Workshop 4: From point measurements to regional assessment

Using spatial analysis to map diffuse pollution

Frederik Priem, Ward Swinnen, Karolien Vermeiren, Ilse Van Keer

International workshop on Emerging policy challenges on New SOil contaminants (**ENSOr**)

2024/03/14

vito

vito.be

From here

To there

And back again

How spatial science can help

At policy / institutional level

- Revealing or confirming spatial correlations of diffuse soil pollution.
- Identifying and understanding spatial and other patterns in soil data.
- Mapping pollution danger and risk, at least indicative, on regional level.
- Offering guidance in monitoring, mitigation and policy strategies.

On the field / at parcel level

- Estimating the expected level of local soil pollution for various substances.
- Indicating the possible source activities of the encountered soil pollution.
- Defining more substantiated intervention areas around polluted sites.
- Making the survey of multiple parcels more time/resource efficient.

Two PFAS case studies, two scales

Why PFAS?

1. Center of attention.
2. Publicly available data.
3. Insights and workflows transferable to other types of diffuse pollution.

1. Case study with **local focus** - From point measurements to comprehensive assessment: upscaling measurements and fingerprinting techniques.
2. Case study with **regional focus** - A regional analysis of PFAS environmental data in support of the Flemish Soil Decree.

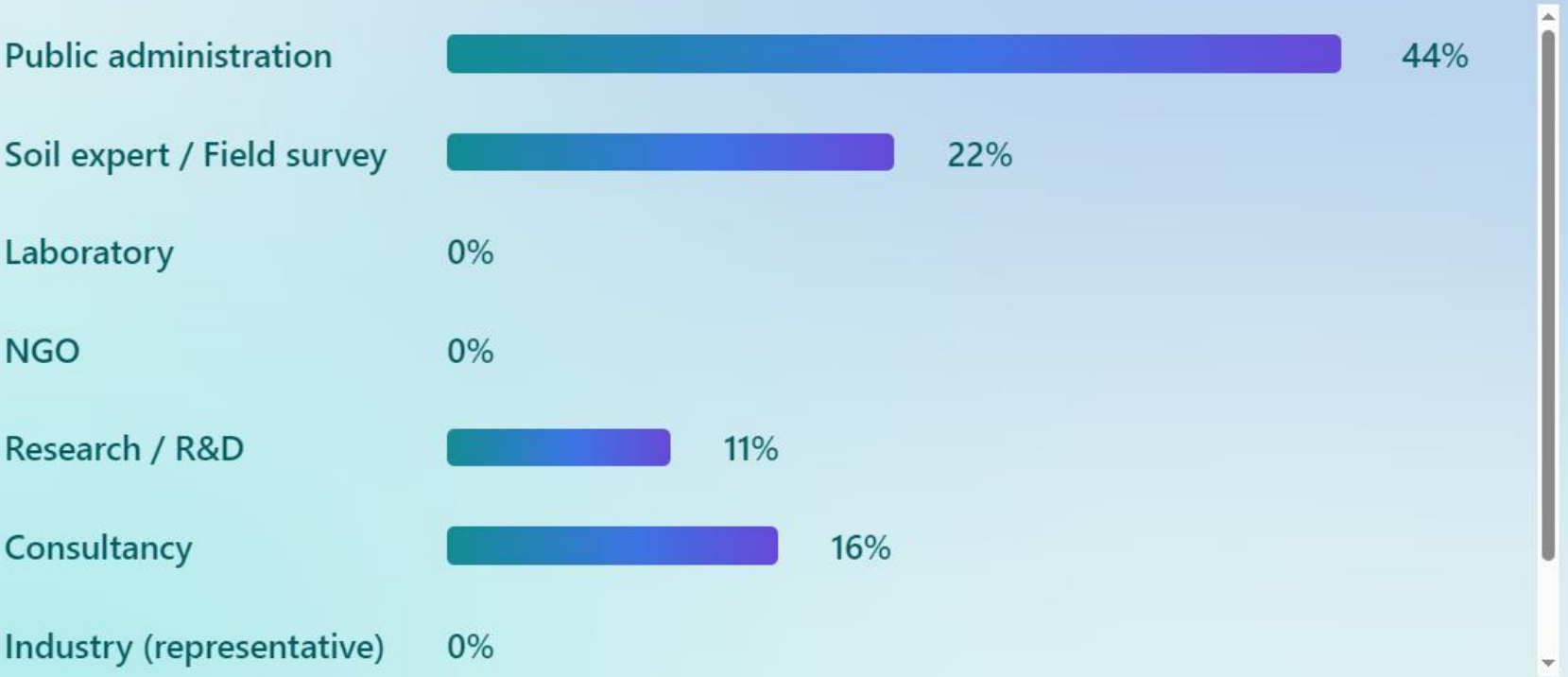
Scan the QR or use link to join

https://forms.office.com/e/rsMwybPJn6

Copy link

18 responses submitted

In what type(s) of organization do you work?



1 of 2

vito

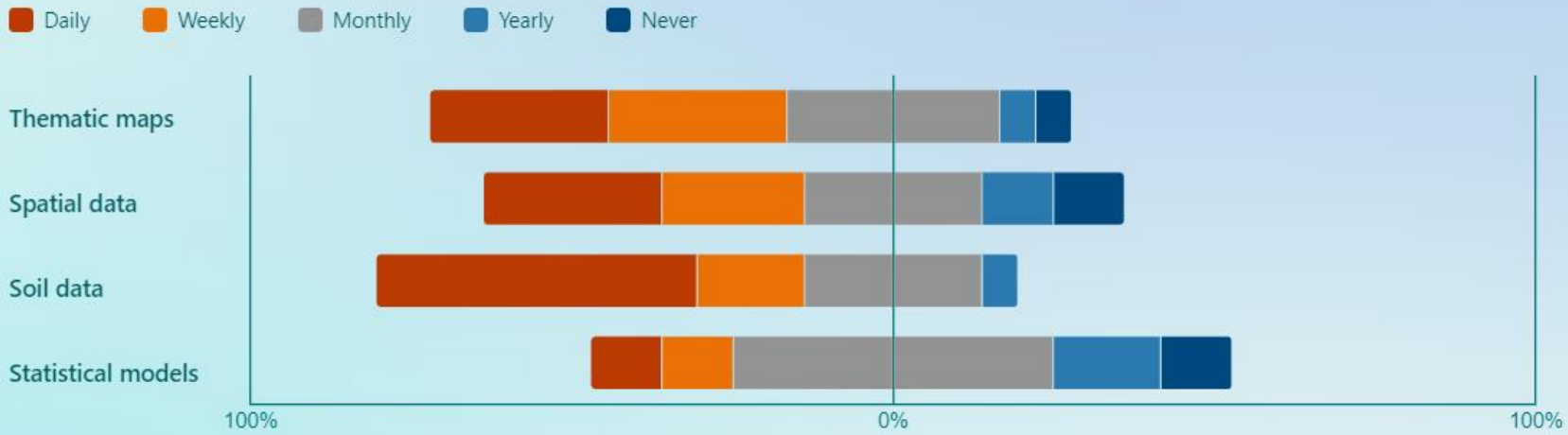
Scan the QR or use link to join

https://forms.office.com/e/rsMwybPJn6

Copy link

18 responses submitted

How often do you or your colleagues use the following products?



vito

Case study 1: From point measurements to comprehensive assessment

Upscaling measurements and fingerprinting techniques

Ward Swinnen

vito

vito.be

Introduction

- Soil and groundwater surveys produce large amounts of data
- More diverse parameters are more challenging to interpret but also provide a wealth information for further analysis (e.g., PFAS)
- Depending on the context, statistical analysis of the obtained data can provide added value
- Statistical techniques can help to discern sources and pathways of contamination and provide insight in patterns found across and between sites

From point measurements to comprehensive assessment

- Further statistical analysis leads to a more in-depth understanding of the patterns within the data → unveil hidden complexities and nuances

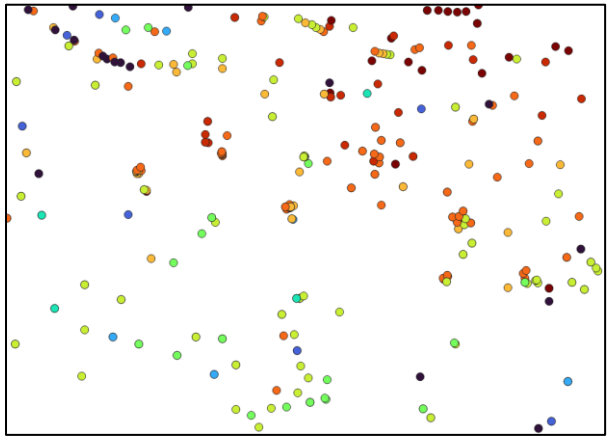
- Focus on two topics:
  - Spatial delineation of contamination
  - Spatial connection: fingerprinting and source identification

- Anonymized case studies from Flanders as examples to demonstrate added value

Part 1: Spatial delineation of contamination

- Statistical interpolation techniques → area-wide estimation of concentrations
- Allows for a more detailed delineation
- Especially useful for larger areas (sampling points spaced more widely)
- Strong differences between techniques

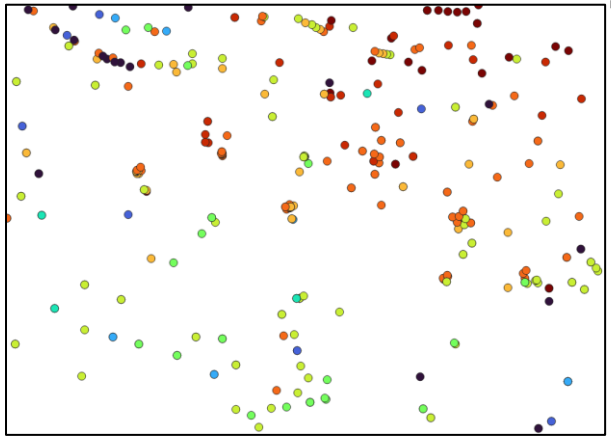
Measured data



Case study: delineation with different interpolation techniques

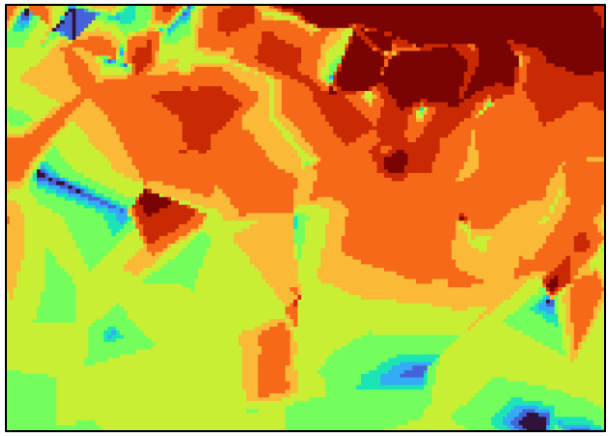
- Statistical interpolation techniques → area-wide estimation of concentrations
- Allows for a more detailed delineation
- Especially useful for larger areas (sampling points spaced more widely)
- Strong differences between techniques

Measured data

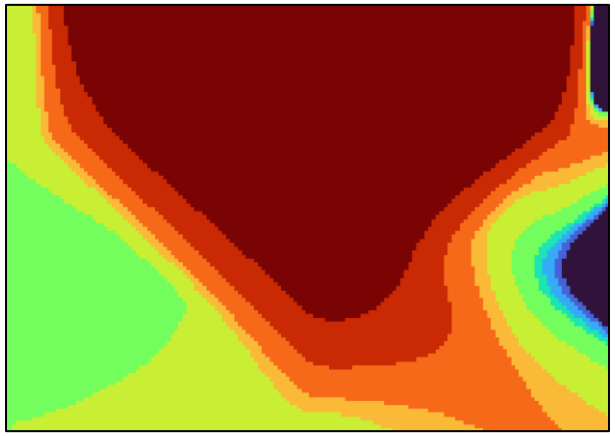


Which one is “correct”?

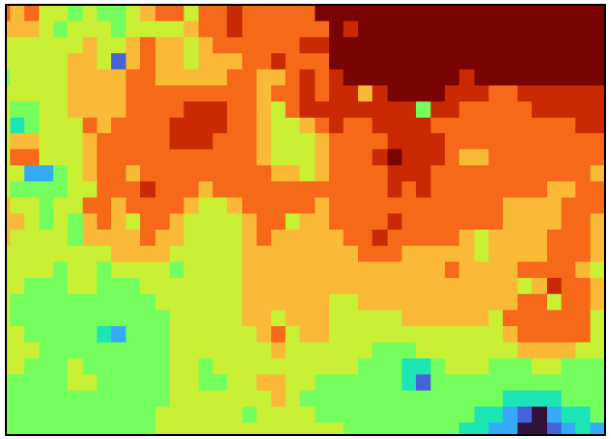
TIN



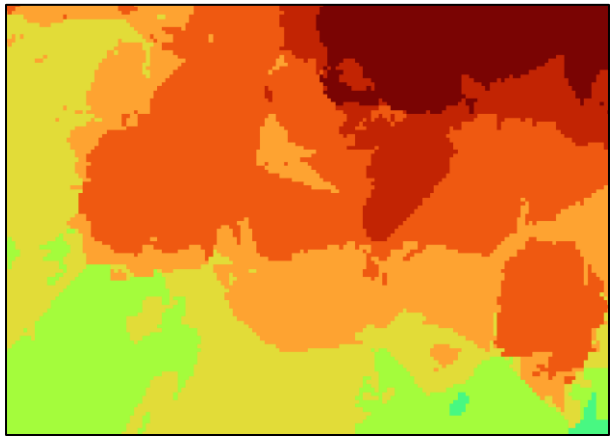
Splines



IDW



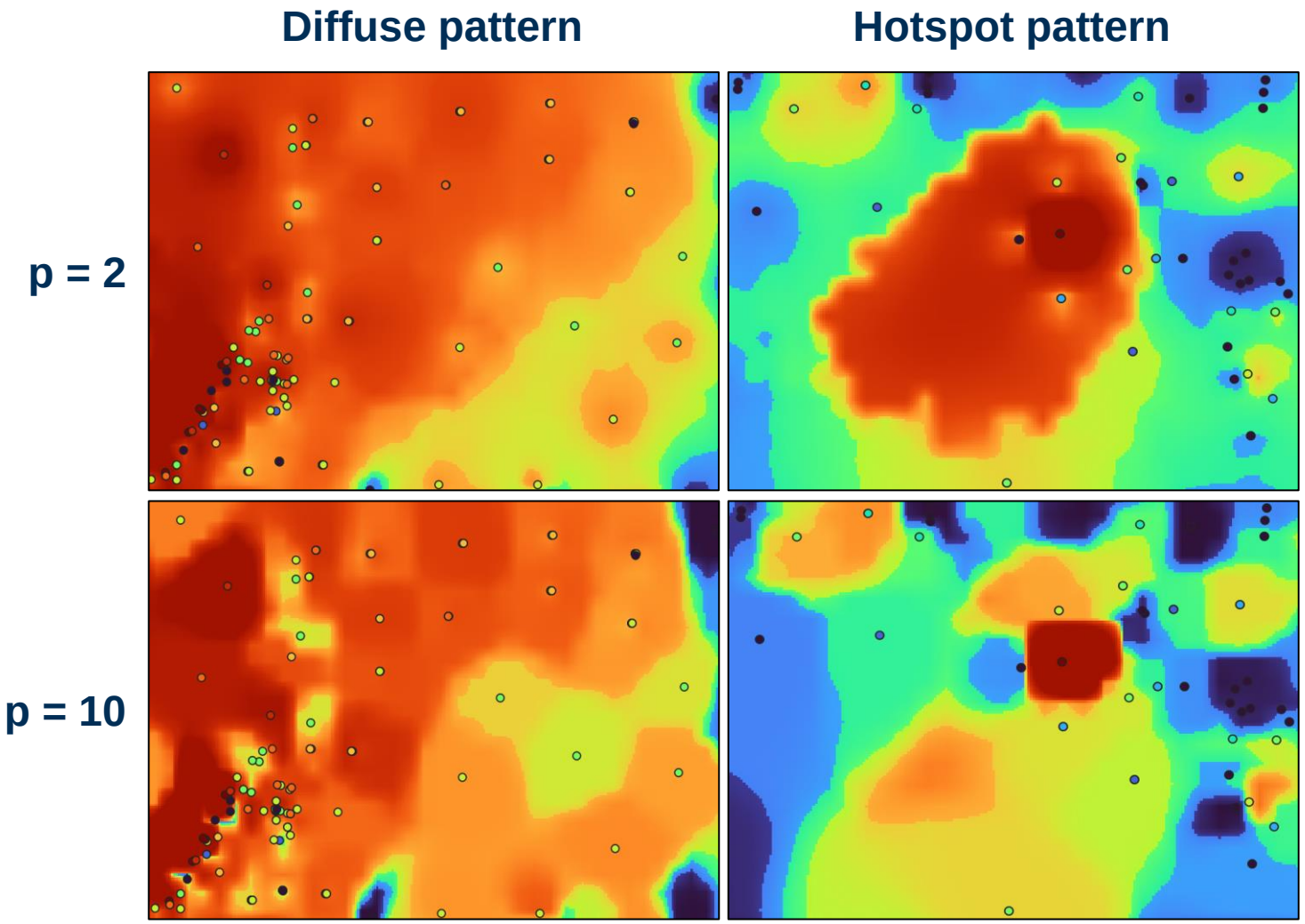
Kriging



vito

Case study: delineation with different interpolation techniques

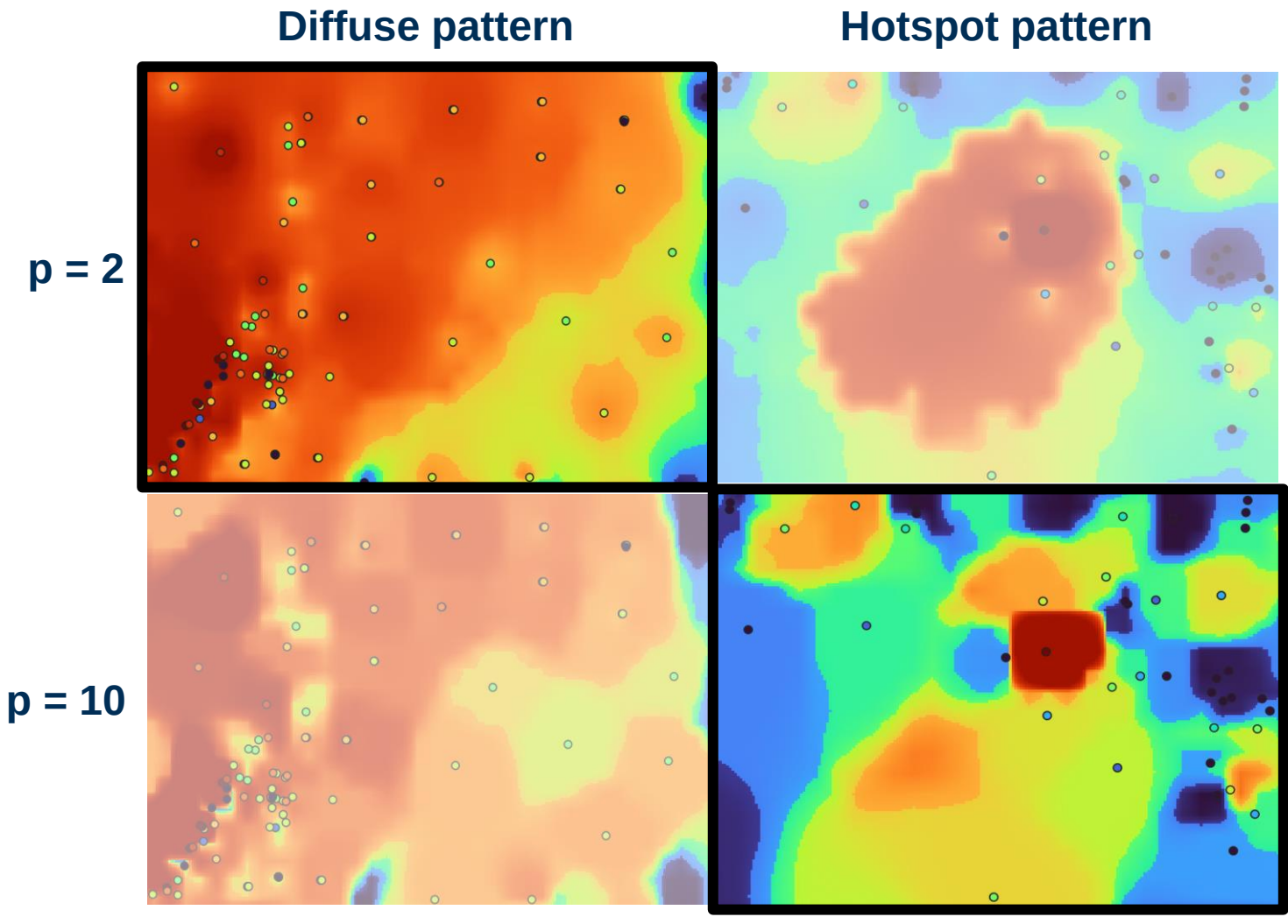
- “Correct” technique depends on type of contamination (pattern)
- Example: contaminated site with multiple sources.
- Interpolated with inverse distance weighting (IDW)
- Power values of 2 and 10
- Low power well-suited for gentle/diffuse patterns
- High power well-suited for hotspots/strong concentration gradients



vito

Case study: delineation with different interpolation techniques

- “Correct” technique depends on type of contamination (pattern)
- Example: contaminated site with multiple sources.
- Interpolated with inverse distance weighting (IDW)
- Power values of 2 and 10
- Low power well-suited for gentle/diffuse patterns
- High power well-suited for hotspots/strong concentration gradients



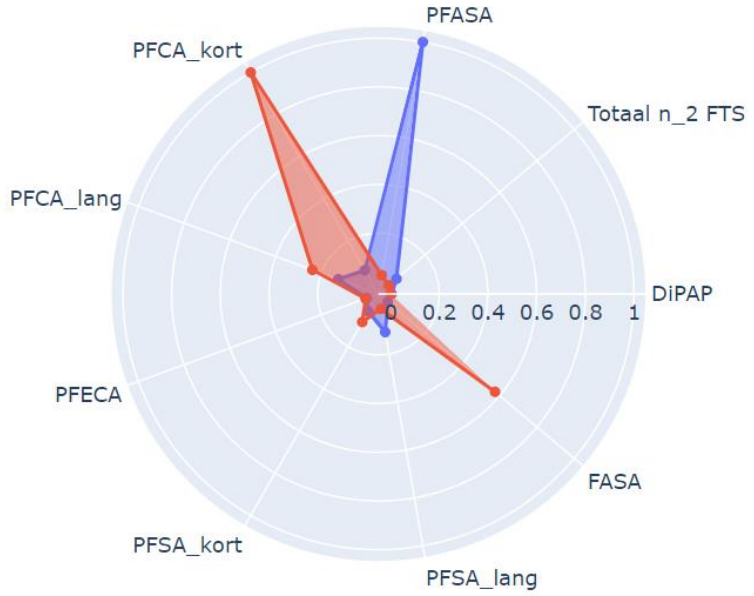
Part 2: Spatial connection: fingerprinting and source identification

- Diverse parameters allow to construct fingerprints for different locations/depths/…
- Different fingerprints in the same area can indicate the potential presence of multiple contamination sources
- Helps identifying pathways
- Presented examples show both simple and more sophisticated techniques.

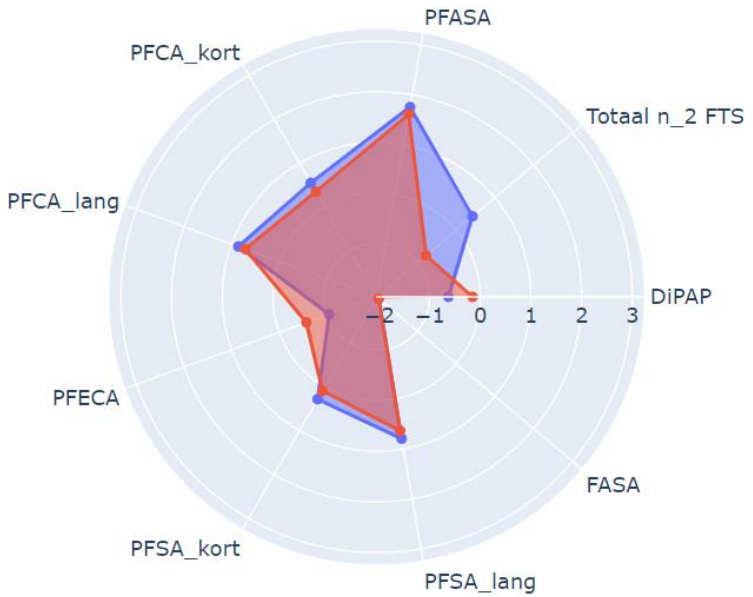
Example: PFAS fingerprint based on functional groups

- PFAS concentrations summed for nine functional groups
- Radar plots of average concentrations to study correspondence between locations/soil layers/…
- Easy to apply and no additional data required

No correspondence

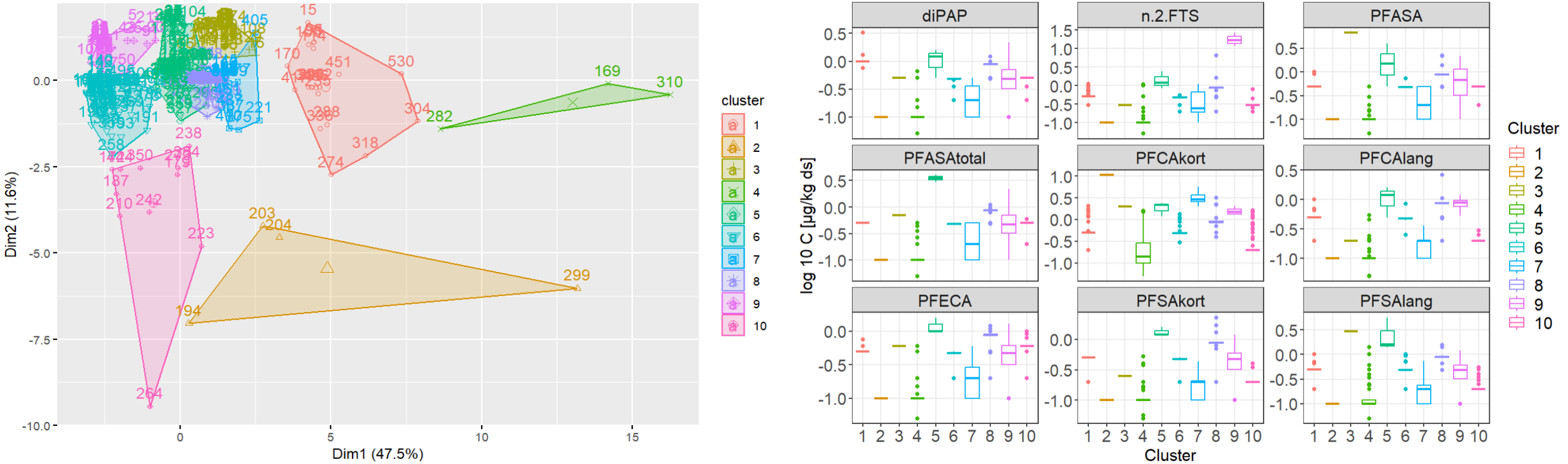


Good correspondence



Example: PFAS fingerprint based on cluster analysis

- Clustering of PFAS data for large amount of different locations
- Group locations based on their PFAS fingerprint
- Insight in typical PFAS compounds for each cluster (indicator compounds)



Conclusion

- Additional statistical analysis is often not required but can improve in-depth understanding of the case.
- Even simple and readily available techniques can already provide added value
- Spatial statistics can assist in contamination delineation if the adequate technique is used
- Fingerprinting techniques can highlight the important elements in the large amount of data produced by diverse parameters such as PFAS.

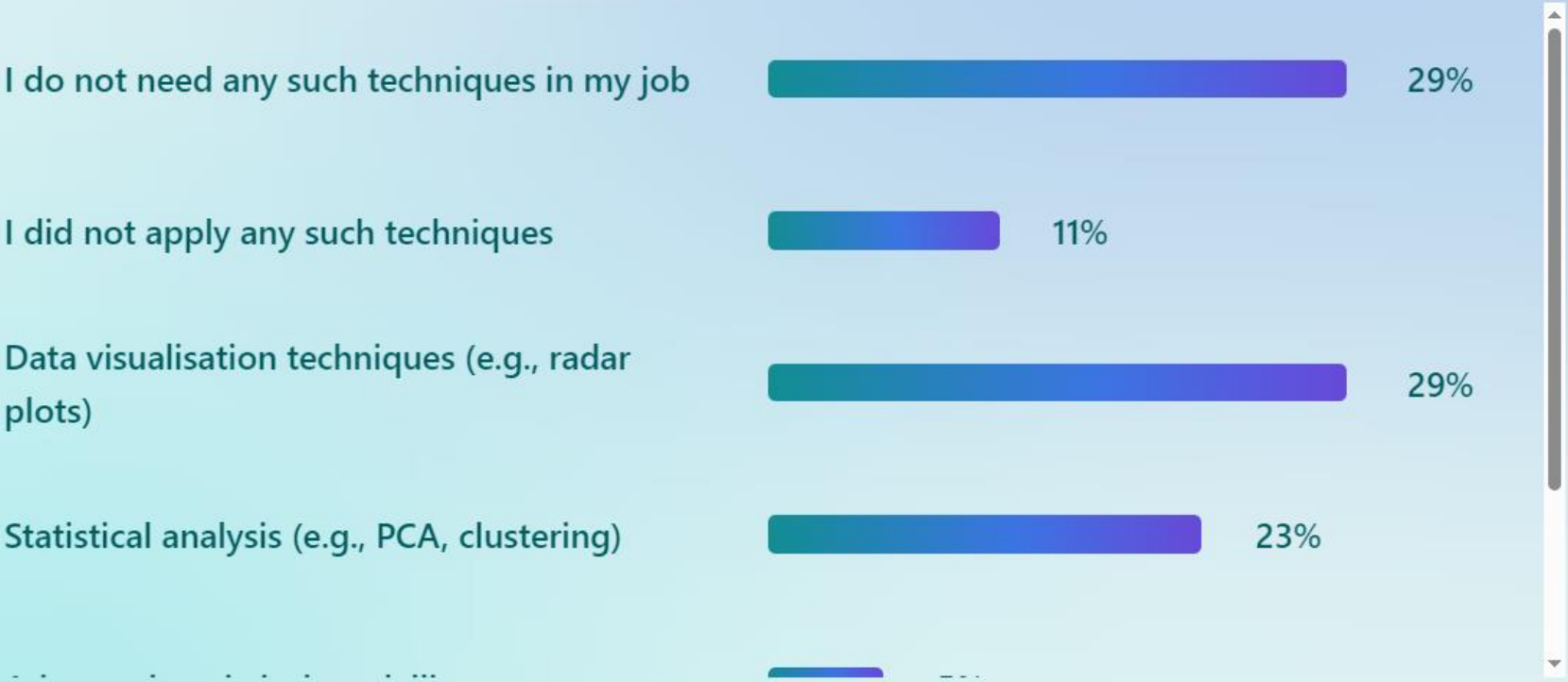
Scan the QR or use link to join

https://forms.office.com/e/4jc48Kcm8p

Copy link

14 responses submitted

Which additional fingerprinting techniques have you used for diverse parameters such as PFAS to gain insights in sources and pathways?



vito

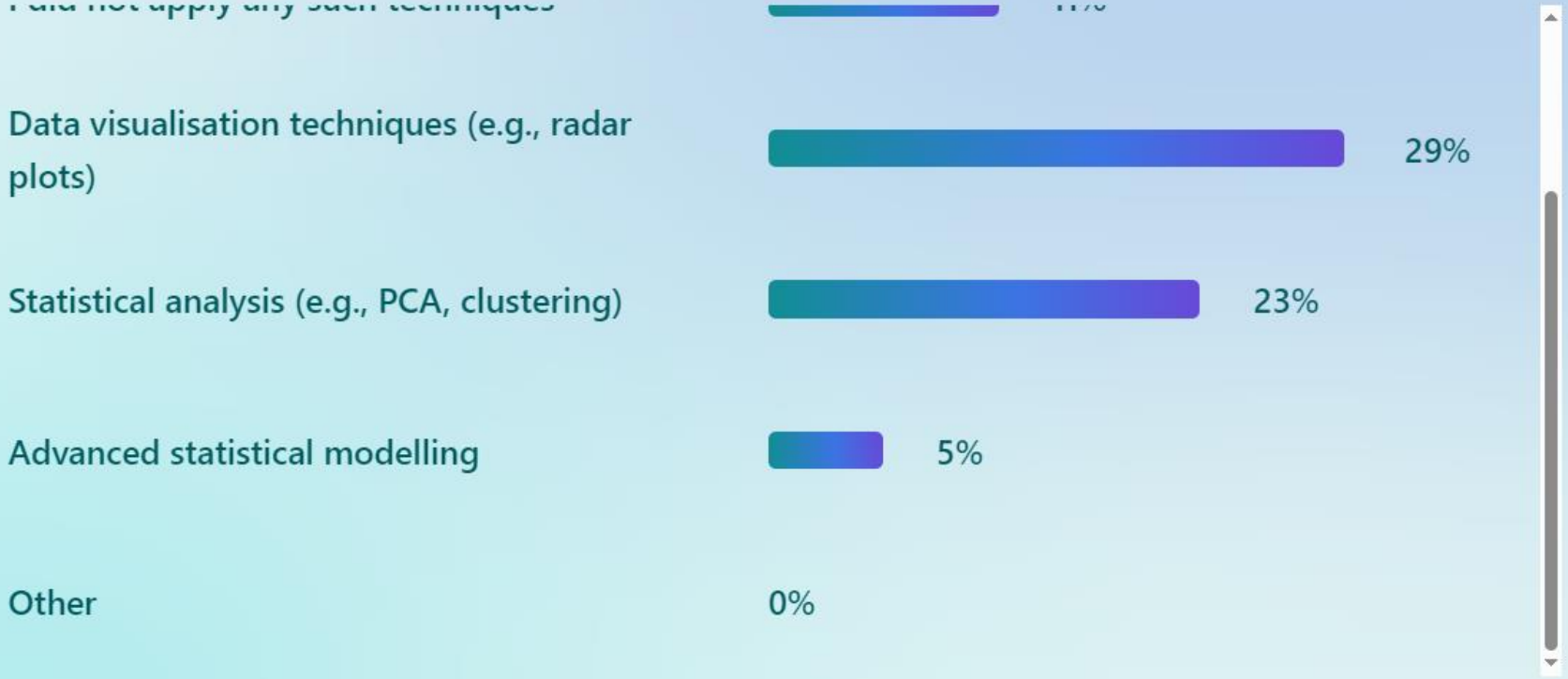
Scan the QR or use link to join

https://forms.office.com/e/4jc48Kcm8p

Copy link

14 responses submitted

Which additional fingerprinting techniques have you used for diverse parameters such as PFAS to gain insights in sources and pathways?



1 of 2

vito

Scan the QR or use link to join

https://forms.office.com/e/4jc48Kcm8p

Copy link

14 responses submitted

After seeing this presentation, how often will you use statistical analysis in soil pollution case studies?

Treemap | Bar

2 of 2

vito

Case study 2: A regional analysis of PFAS environmental data in support of the Flemish Soil Decree

Frederik Priem, Wim Clymans, Frank Sleeuwaert, Karolien Vermeiren

vito

vito.be

Objectives of this study

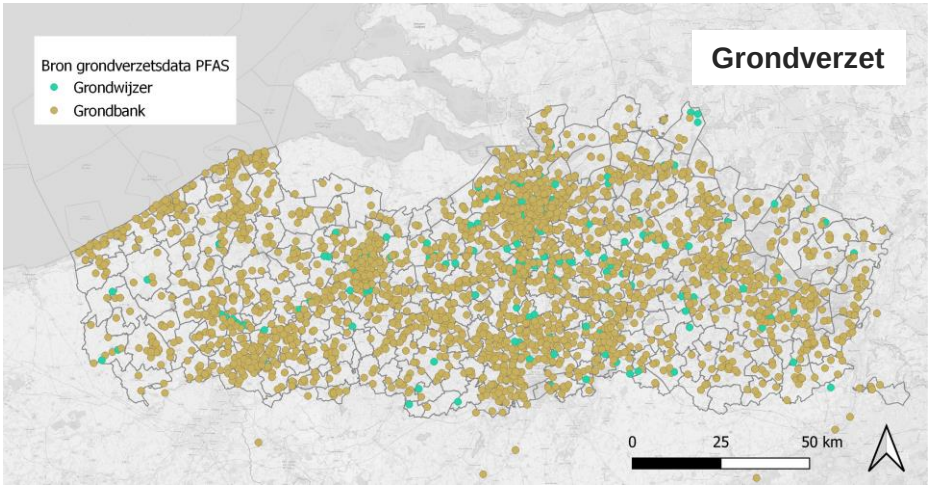
Assess regional PFAS soil pollution in Flanders to support policy review.

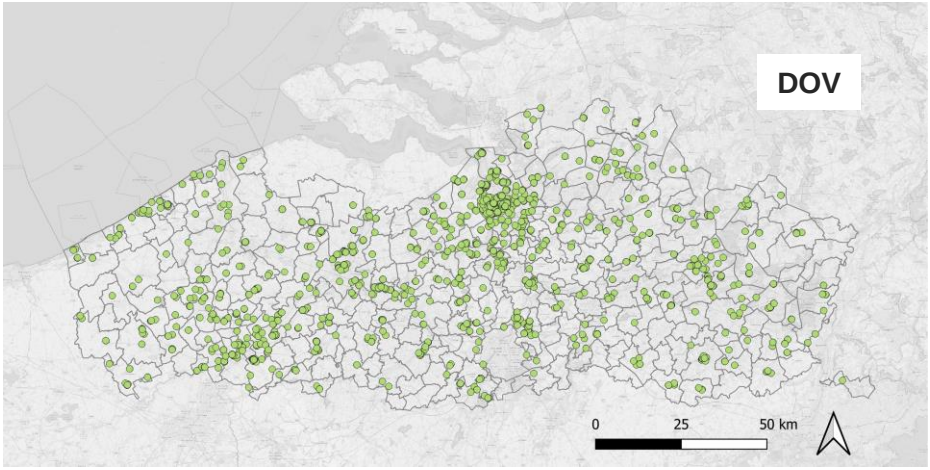
1. Collect and consolidate Flemish PFAS data on:
   - Geocoded soil concentration measurements.
   - **S**uspected **A**reas (**SA**).
2. Spatially overlay data to quantify / qualify pollution:
   - **Within** SA.
   - **Near** SA.

Data

PFAS soil measurements

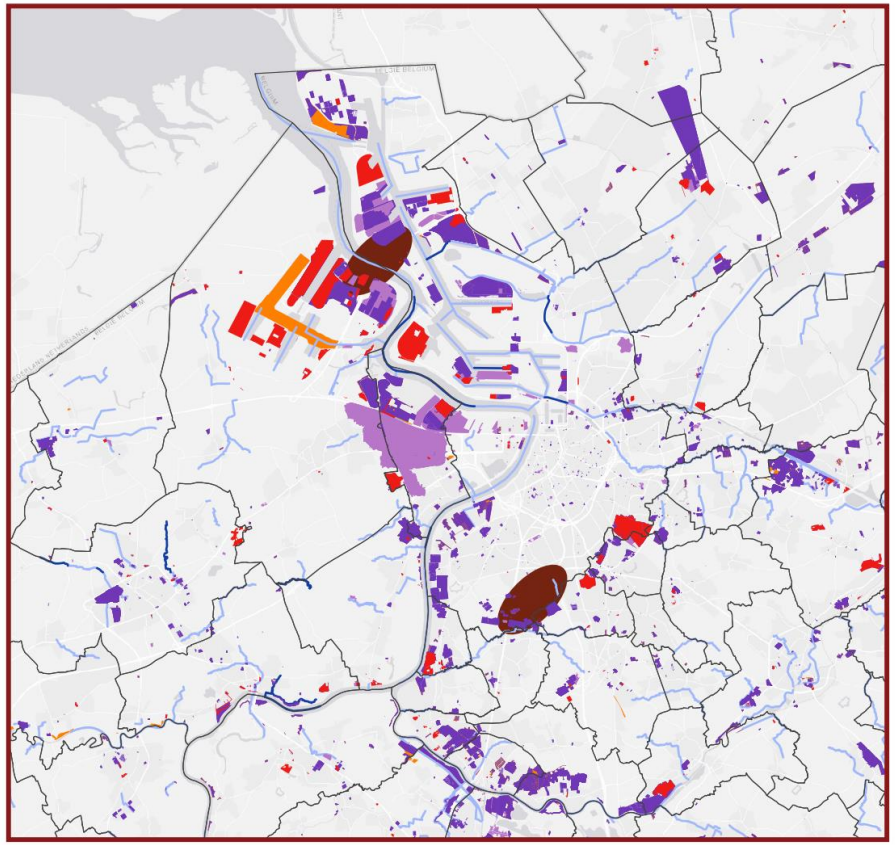
Dataset	Focus	# substances measured	# points measured
Grondverzet	Detecting PFAS soil pollution at groundworks and dredging sites.	3	2945
DOV database	OVAM surveys of areas with suspected PFAS soil pollution.	48	3736
Witteveen & Bos	Determining PFAS background concentrations in soils.	54	74





Data

Suspected areas



Suspected areas

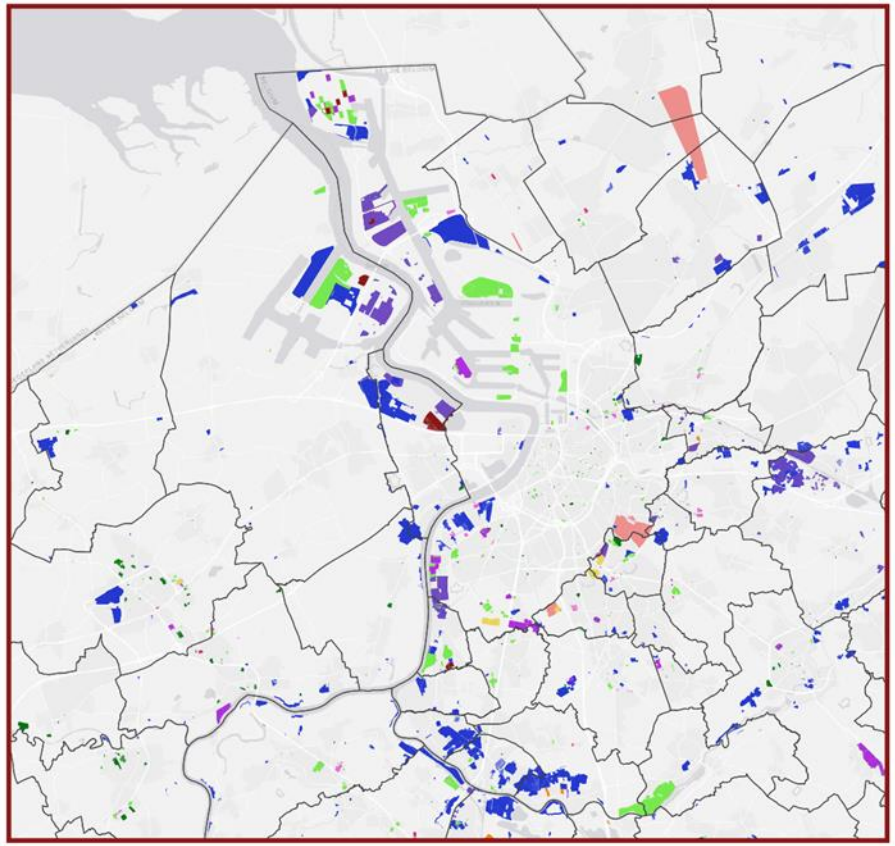
- Firefighting
- Areas with suspected PFAS activity (screening)
- Other OVAM casefiles
- River soils with permitted PFAS emission
- River soils with suspected PFAS emission
- Dumpsites/landfills
- Solid waste processing plant (ellipse)

- Municipality

Data

Suspected area screening

Suspected/permitted use of PFAS ≠ effective use ≠ effective emission



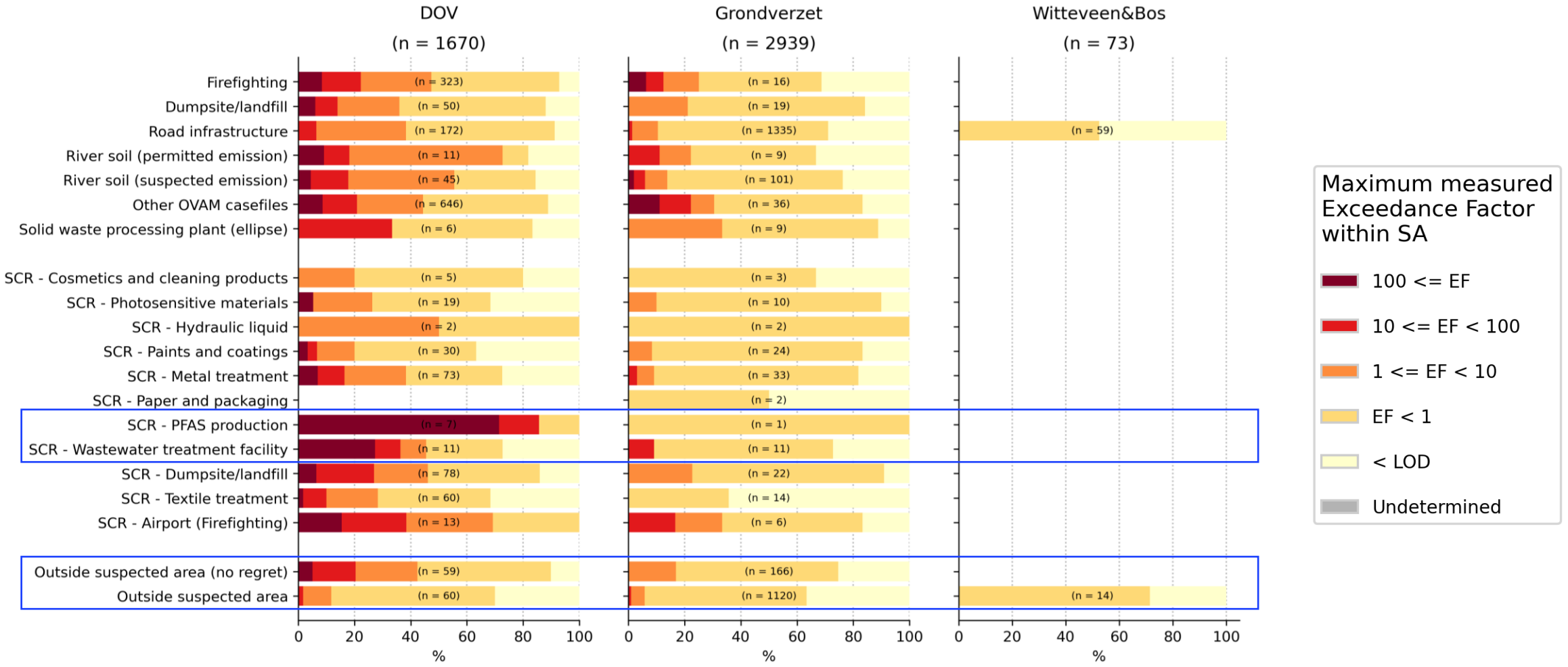
Areas with suspected PFAS activity (screening)

- PFAS production
- Cosmetics & cleaning products
- Paper & packaging
- Metal treatment
- Textile treatment
- Photosensitive materials
- Hydraulic liquids
- Paints & Coatings
- Wastewater treatment facility
- Dumpsite / landfill
- Airport (firefighting)

Municipality

PFOS exceedance within different SA types

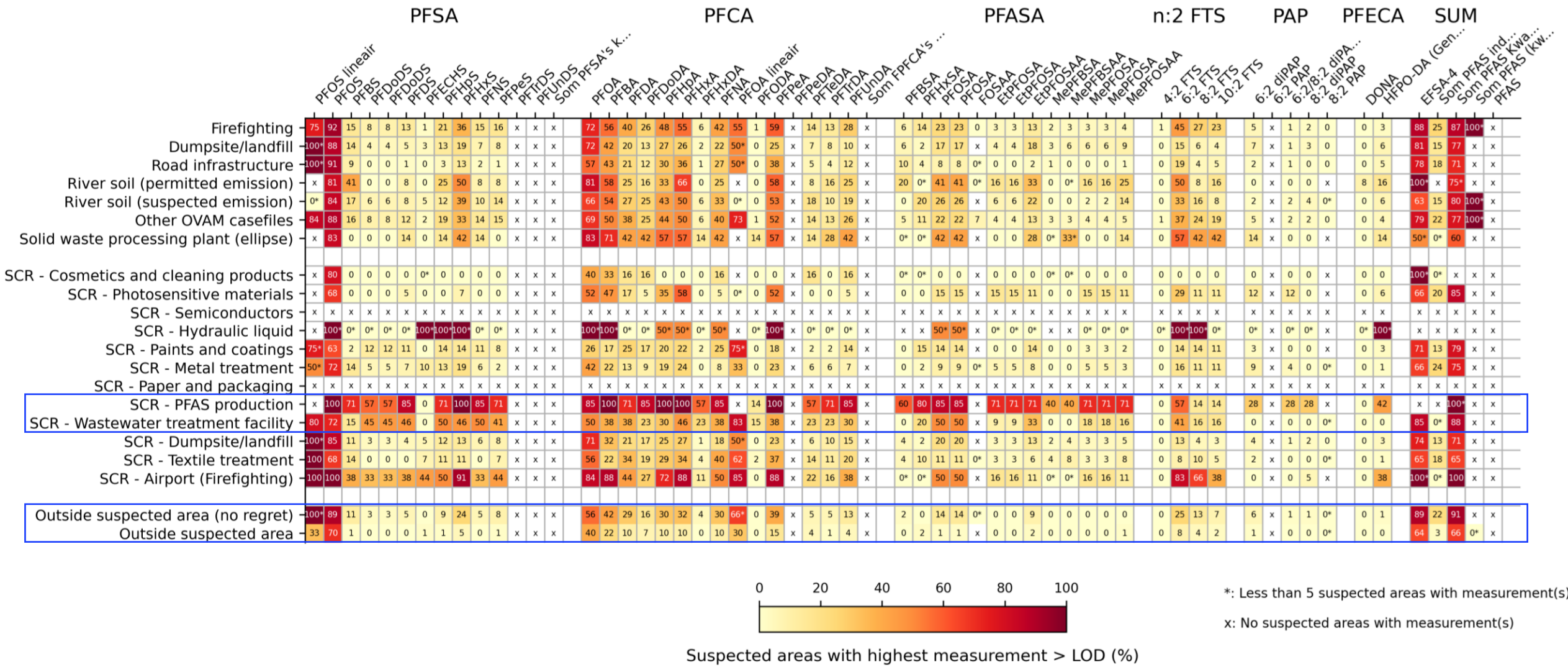
$$EF_{PFOS,\,soil} = \frac{measurement}{[3\ \mu g \backslash \mathrm{kg}\ DM]}$$



vito

vito.be

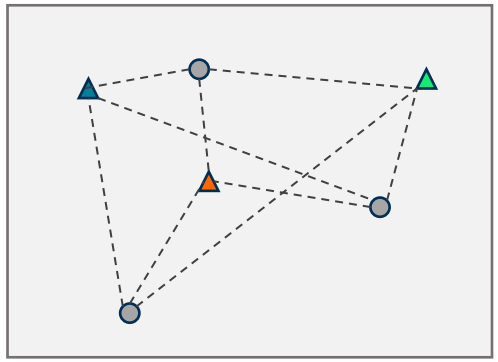
Detection of PFAS substances within different SA types



PFAS pollution near SA

Workflow

Spatial join of measurement points and SA



Measurement

SA (type X)

Distance quantification

Regression dataset

Point ID	Soil concentrations			Min. Distance to SA		
	PFOS	PFOA	…	WWTF	FF	…
1	1.1	0.5	…	550	2300	…
2	24.0	8.2	…	40	4300	…
3	0.04	0.006	…	5600	7100	…
…	…	…	…	…	…	…

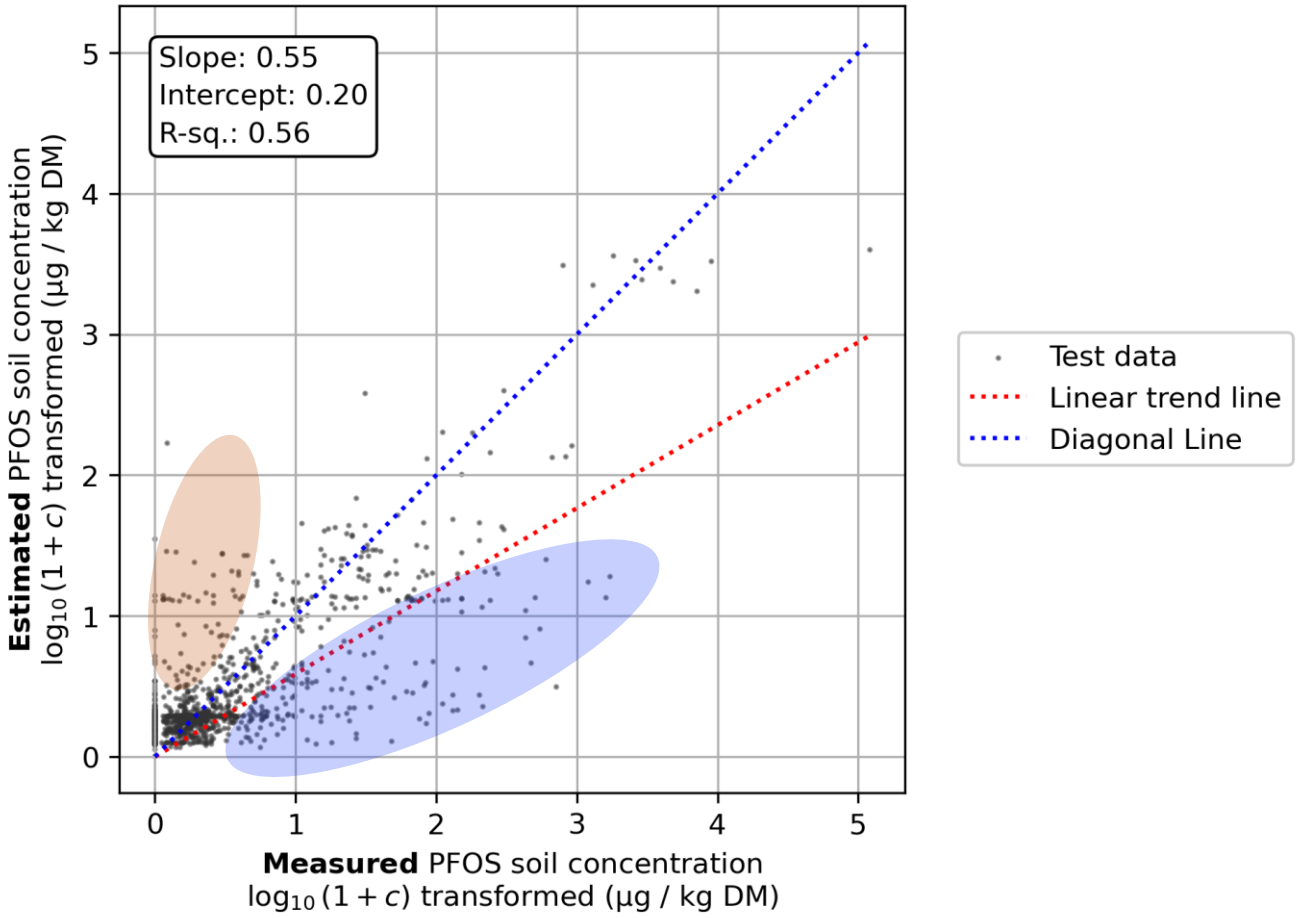
80% of observations randomly sampled to train machine learner (SVR) targeting a specific substance

Other 20% used to evaluate model performance

Performance of predictive PFOS soil concentration model

Underestimation due to missing SA data (coastal + farmland).

Overestimation due to SA without emission?



From predictive model to regional soil PFAS map?

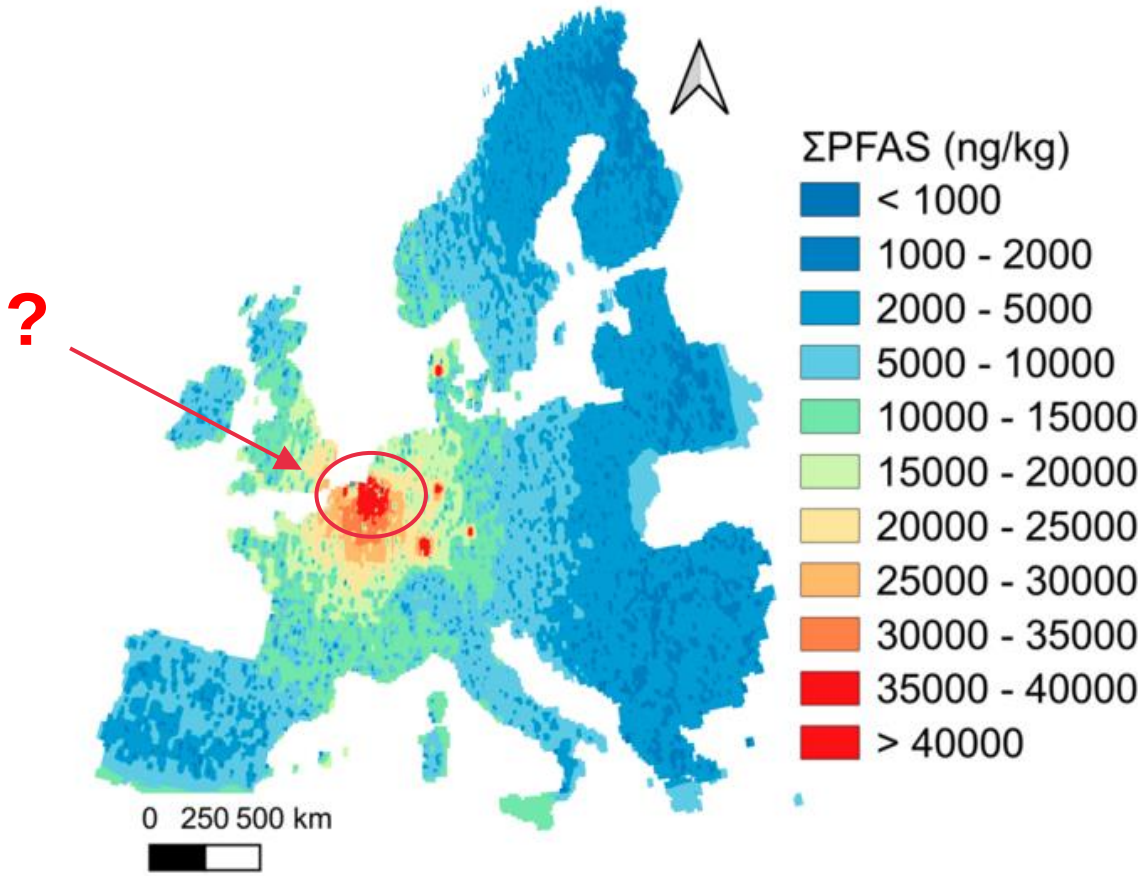


Figure 2. Geo-spatial map of predicted PFAS [∑PFAS (nanograms per kilogram)] concentrations in European soils. The different colors represent different PFAS soil concentrations.

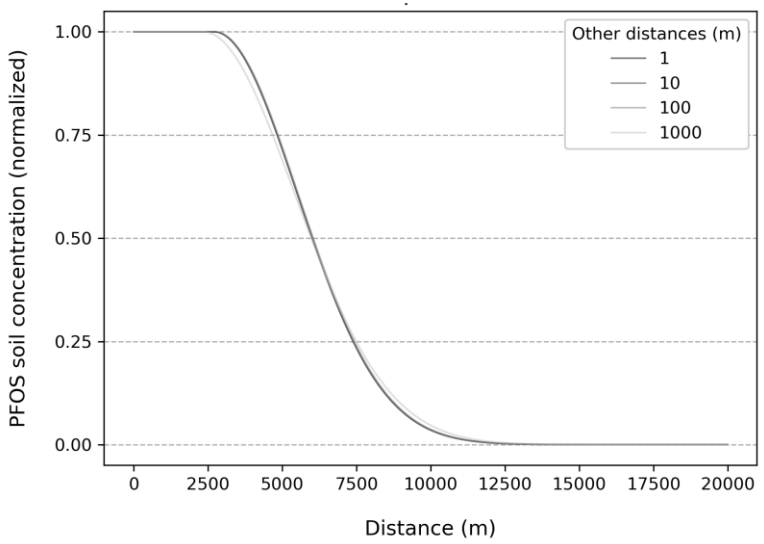
Moghadasi et al., 2023

https://doi.org/10.1021/acs.estlett.3c00633

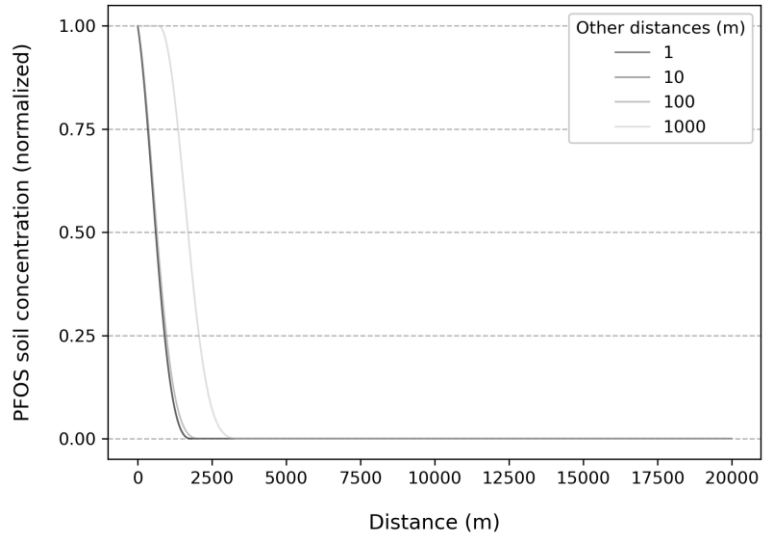
Modelled PFOS distance decay trends per SA type

These trends aren't necessarily representative for individual SA!

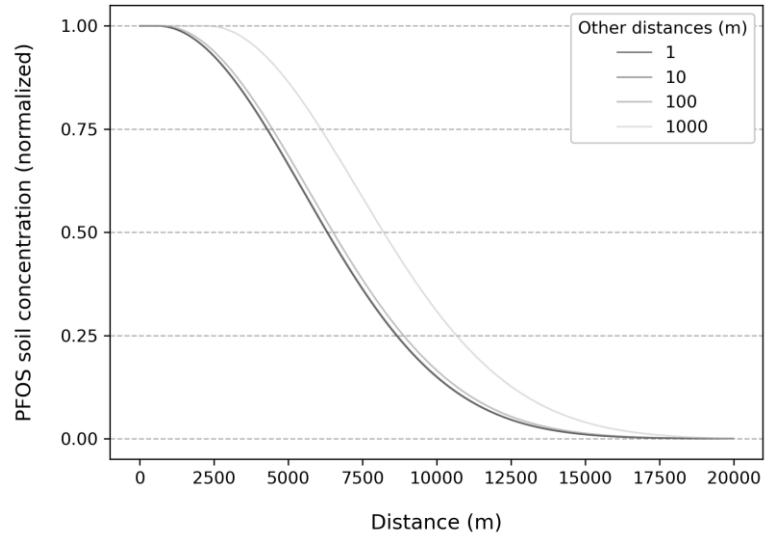
PFAS production



Firefighting



Paper and packaging



Conclusions and outlook

- The recent efforts of the Flemish, local governments and OVAM create potential for more data-driven PFAS policy support.
- The identified SA generally have elevated soil PFAS values within and around the grounds.
- We observe varying soil PFAS compositions and distance decay trends per SA type.
- Insights gained from regional analysis can support local applications.
- Some municipalities, SA types and PFAS substances still have limited data coverage.
- Envisioned model improvements: coastal & farmland, wind direction, elevation, soil types …

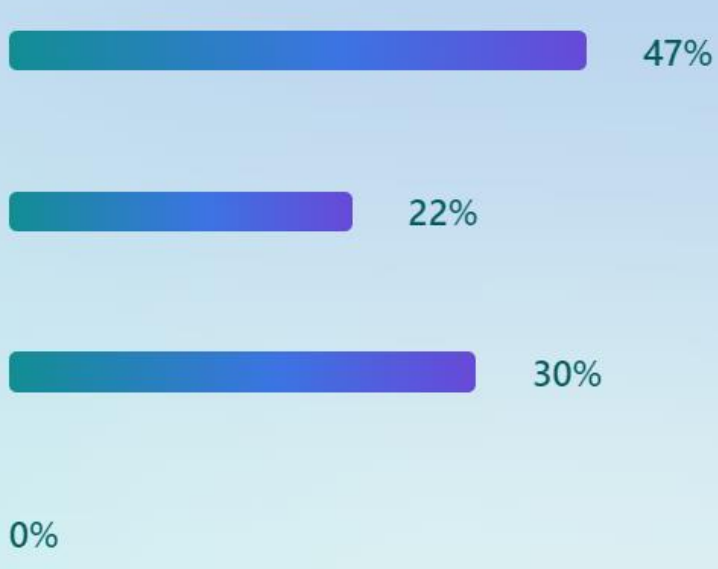
Scan the QR or use link to join

https://forms.office.com/e/sukerCj6wm

Copy link

18 responses submitted

Which of the following research outputs could be interesting for your work or organization?



1 of 2

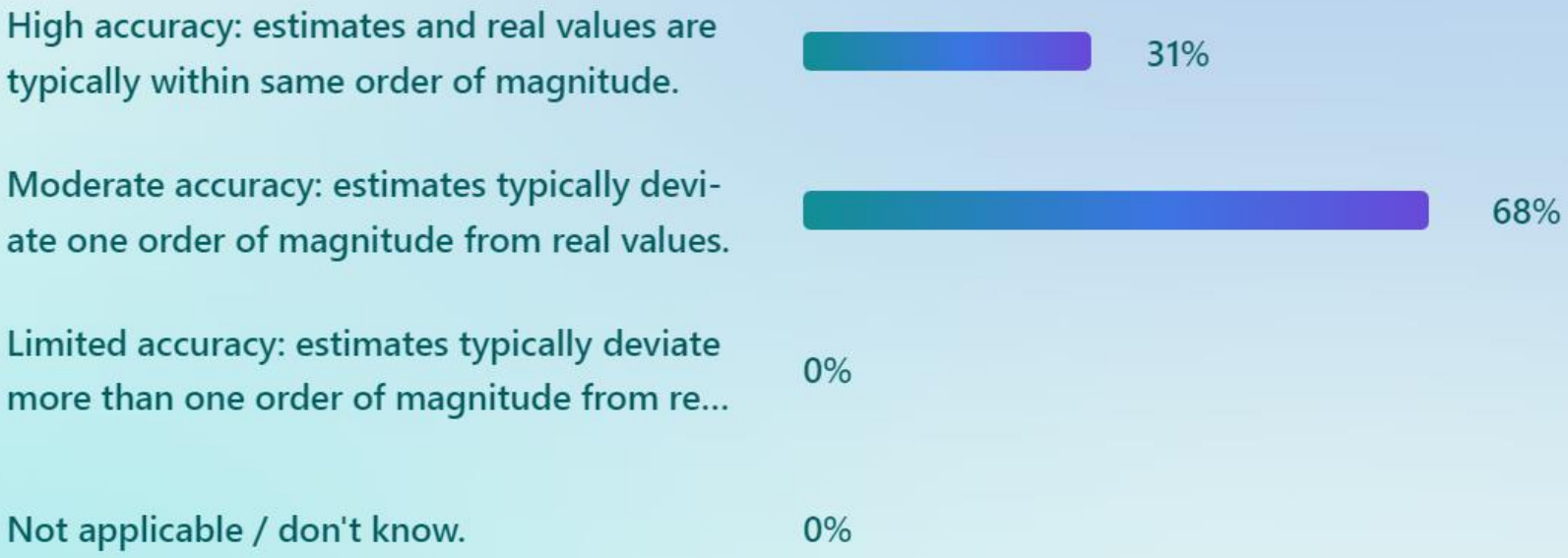
Scan the QR or use link to join

https://forms.office.com/e/sukerCj6wm

Copy link

18 responses submitted

At which level(s) of accuracy could PFAS soil concentration maps be useful for your work or organization?



2 of 2

vito

Take-away messages of this workshop

- Interpretation of diffuse soil pollution is very challenging and requires handling and integrating large numbers of diverse data from different sources.
- Comprehensive soil data management and increasing the spatial scale of analysis can help us to gain valuable insights.
- Lessons can be learned both on local and regional levels and can then be exploited back on parcel-level.
- More dialogue is needed to align probabilistic outputs of science with the stakeholders' need for clarity.

Thank you!

frederik.priem@vito.be

ward.swinnen@vito.be

ilse.vankeer@vito.be

karolien.vermeiren@vito.be