regulatory relevant classes: **<0.1 µg/L / >0.1-10 µg/L / >10 µg/L**, modelling and measurements results in the same class are found for the majority of metabolites (**59-65 %**): Highest agreement was reached with previous EU endpoints.
- For 28-35 % of the metabolites, higher modelling results in different regulatory classes occur: It ensures a safe prediction of leaching, but could require higher tier refinements.

Results of Comparison Analysis - Metabolites

Fraunhofer IME



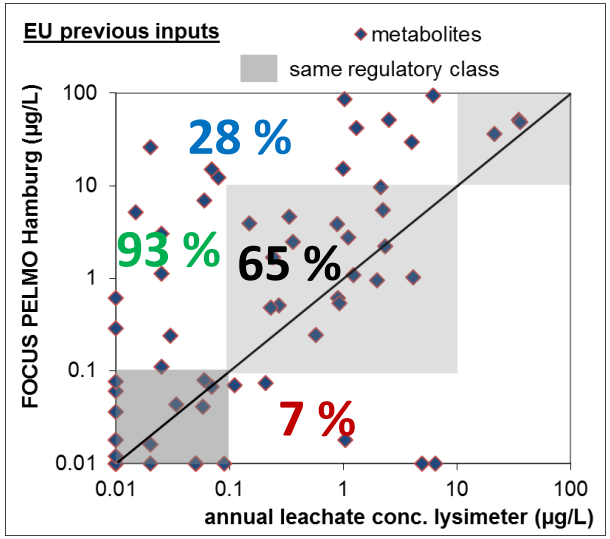


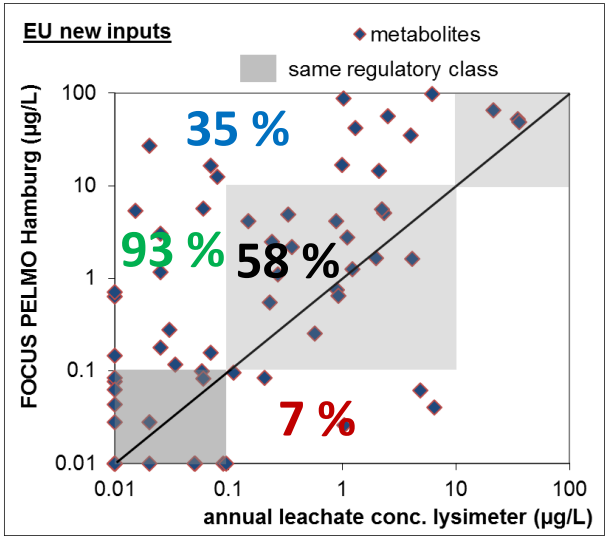


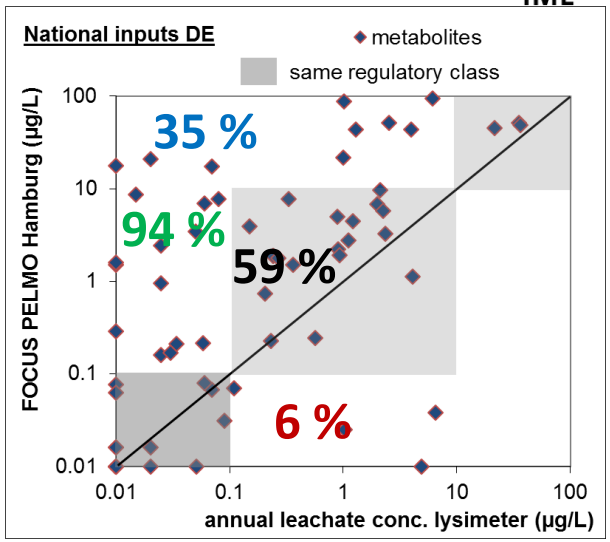
- Considering regulatory relevant classes: **<0.1 µg/L / >0.1-10 µg/L / >10 µg/L**, modelling and measurements results in the same class are found for the majority of metabolites (**59-65 %**): Highest agreement was reached with previous EU endpoints.
- For 28-35 % of the metabolites, higher modelling results in different regulatory classes occur: It ensures a safe prediction of leaching, but could require higher tier refinements.
  - A safe prediction complies for **93 %** (both EU) and **94 %** (DE) of the metabolites.

Results of Comparison Analysis - Metabolites

Fraunhofer IME







- Considering regulatory relevant classes: **<0.1 µg/L / >0.1-10 µg/L / >10 µg/L**, modelling and measurements results in the same class are found for the majority of metabolites (**59-65 %**): Highest agreement was reached with previous EU endpoints.
- For 28-35 % of the metabolites, higher modelling results in different regulatory classes occur: It ensures a safe prediction of leaching, but could require higher tier refinements.
  - A safe prediction complies for **93 %** (both EU) and **94 %** (DE) of the metabolites.
- For **6-7 %** of the metabolites FOCUS PELMO estimates leaching below 0.1 µg/L, but lysimeters show measurements between 0.1 µg/L and 10 µg/L. Relevance assessment would be triggered for all those cases from lysimeter results, only.

Results of Comparison Analysis – Metabolites

Fraunhofer IME

22 Metabo-lites	Direct comparison		Regulatory relevant		
	FOCUS H ≥ Lys.	FOCUS H < Lys.	FOC.H < 0.1µg/L Lys. ≥ 0.1µg/L	FOC.H < 0.1µg/L Lys. ≥ 10 µg/L	FOC.H ≥ 0.1µg/L Lys. ≥ 0.1µg/L
Prev. EU	**13**	**9**	**2**	**0**	**0**
New EU	**15**	**7**	**2**	**0**	**0**
National	**17**	**5**	**2**	**0**	**0**

- Deviating national endpoints from EU have been evaluated for 22 metabolites.
- Uncertainties to leachate prediction (Lysimeter > FOCUS Hamburg) was obtained for a smaller subset of those 22 metabolites with national endpoints (5) compared to EU endpoints (7 or 9).
- However, taking into account regulatory relevant limit values, uncertainties with FOCUS modelling remain for 2 of those metabolites, independent of the endpoint selection.

Results of Comparison Analysis – Inverse Modelling

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- Success of inverse modelling depends on the quality of available data from the experiment (e.g. weather data). Expert judgement is needed.
- The methodology causes uncertainties, because a high degree of freedom exists for parameter definition. Even higher uncertainties remain for metabolite estimations.
- No standardised recommendations could be derived from the investigated cases, how to overcome uncertainties of measured lysimeters concentrations in relation to single applications and short study durations.
- Some evaluations show, that lysimeter studies could be still interpreted as endpoint studies: if they are conducted close to FOCUS Hamburg conditions, if they are comparable to the conditions of the intended use, for (very) mobile compounds.
- Inverse modelling is not recommended to be applied as standard method for FOCUS tier 3c assessment.
- It´s rather recommended as possibility to investigate reasons for high deviations between modelled and measured results, if those occur.

Summary of Results

- The direct comparison of absolute values from modelling & lysimeters
  - gives evidence for a high percentage of safe predictions for active substances & metabolites (about **80 %**) by FOCUS modelling for sandy soils.
  - Higher leachate concentrations are measured in lysimeters for several compounds (about **20 %** of the investigated cases).
  - The effects from the three different investigated endpoint selection approaches are rather small. A slightly more conservative prediction by modelling was reached with national and new EU endpoints (geometric mean kfoc values).
- Taking into account regulatory limit values,
  - the agreement between modelling and lysimeter results is much higher.
  - The different endpoint selections lead to comparable results.
  - Uncertainties remain for the calculation of leachate concentrations for metabolites (about **7 %** of the investigated cases).
- Uncertainties for FOCUS Hamburg modelling could still be higher in terms of the lysimeter study critique in FOCUS (2009), that they can underestimate the leaching potential of several compounds due to single applications and short study durations.
- The conducted investigations could not give a profound answer to that.

Regulatory Conclusions

- Because the national endpoint selection procedure does not lead to significant different regulatory results and mainly for harmonization reasons, EU endpoints for FOCUS modelling are going to be accepted for national groundwater risk assessment.
- However, there are still concerns about the identified uncertainties with FOCUS modelling, especially for a safe prediction of metabolite leaching in sandy soils.
  - The FOCUS modelling using averaged endpoints may not cover all cases in reality.
  - Finally no conclusions can currently be drawn on how the new EU approach to derive degradation endpoints (EFSA 2014) will affect the system.
- The analysis further shows, that lysimeter studies can be regarded as legitimate part of the risk assessment for groundwater.
- For national risk assessment, they are still used as endpoint studies for (very) mobile compounds, if their experimental design ensures a comparison to the conditions of the intended use and FOCUS Hamburg conditions.
  - Long-term FOCUS Hamburg modelling could help to identify possible uncertainties of lysimeter studies regarding study duration and single application in relation to the properties of the compound which needs to be assessed.

Thanks for your attention!

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