

Semi-Quantitative Direct-Push Data Can Improve Contaminant Delineation and Mass Discharge in Groundwater

Detector signals become a probability field that constrains where the contaminant plume is interpolated

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NIRAS

THE PROBLEM

Data is stranded

Advanced investigation methods are increasingly used in contaminated soil- and groundwater site investigations.

Hard to trust Heterogeneous geology, detection limits, temperature, calibration, background noise

Only used qualitatively For refining the conceptual model and guide sampling

The goal Utilize increased quantity, quality and resolution of data

- Integrate it directly into plume interpolation and contaminant mass discharge estimation — without overinterpreting it



BEFORE WE START

Risk assessment and POC

Concentrations at a point of compliance are compared with threshold values

- Basis of most risk assessment tools

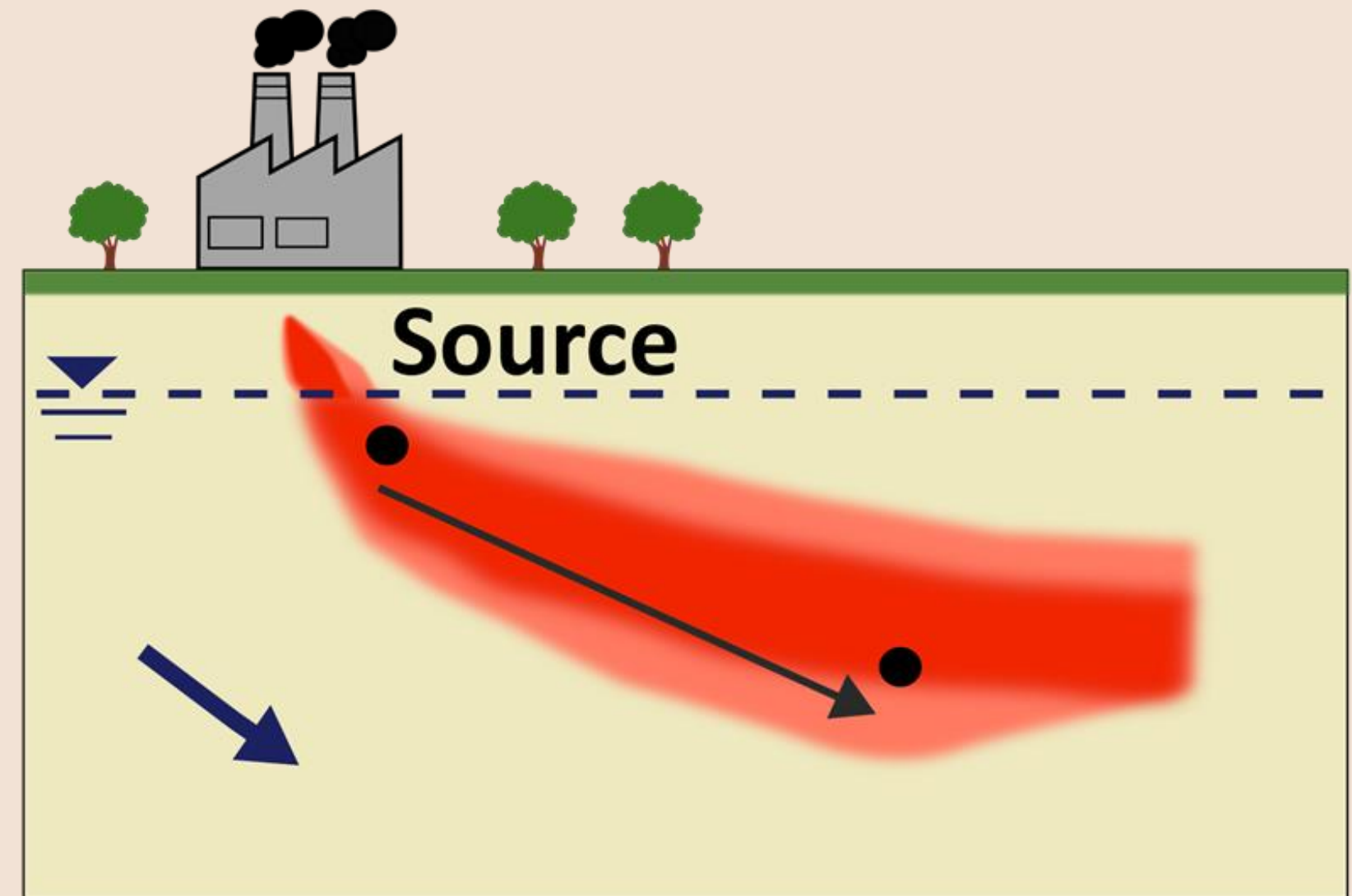
Fail to capture total mass of pollutant

- i.e. the volume of affected water

Contaminant Mass Discharge (CMD)

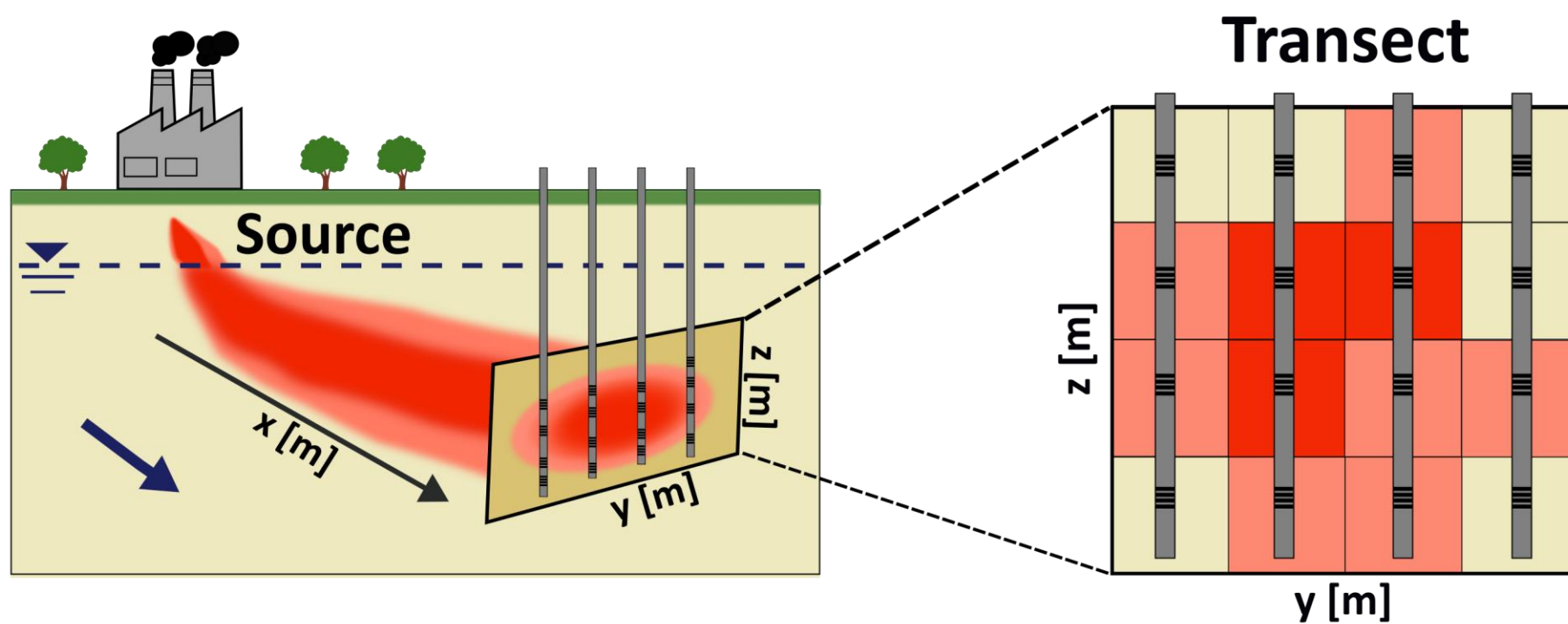
Combines contaminant concentration with groundwater flow

- Mass per time (e.g. kg/yr)
- Measure of the load on downgradient receptors



BACKGROUND

CMD: The transect method



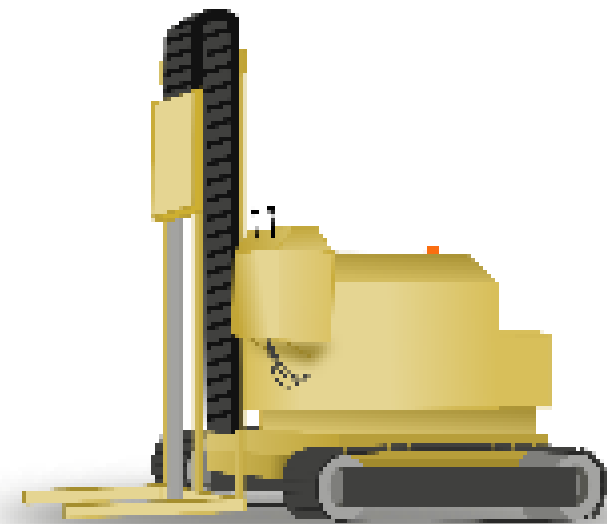
$$CMD = \sum_i C_i \cdot q_i \cdot A_i$$

C : concentration · q : Darcy flux · A : sub-area · i : index of the i -th sub-area

Uncertainty can be described with geostatistics — but the result still depends on number of samples

THE TOOL

MiHPT: Contamination and permeability in one push



Direct-push probing

Continuous, *in-situ* and cheap relative to drilling.

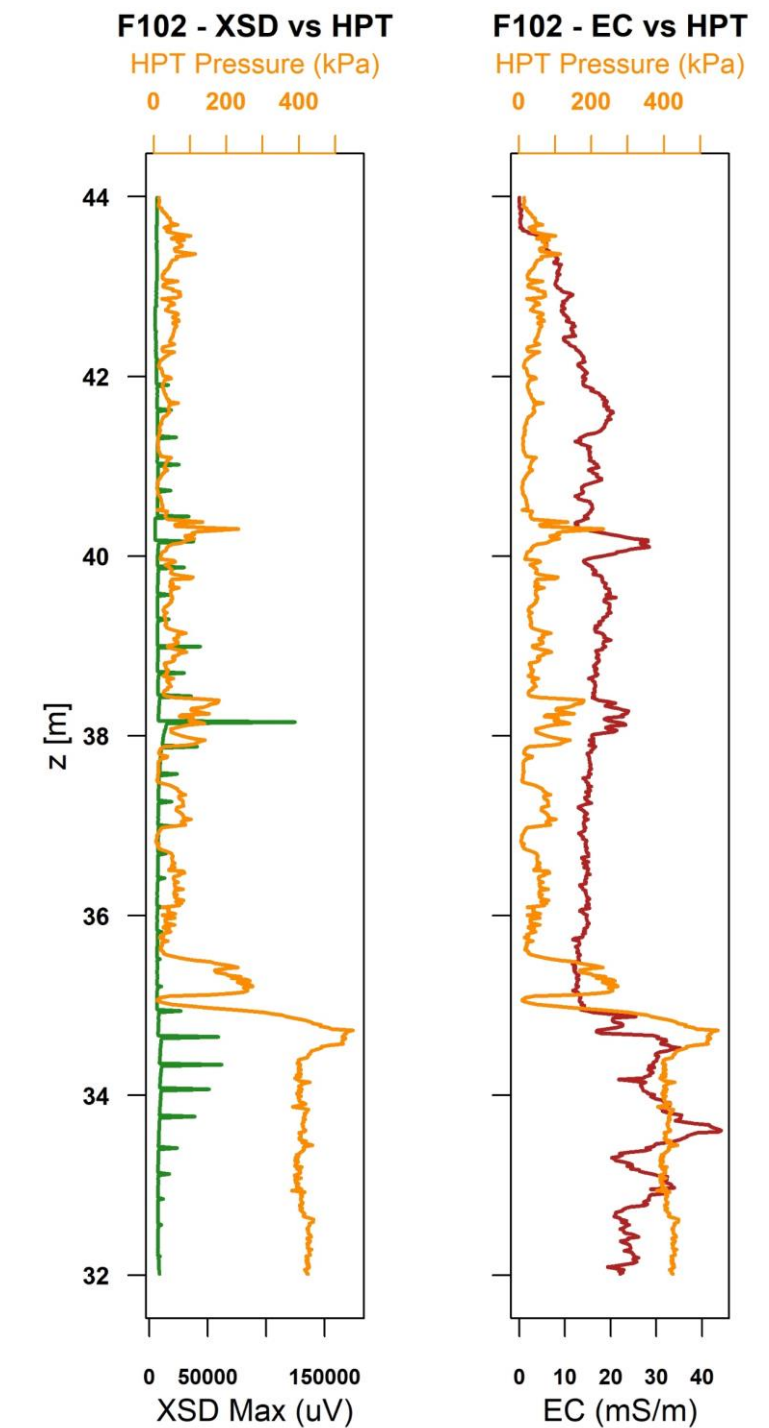
MIP

A *relative* response: Where there is contamination, roughly the magnitude — and, importantly, where there is none

HPT

Pressure needed to sustain flow into the formation.

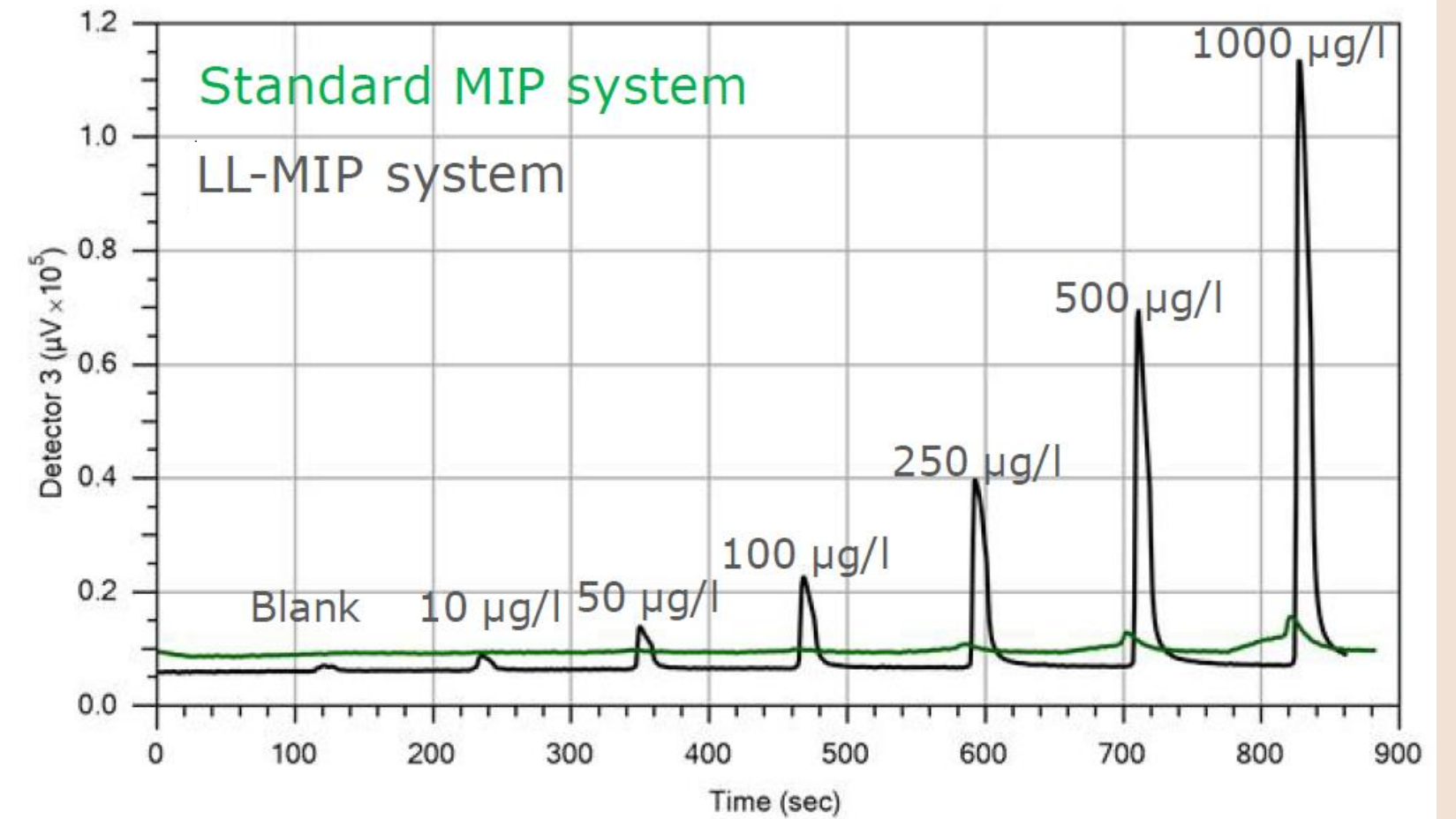
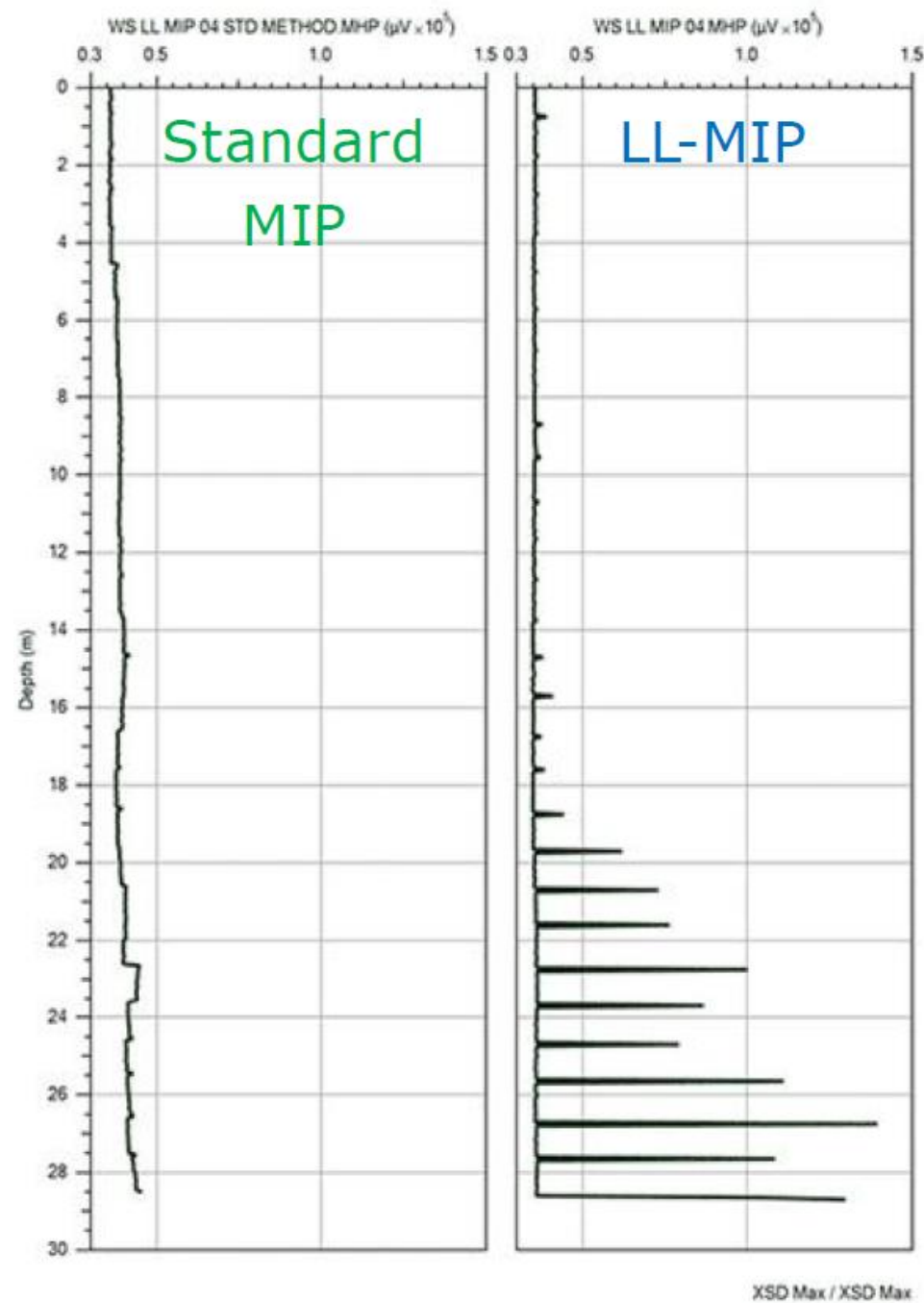
Sand = low pressure, clay = high pressure



THE TOOL

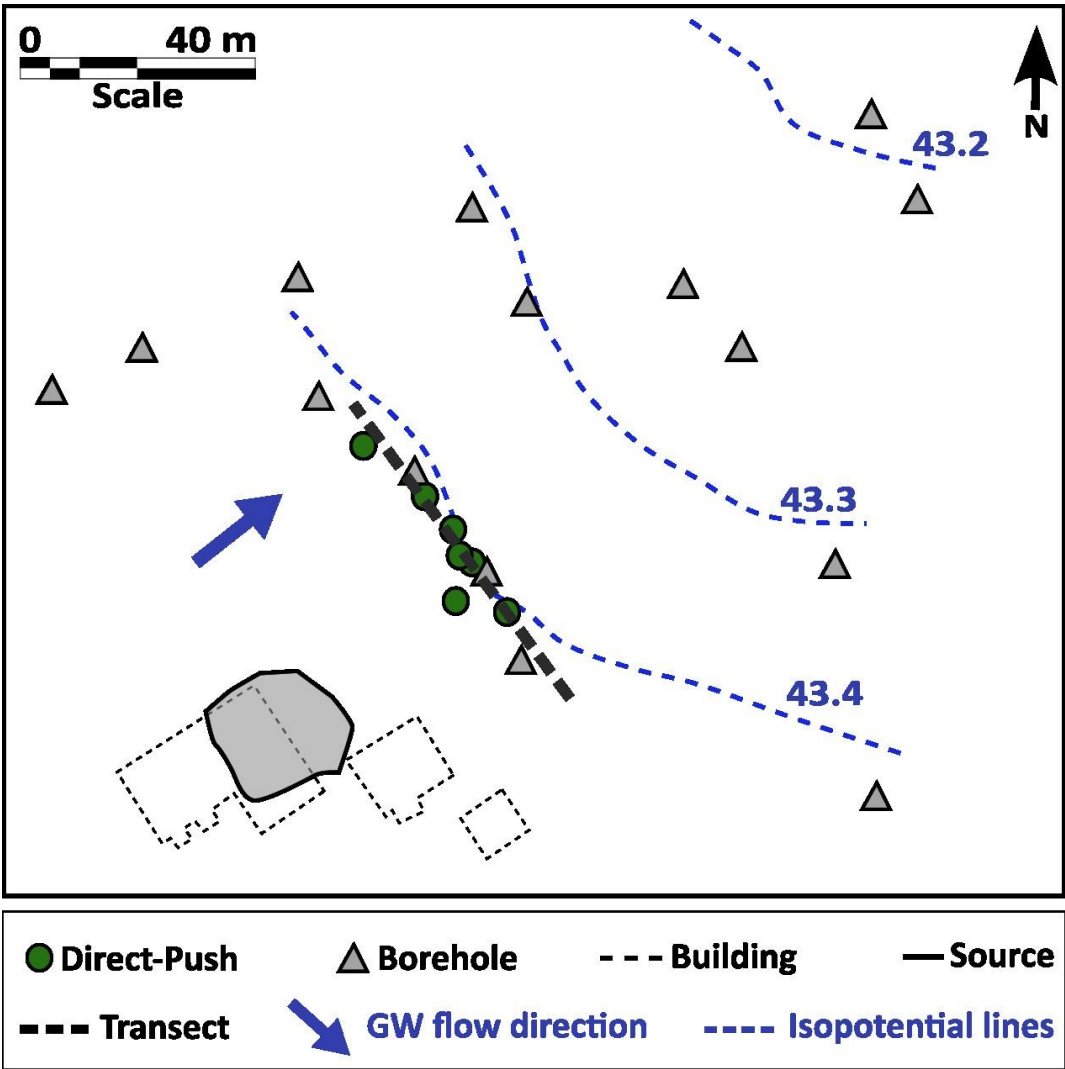
LL-MiHPT reaches low $\mu\text{g/L}$

Near-continuous logging every ~ 0.3 m, $10\text{--}50\times$ the sensitivity of standard MIP.



THE SITE

Håndværkervænget



Ongoing investigation

Complex geology, difficult fieldwork.
Soil, vapor and groundwater analysis

$>1500 \mu\text{g/L}$

TCE in the source zone
from old industry

2.8‰

Hydraulic gradient

40 m

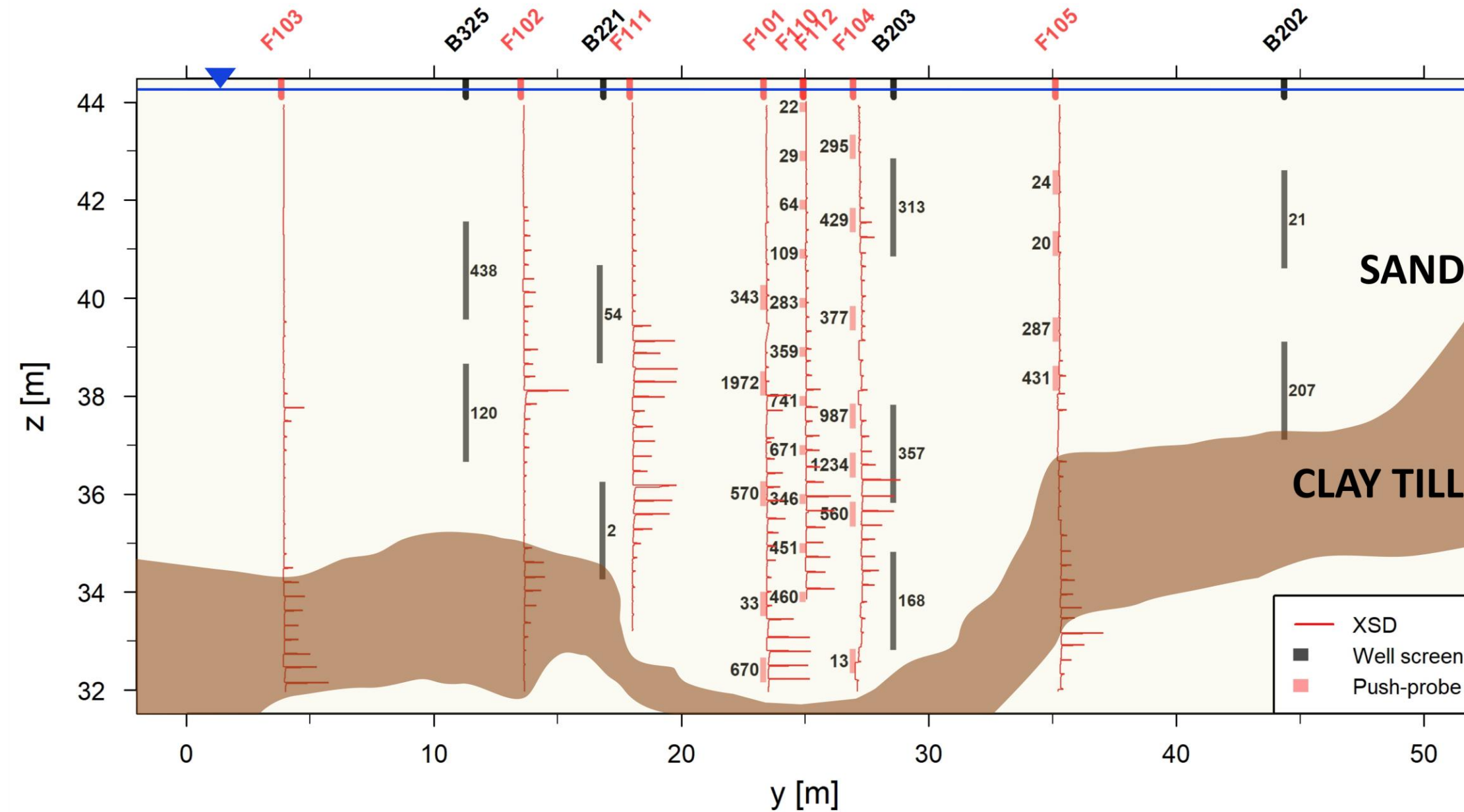
Transect downstream
of source

$4.3 \times 10^{-5} \text{ m/s}$

Geometric mean K ,
sandy aquifer

THE DATA

One transect, two datasets



9 Samples — small dataset, traditional wells only

36 Samples in total — large dataset, wells and push-probe

232 XSD signals from seven logs, ~ 0.3 m spacing

STEP 1 · ONE STEP BACK

Yes or no

$I = 1$ if $XSD > XSD_{lim}$
 $I = 0$ otherwise

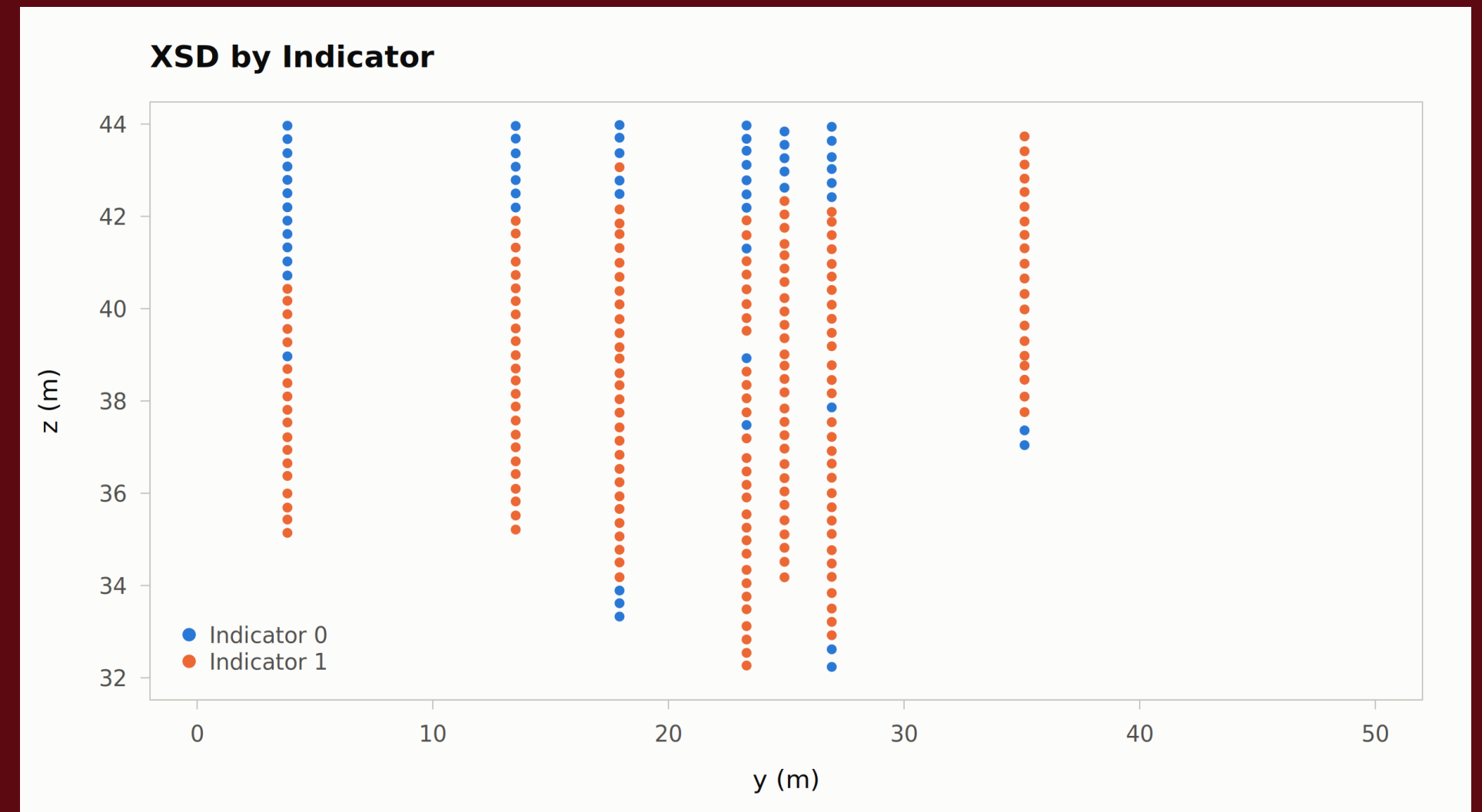
Signals are normalised to each probe's background noise.

- $XSD_{lim} \approx 2$ mV, from blanks against a $10 \mu\text{g/L}$ TCE standard.

Direct correlation to concentration is unreliable.

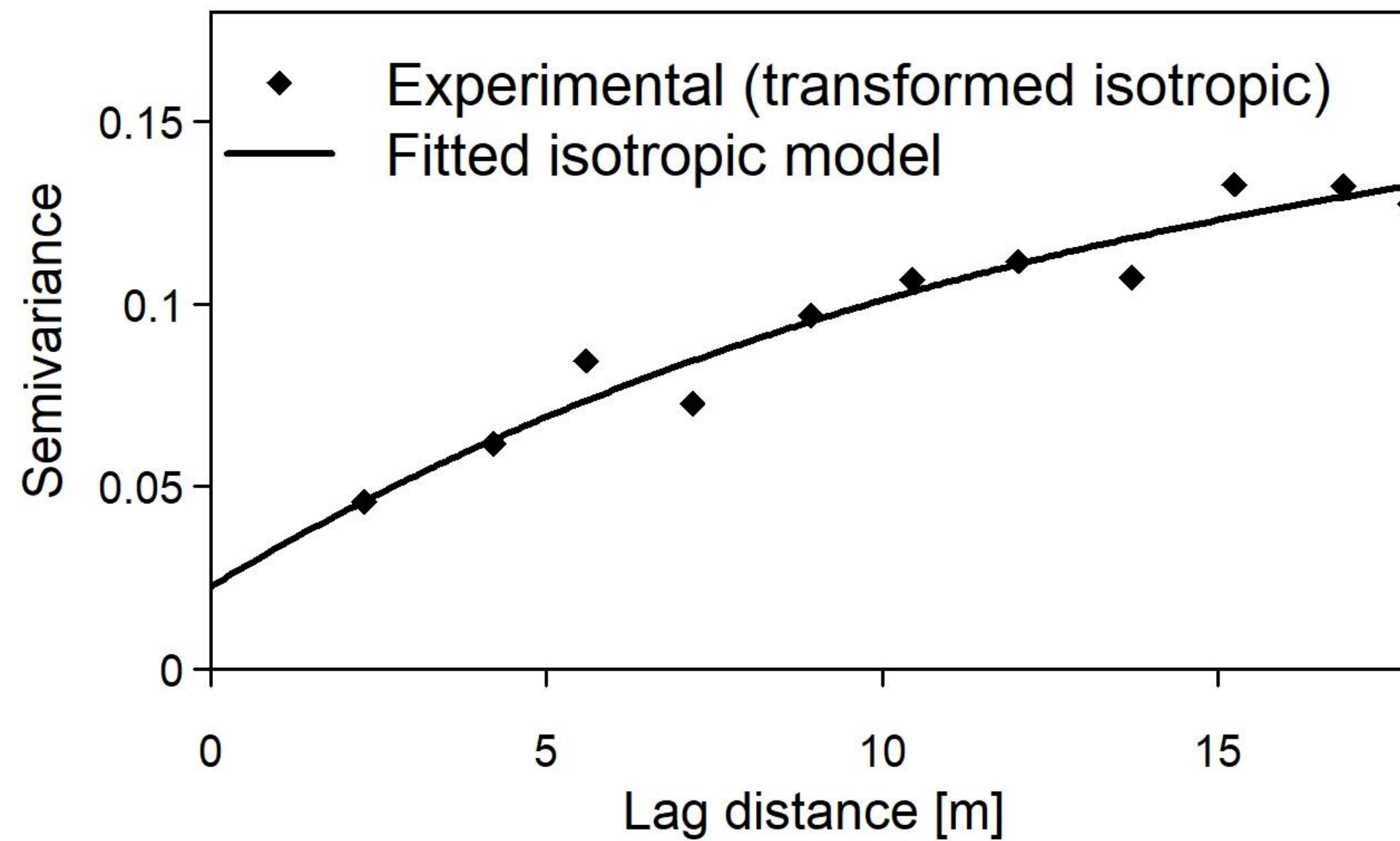
- We do not trust the size of the signal — only whether contamination is there.

Conservative by design: a non-detection is trusted, a high signal is not quantified.



STEP 2 · SPATIAL STRUCTURE

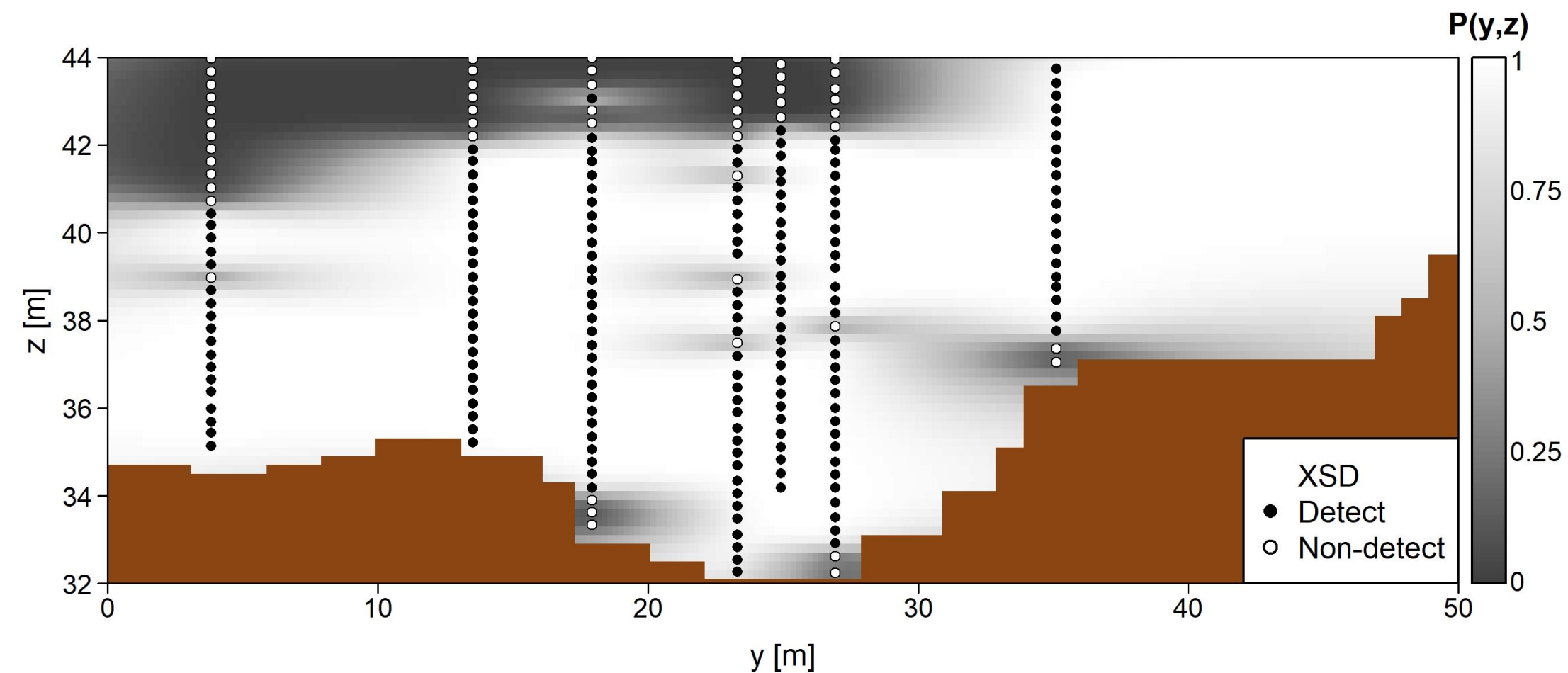
Contaminant presence is spatially correlated



STEP 3 · INDICATOR KRIGING

Where is contamination likely?

Areas far from XSD data defaults to probability 1 and nothing is censored → Unsampled areas stay fully uncertain.



High-probability core

$P = 0.75\text{--}1.0$ through the central parts of the aquifer, matching observed concentrations.

Upper-left area

A connected $P < 0.25$ region with no groundwater samples, the gap XSD-signals fills.

Non-detections at depth

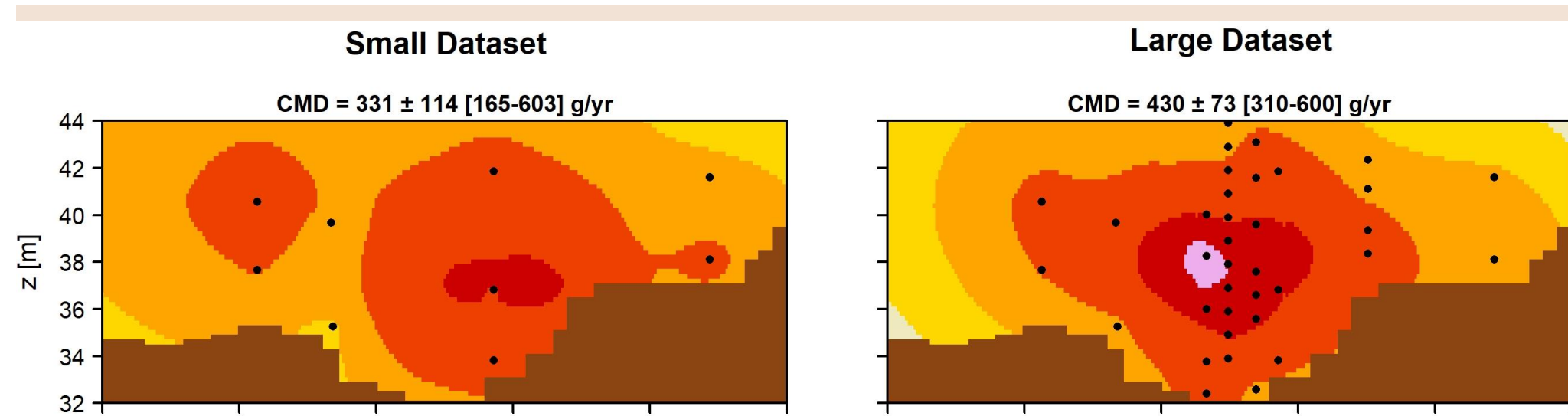
Non-detects above the clay till create thin, flat low-probability lenses — short vertical correlation keeps them confined to the base.

The probability field masks the plume

The corrected concentration is the interpolated value with probability P

$P \rightarrow 1$	Detections nearby, or no XSD data. Interpolated plume is sustained.
$P \rightarrow 0$	Consistent non-detections. Concentration suppressed toward zero.
Ensemble	22,500 simulations per dataset on a 0.2×0.2 m grid Full CMD distribution

P is bounded 0–1, so censoring can only reduce a CMD estimate. It corrects overestimation but never adds mass.



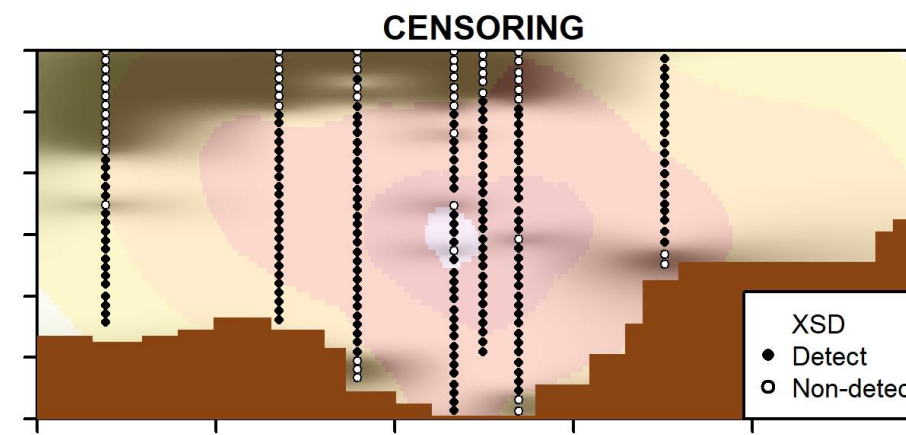
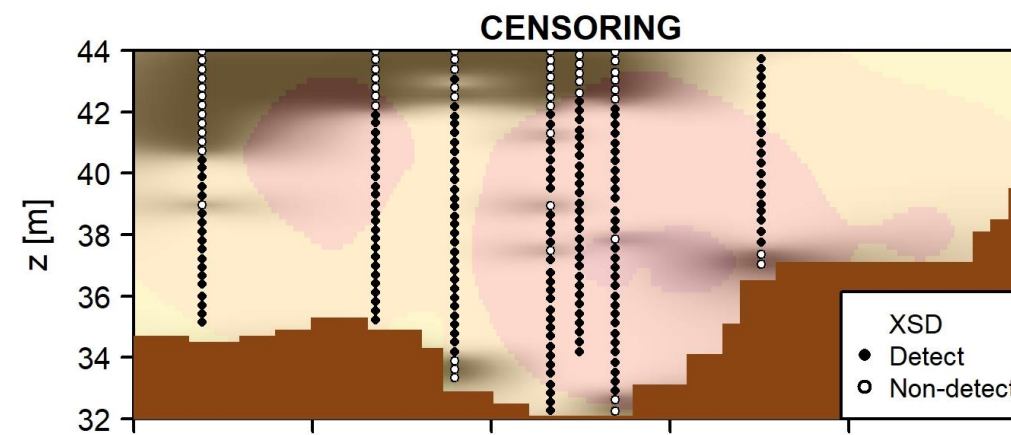
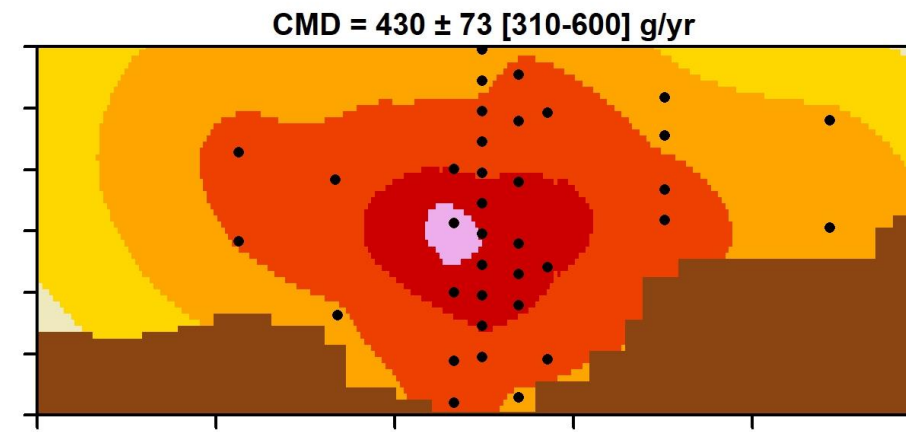
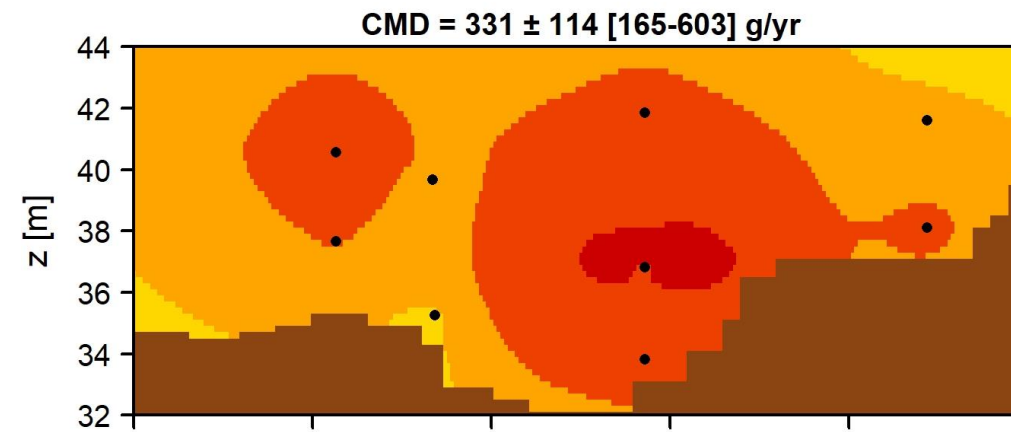
RESULTS · INTERPOLATION

Fringes sharpen, the core remains

Neither uncensored field has a clear plume boundary.

Small Dataset

Large Dataset



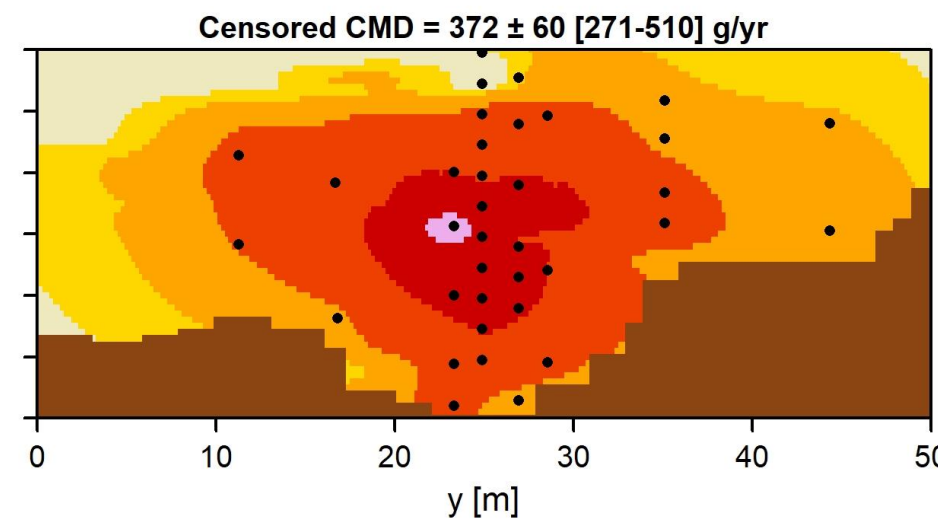
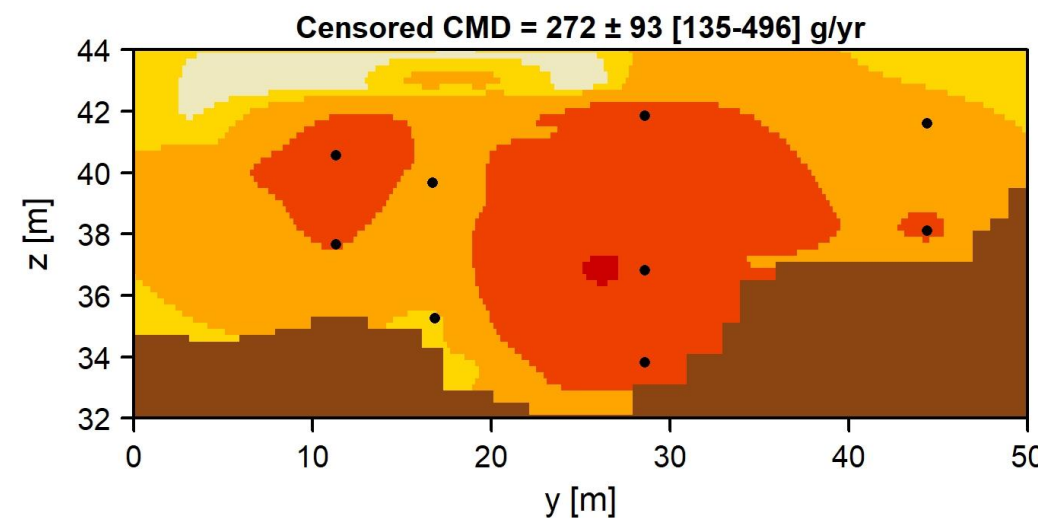
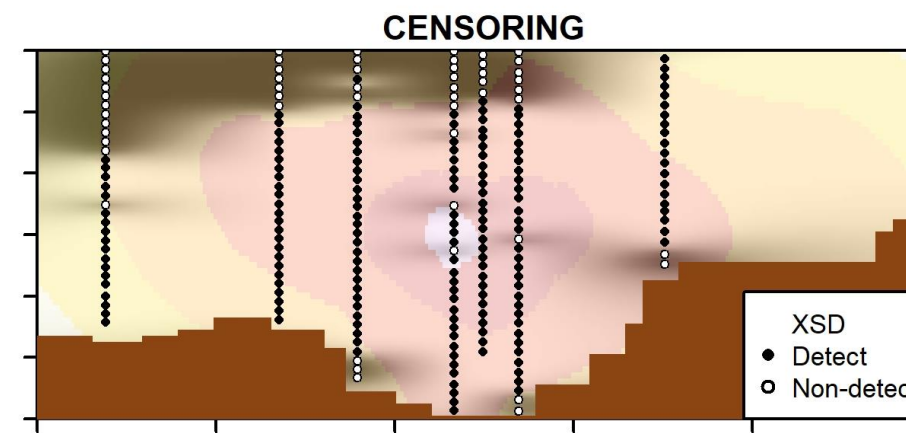
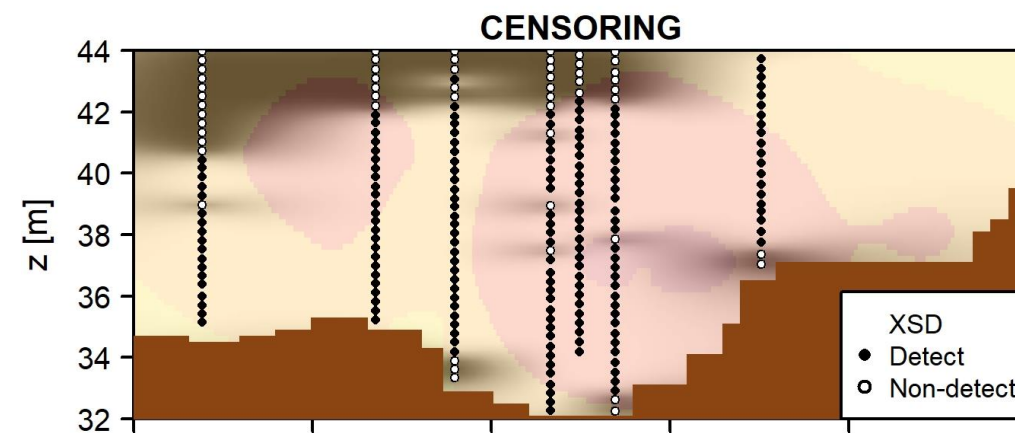
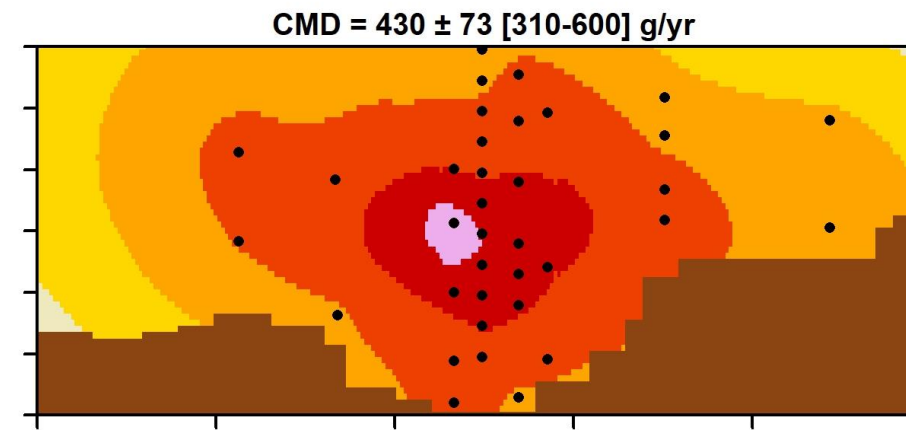
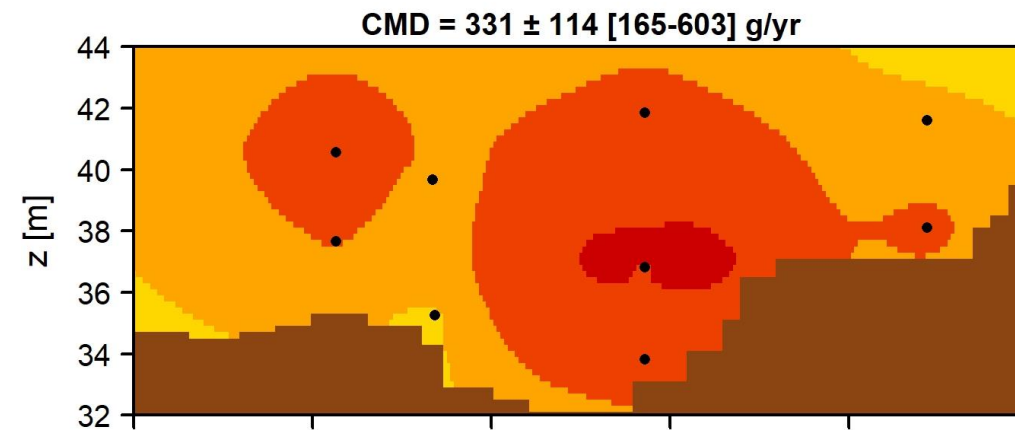
RESULTS · INTERPOLATION

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Small Dataset

Large Dataset



RESULTS · INTERPOLATION

Fringes sharpen, the core remains

Neither uncensored field has a clear plume boundary. Censoring acts as a boundary constraint but does not change the plume core.

+85% area below $10 \mu\text{g/L}$, small dataset (72 $\rightarrow$ 133 m^2)

+41% area below $10 \mu\text{g/L}$, large dataset (140 $\rightarrow$ 198 m^2)

RESULTS · CONTAMINANT MASS DISCHARGE

CMD decrease 13–18%, relative uncertainty unchanged

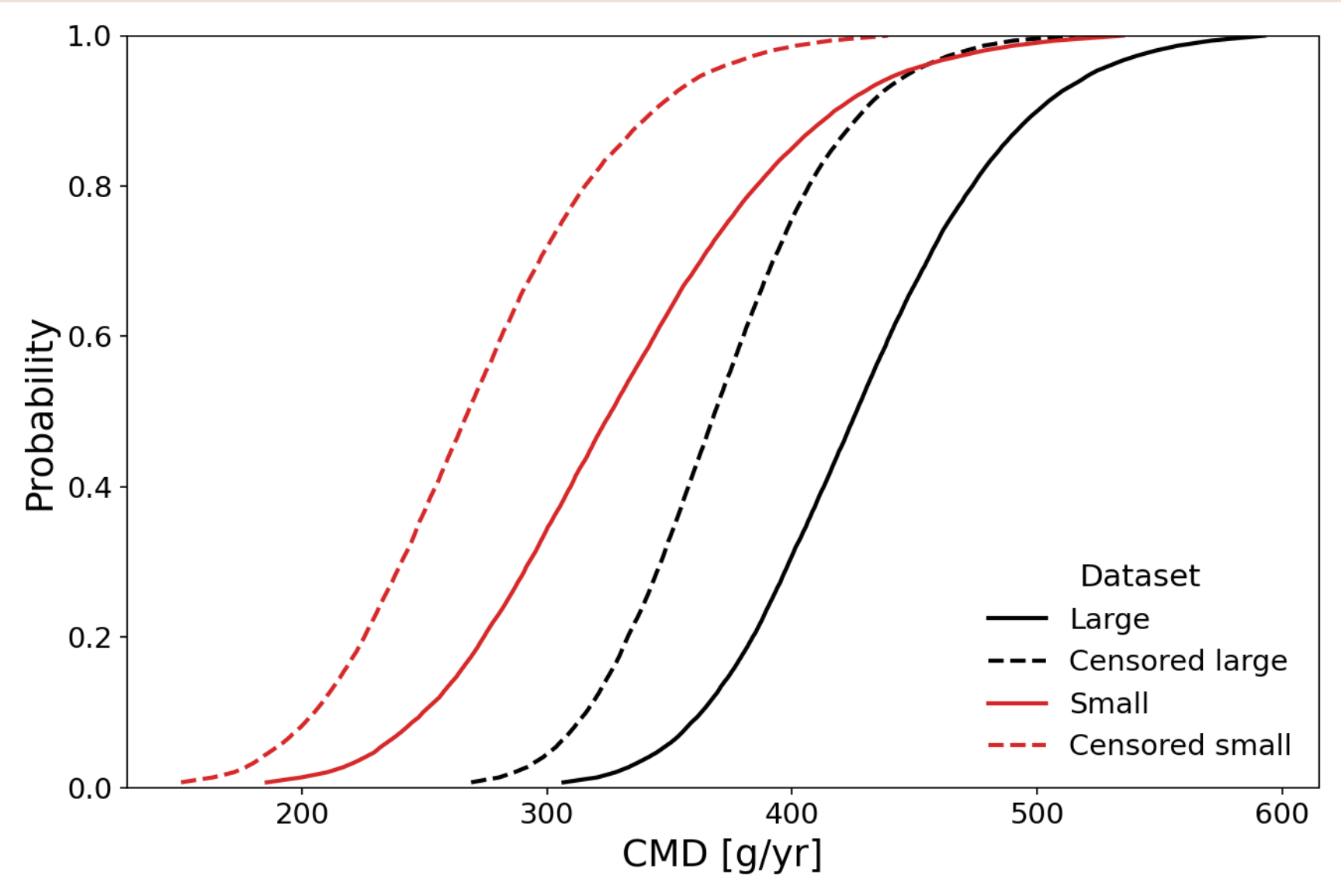
DATASET	MEAN CMD	95% CI G/YR	REL. UNC.
Large (36 samples)	430	310–600	17.0%
Censored large	372 (–13.5%)	271–510	16.1%
Small (9 samples)	331	165–603	34.4%
Censored small	272 (–17.8%)	135–496	34.2%

Sparser data, larger effect

Censoring is most effective where spatial support is weakest.

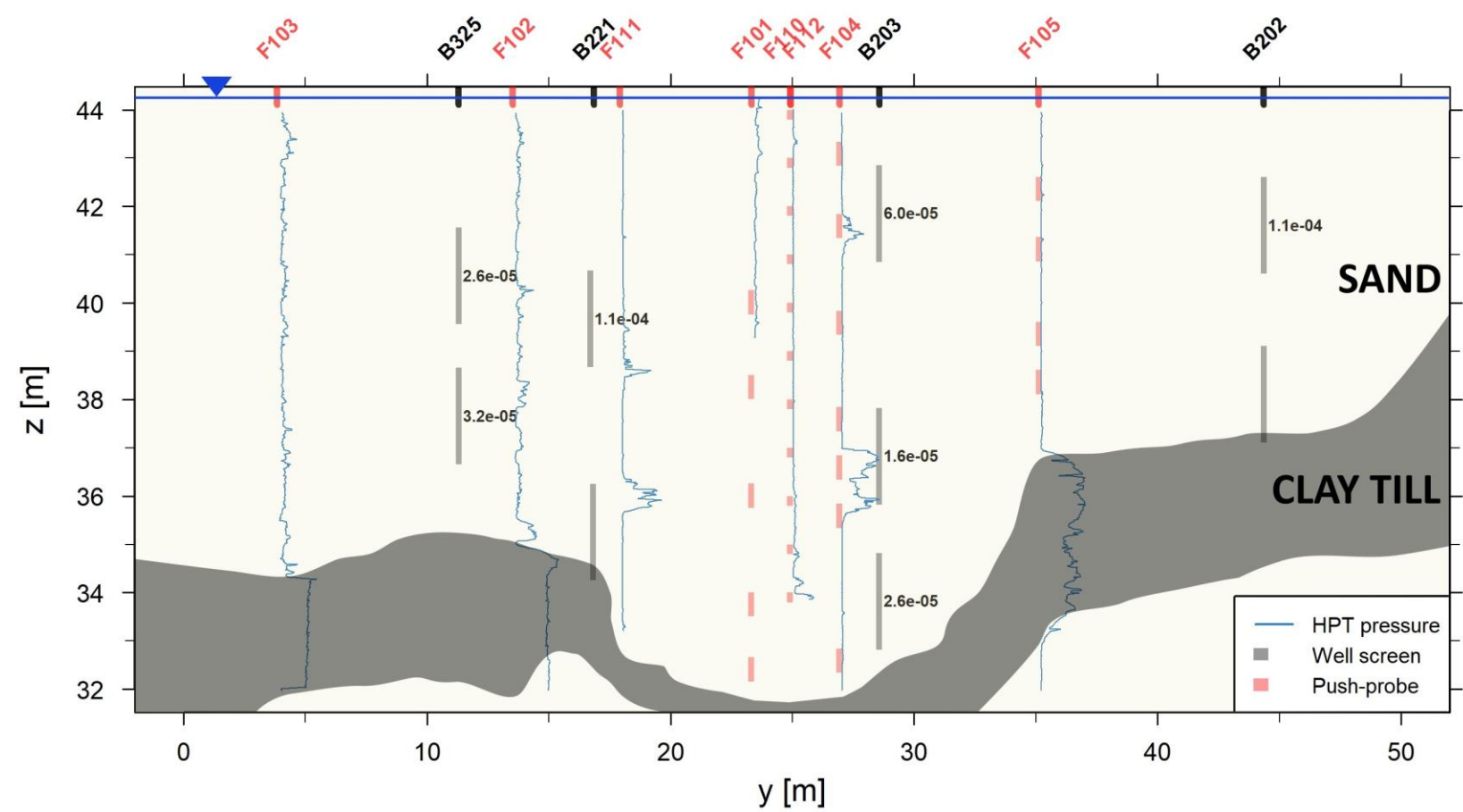
Not a narrower interval

Absolute CIs decrease; relative uncertainty does not. Uncertainty is driven by the plume centre.

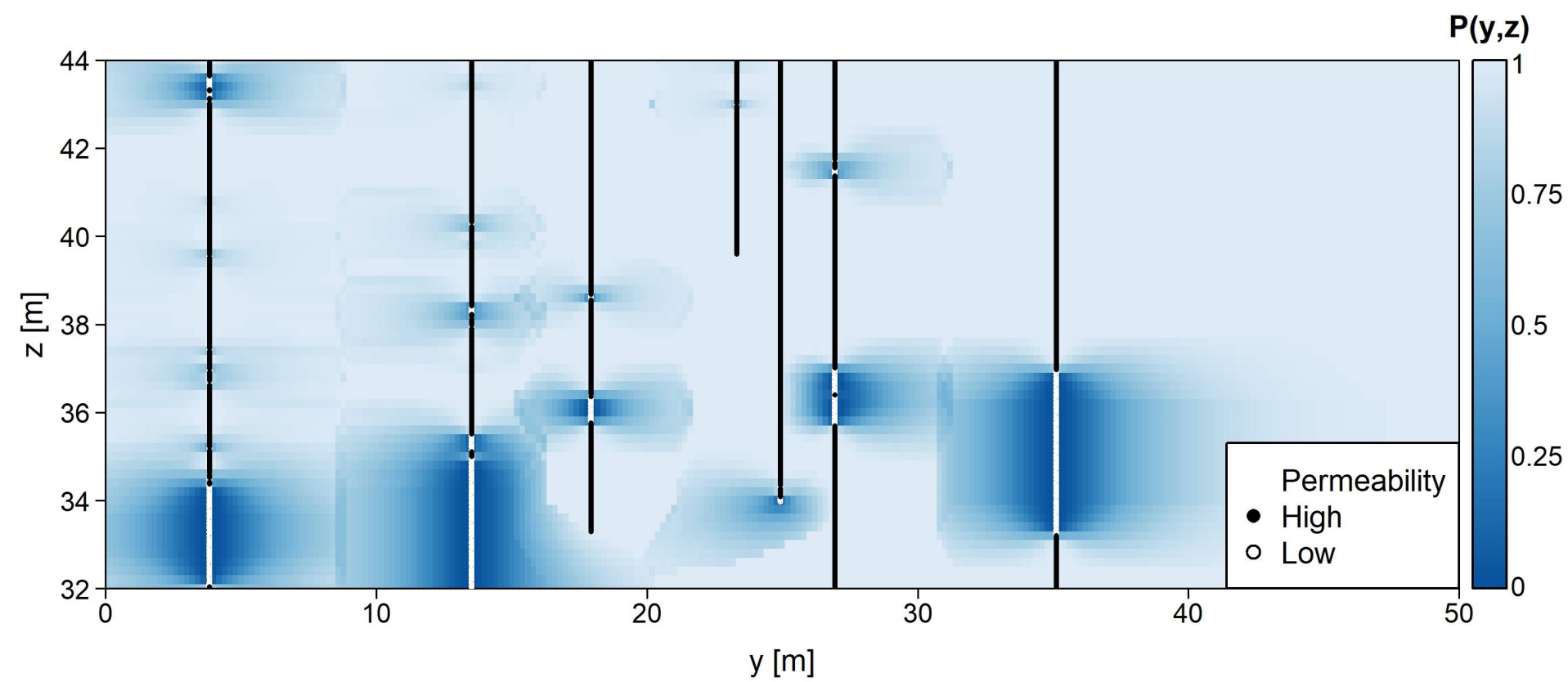


RESULTS · TRANSFERABILITY

It also works on HPT and K



A coarse K -field from slug tests is overlaid with the relative permeability indication from HPT pressure, capturing low-permeability zones slug tests fail to capture



TAKEAWAYS

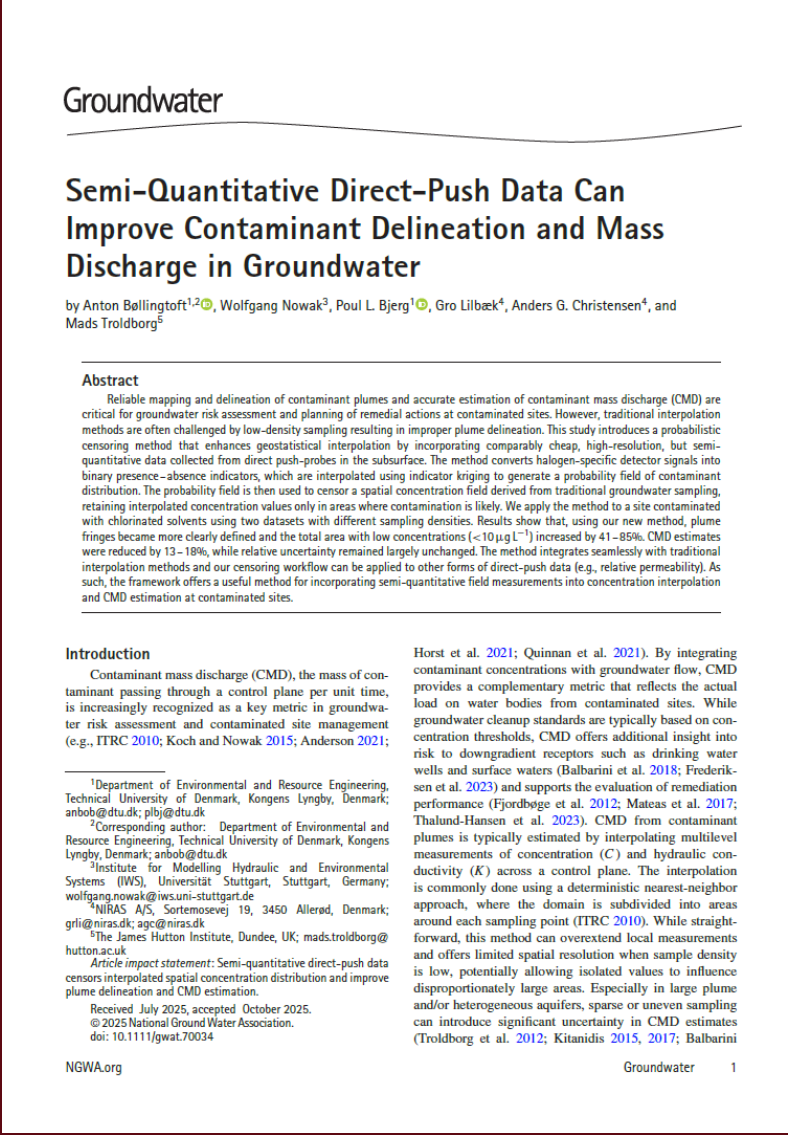
Semi-quantitative data improves site investigations

- 01 Data driven: spatial information from soft data, used without overinterpretation.
- 02 Integrated directly into plume interpolation, not just the conceptual model.
- 03 Improved plume delineation and a better-supported CMD estimate.
- 04 Standard geostatistical tools, modest preprocessing, developed on a real site.
- 05 Transferable to other soft data (e.g. HPT) and to other purposes.

The detection limit is a key step: it simplifies the signal but determines where contamination is confidently detected. Field-specific limits, lowered where possible, would improve the indicator classification

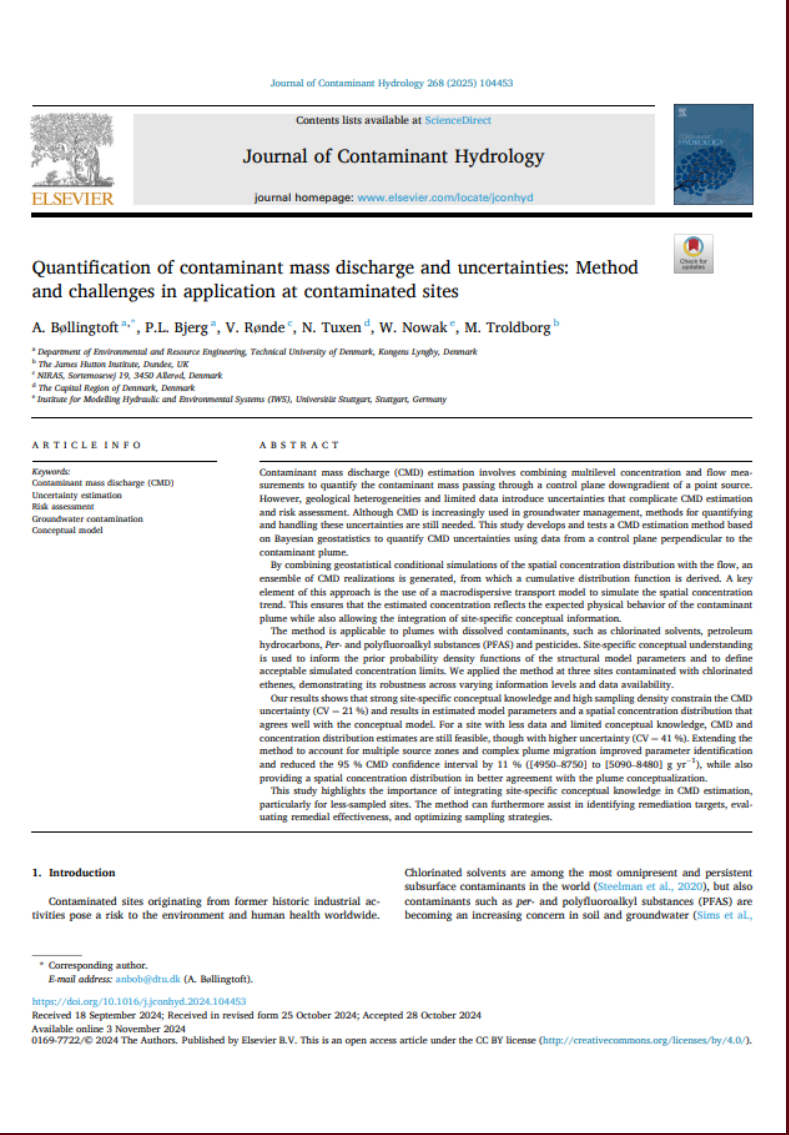
CURIOUS?

Semi-quantitative data



<https://doi.org/10.1111/gwat.70034>

Geostatistical method



<https://doi.org/10.1016/j.jconhyd.2024.104453>



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- Louise Rosenberg and Henriette Kerrn-Jespersen from the Capital Region of Denmark for access to the site
- Bettina Olsen from DMR for interpretation of the site data

Funding provided by the Capital Region of Denmark and DTU Sustain at the Technical University of Denmark

Geostatistical CMD-estimation method is published as open-source:

Code for Contaminant Mass Discharge Quantification and Uncertainty Estimation in Groundwater

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citations

Is supplement to

[Quantification of contaminant mass discharge and uncertainties: Method and challenges in application at contaminated sites](#)

Is supplement to

[Application of Bayesian geostatistics for evaluation of mass discharge uncertainty at contaminated sites](#)

DTU Data

- a service from DTU Library

This software analyses the spatial variability of multilevel concentration data from a transect located downstream of a contaminated site.

This is version 1.0 of the software.

It uses a geostatistical framework to estimate the contaminant mass discharge (CMD) and its uncertainty. The method is published and described in detail in Bøllingtoft et al. (2025) and is a continuation of the work originally published by Trolborg et al. (2012).

The method combines:

- An analytical trend model (Domenico & Palciauskas, 1982) to estimate the mean concentration field and generate concentration residuals which are then transformed used Box-Cox transformation
- Bayesian model parameter calibration using Markov-Chain-Monte-Carlo (MCMC) is used to determine the best fit of variogram, transformation and analytical trend model parameters
- These residuals are then used for spatial simulation via kriging and conditional simulation

The code is modular and designed for practitioners working with subsurface contaminant data.

<https://doi.org/10.11583/DTU.29891264>

The logo for the Technical University of Denmark (DTU), consisting of the letters "DTU" in a bold, sans-serif font above a stylized graphic of three horizontal, overlapping, curved shapes.

The logo for NIRAS, featuring the word "NIRAS" in a bold, sans-serif font with a stylized graphic element above the "A" that resembles a curved line or a stylized letter "N".