

Kan semikvantitative data udnyttes bedre ifm. forureningsundersøgelser?

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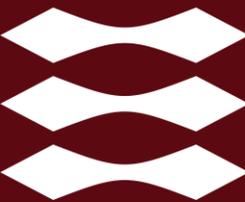
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ATV Vintermøde – Marts 2026

DTU



NIRAS

Semi-kvantitative data

Avancerede undersøgelsesmetoder anvendes i stigende grad ifm. forureningsundersøgelser

- Geofysik, Direct-push sonderinger (Geoprobe), droner ...
- Højt-opløseligt 'bløde' data → *semi-kvantitativt*
- *Et supplement*

Svært at korrelere til 'almindelige' parametre

- Heterogen geologi
- Detektionsgrænser
- Temperatur
- Kalibrering af sensorer
- Baggrundsstøj
- Osv.

Anvendes typisk *kvalitativt*

- Konceptuel model og guide prøvetagning

Et uforløst potentiale – Data 'strander'

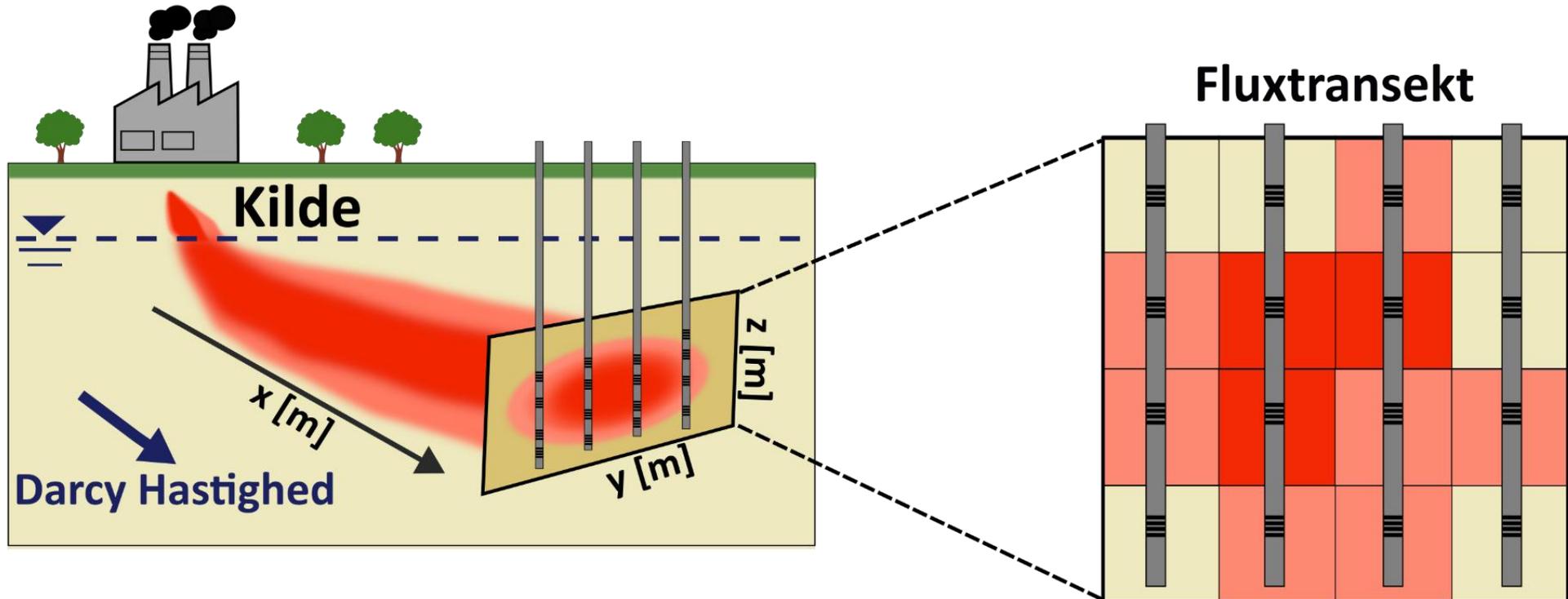


Forureningsflux – Transektmetoden

- Masse pr. tid (fx. kg/år)
- Et transekt opdeles i 'kasser' der tilegnes hhv. C , i og K
- Usikkerheden kan beskrives vha. *geostatistik*

C : Forureningskoncentration
 A : Areal
 q : Darcy flux
 i : Index som beskriver the i^{te} delareal

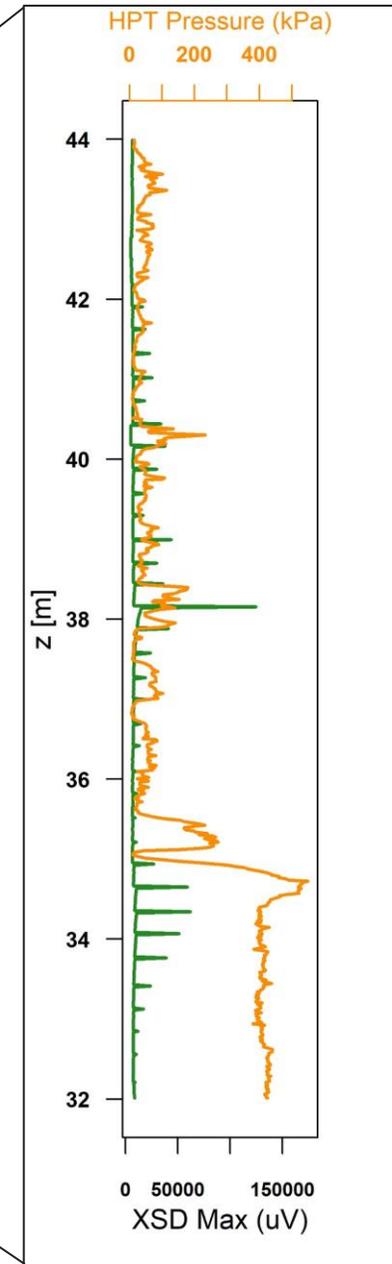
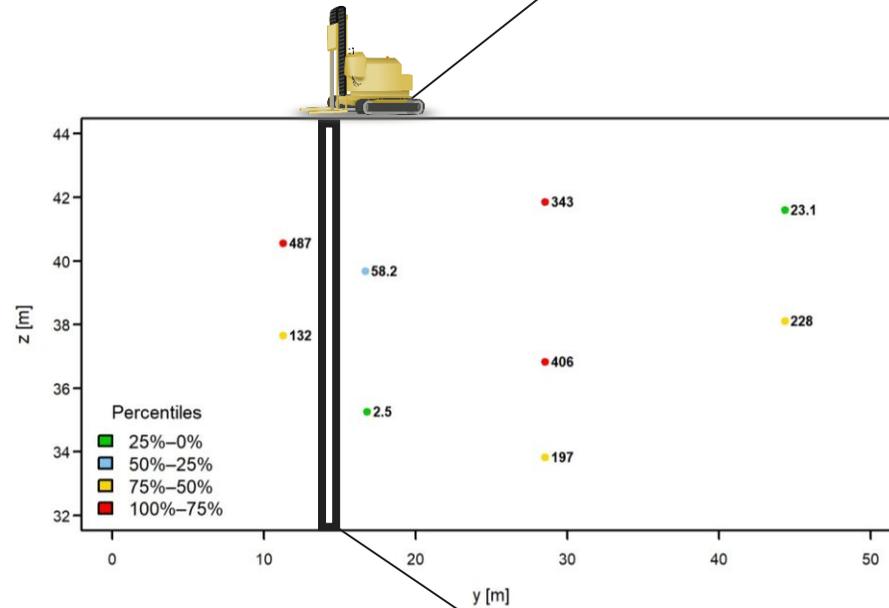
$$J = \sum_{i=1}^n C_i \cdot A_i \cdot q_i$$



Direct-push: MiHPT

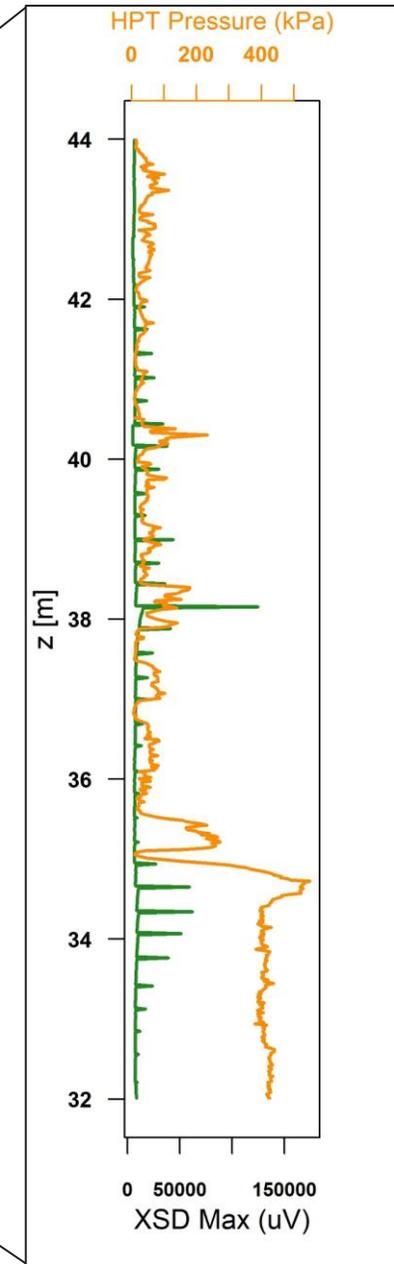
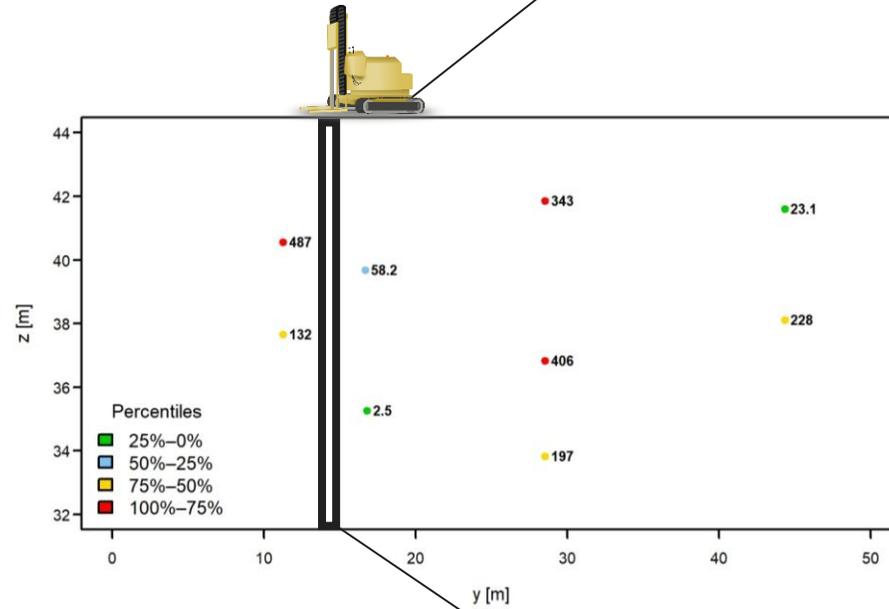
- Membrane Interface Probe (MIP) with Hydraulic Profiling Tool (HPT)
- Direct push sondering → kontinuerlige data, måling *in-situ*
- MIP: Hvor og hvor meget forurening
 - Samt hvor er den *ikke*
 - *Relativ* respons på koncentration
- HPT tryk: Det nødvendige tryk for at opretholde strømning af vand ud i formationen

Sand = lavt tryk
Ler = højt tryk



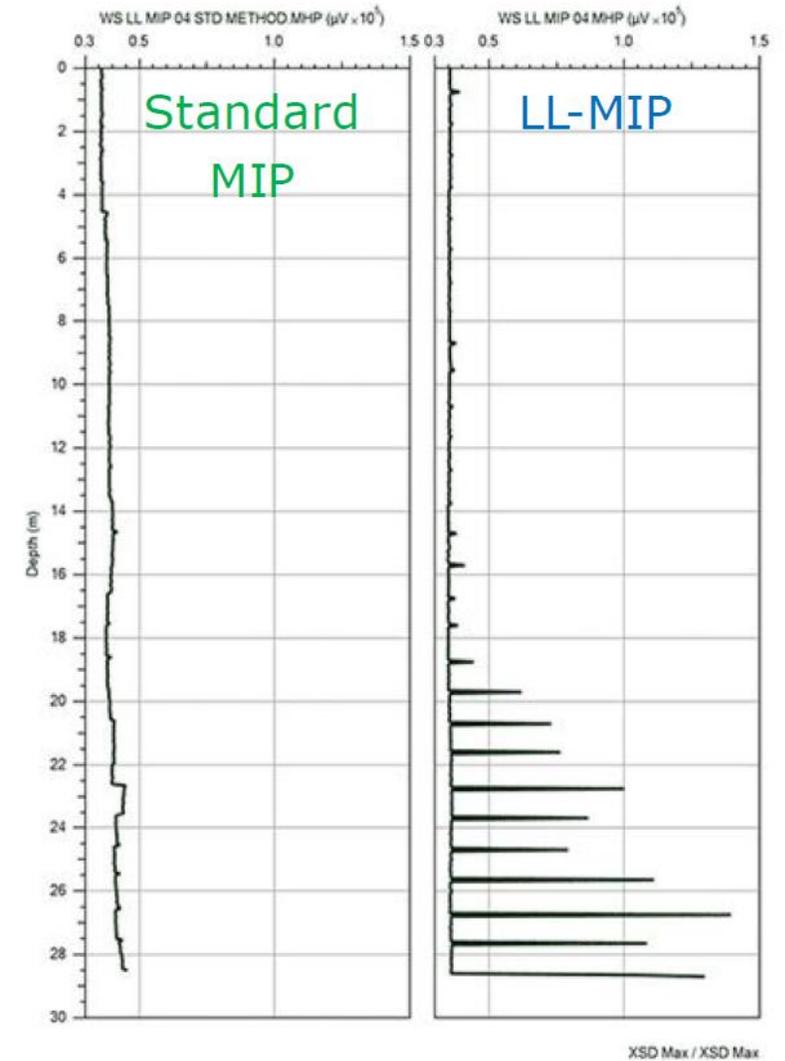
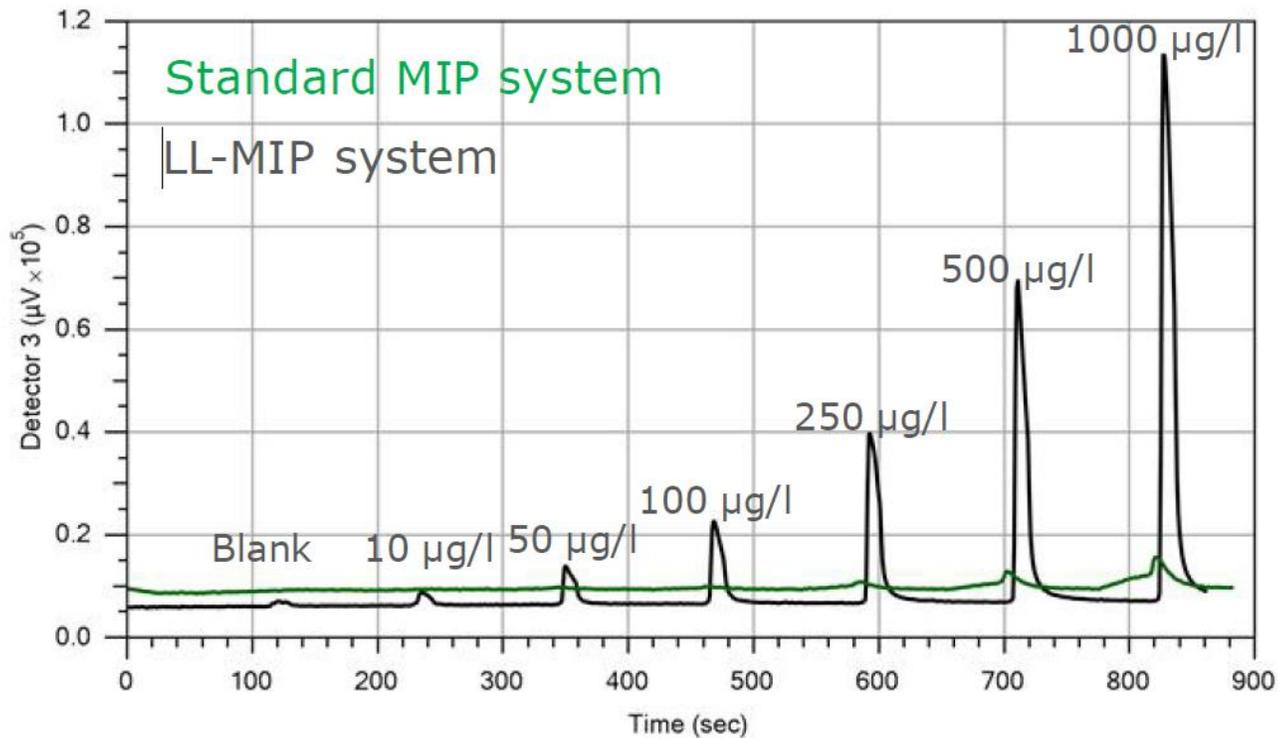
Direct-push: MiHPT

- Mængden, kvaliteten og opløsningen af data stiger
- Udnytte dette systematisk vha. mere avancerede metoder
 - Eksempelvis geostatistik
- Integrere semi-kvantitative data direkte i 'almindelige' forureningsundersøgelser
 - Interpolation af forureningsfane eller grundvandsstrømning



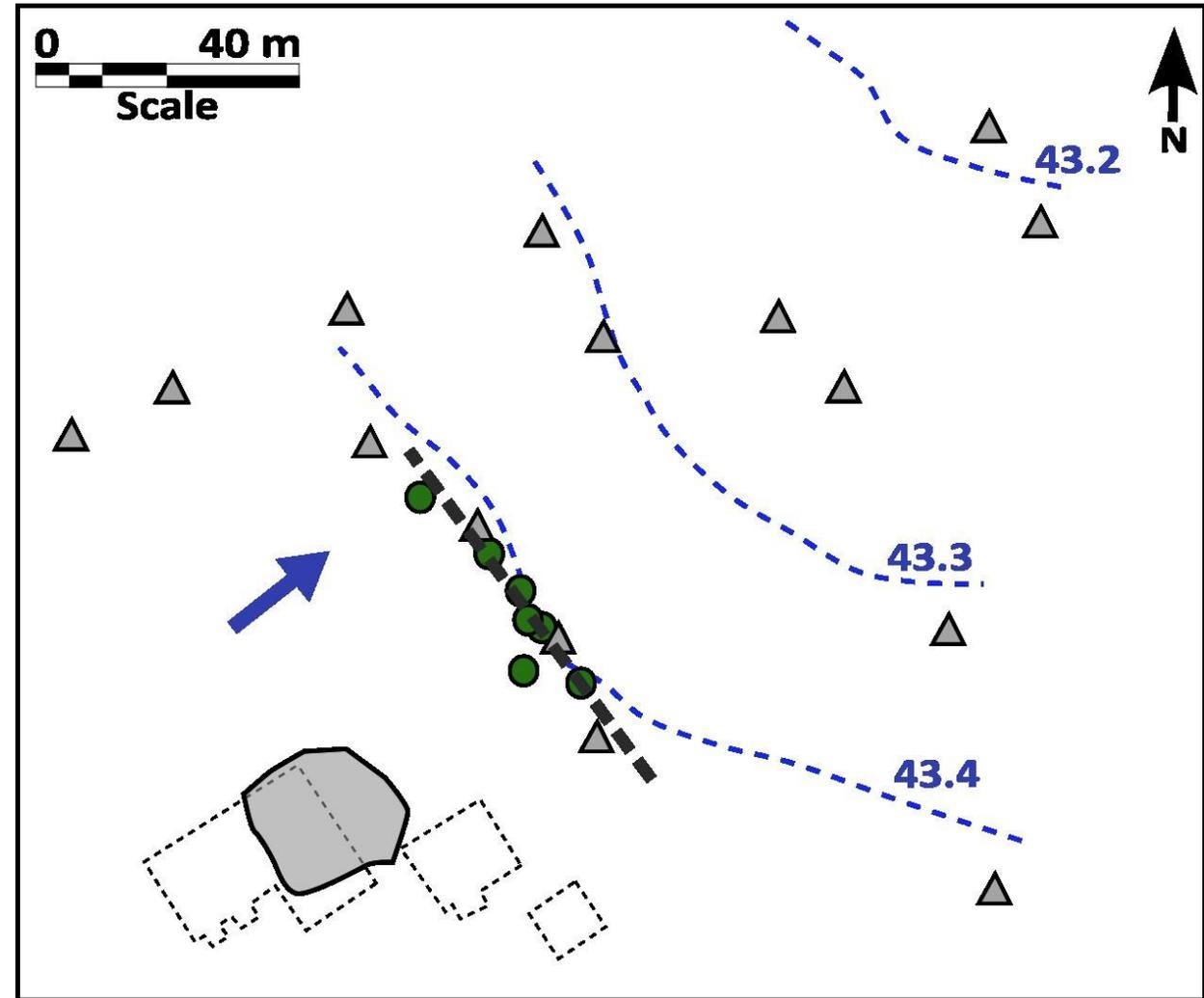
Direct-push: LL-MiHPT

- MIP/MIHPT → kontinuerlige målinger
- LL-MIP (low level) → måling ~ hver 0,3 m
- LL-MIP-systemet har en øget følsomhed (10-50 gange) i forhold til standard MIP-system
- Koncentrationer på lavt µg/L niveau kan observeres



Lokaliteten – Håndværkervænget

- Klorerede opløsningsmidler fra diverse industri siden 1960'erne
- Kilden er afgrænset pba. jordprøver, poreluft og grundvandsanalyser
- Primært TCE (>1500 µg/L)
- Gradient 2.8‰
- Fluxtransekt ca. 40 m nedstrøms



● Direct-Push ▲ Borehole - - - Building — Source
- - - Transect → GW flow direction - - - - Isopotential lines

Stort tak til Bettina Olsen fra DMR for hjælp med felt og data!

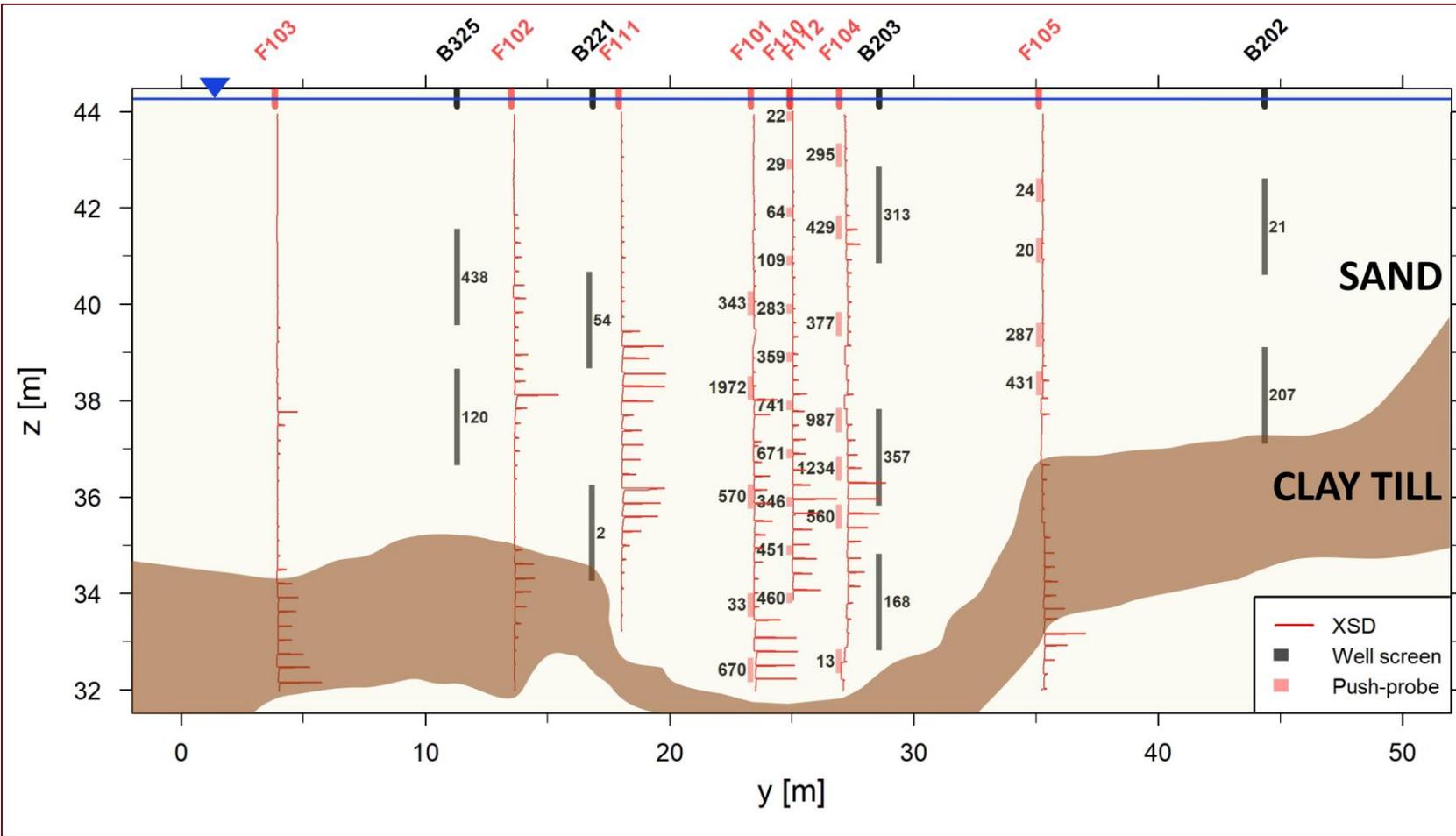
Lokaliteten – Håndværkervænget

- Klorerede opløsningsmidler fra diverse industri siden 1960'erne
- Kilden er afgrænset pba. jordprøver, poreluft og grundvandsanalyser
- Primært TCE ($>1500 \mu\text{g/L}$)
- Gradient 2.8‰
- Fluxtransekt ca. 40 m nedstrøms
- Komplex geologi og skrånende terræn
 - Vanskeligt feltarbejde!



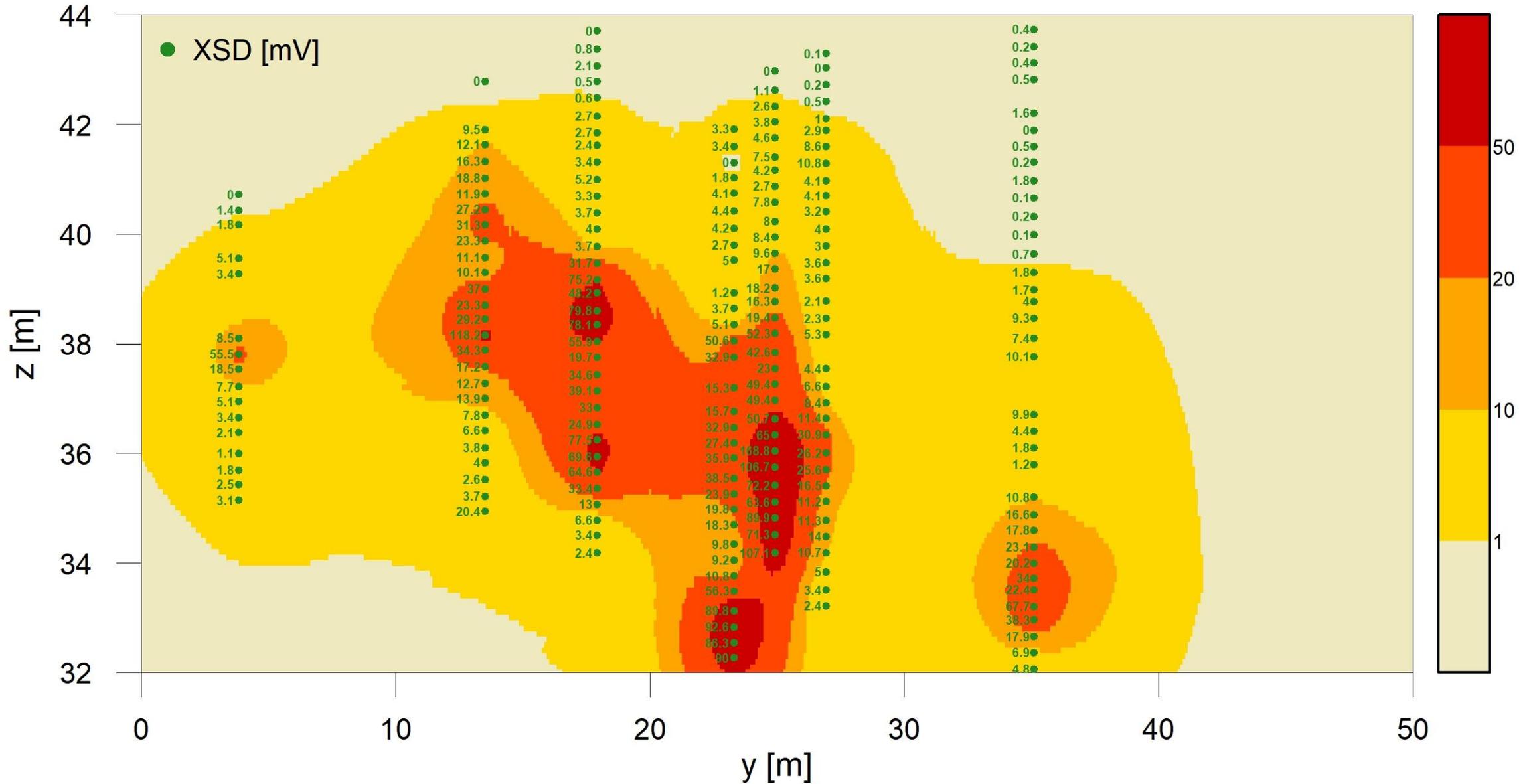
Lokaliteten – Håndværkervænget

Transektet



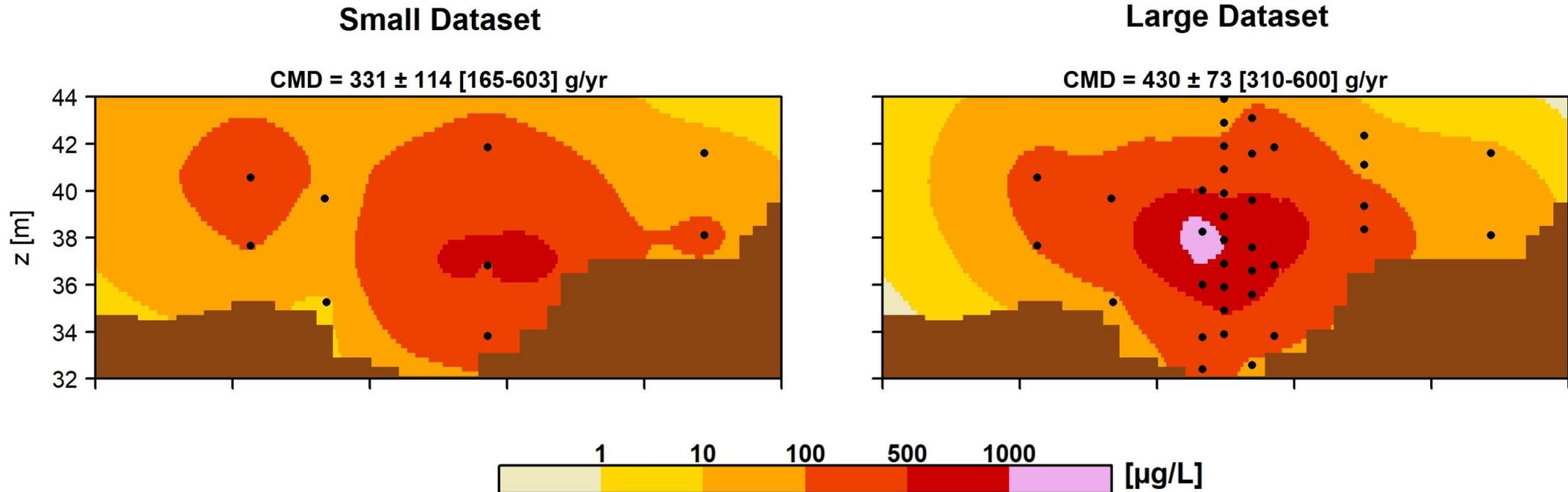
- Fire traditionelle boringer (B-boringer)
 - 9 analyser
- Syv LL-MiHPT sonderinger (XSD) hvoraf fire suppleret med niveauspecifikke vandprøver (F-boringer)
 - 36 analyser
 - 232 XSD-udslag
- Stort (9+36 = 45 analyser) vs. lille (9 analyser) dataset

Lokaliteten – XSD udslag



Lokaliteten – Forureningsfluxen

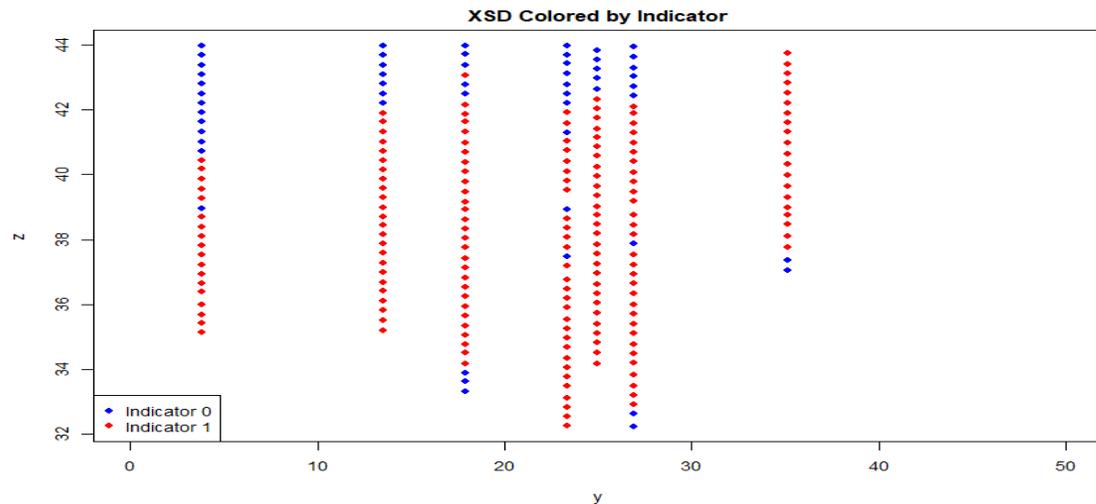
- Fanerne er ikke afgrænsede
- Lille dataset fanger ikke fanens centrum



Metoden – Og hvorfor geostatistik?

- OBS: Direkte korrelation var jo ikke muligt
- Et skridt tilbage – konservativt
- XSD signaler konverteres til en tilstedeværelses/fraværs-indikator
 - Fjerner baggrundsstøj
 - Stoler ikke på *størrelsen* af udslaget, men derimod *om hvorvidt forurening er tilstede*

JA/NEJ

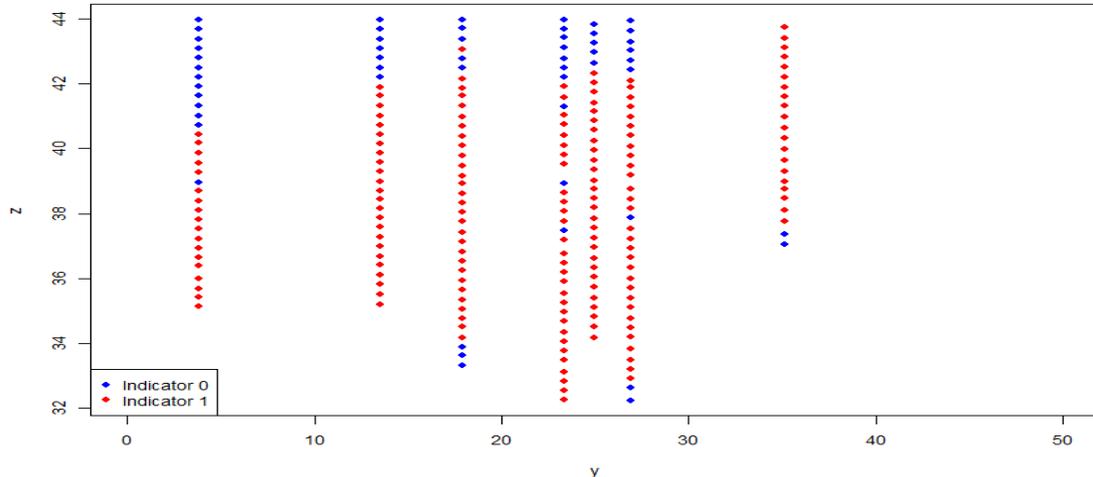


Metoden – Og hvorfor geostatistik?

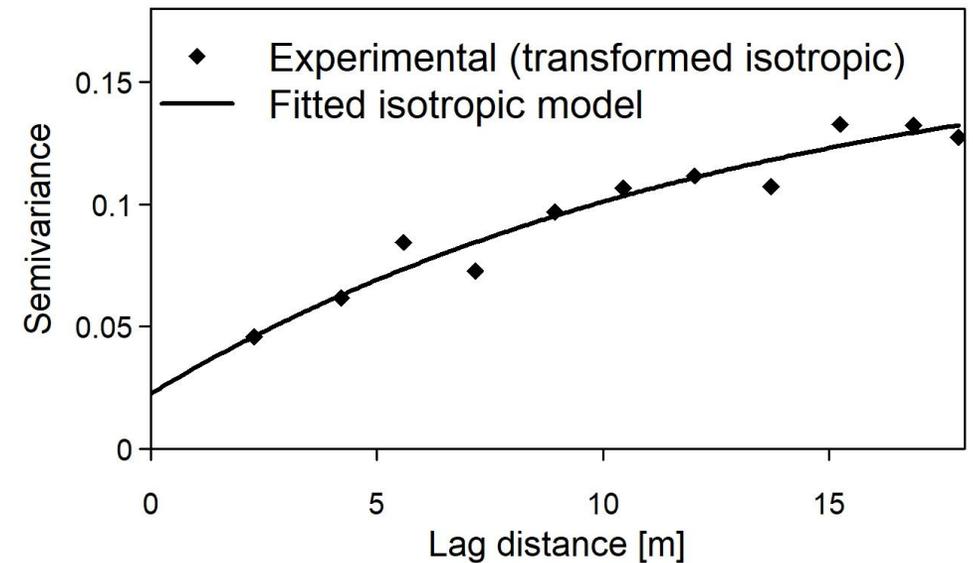
- OBS: Direkte korrelation var jo ikke muligt
- Et skridt tilbage – konservativt
- XSD signaler konverteres til en tilstedeværelses/fraværs-indikator
 - Fjerner baggrundsstøj
 - Stoler ikke på *størrelsen* af udslaget, men derimod *om hvorvidt forurening er tilstede*
 - Variogram: Et geostatistisk værktøj → *sandsynligheden* for JA/NEJ væk fra sonderinger

JA/NEJ

XSD Colored by Indicator



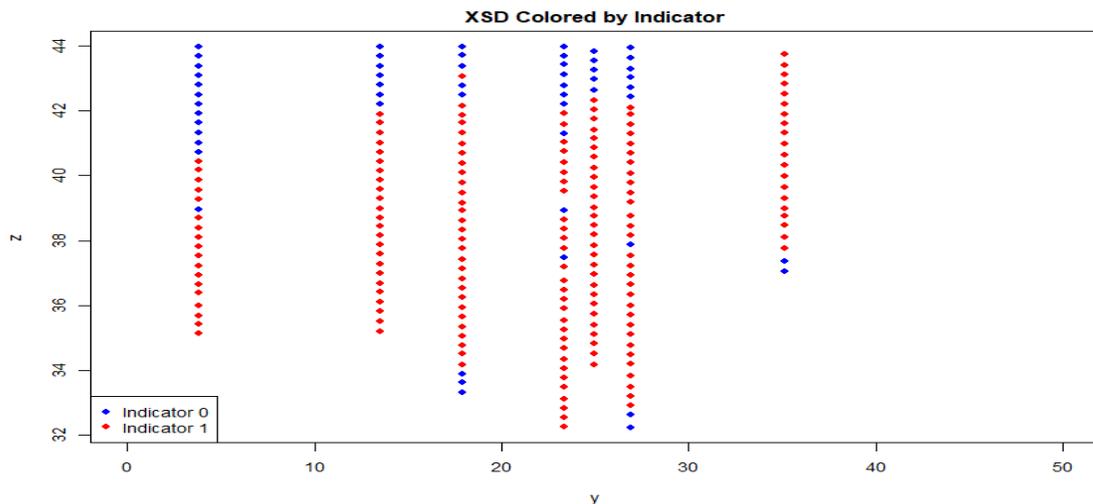
Rumlig sammenhæng



Metoden – Og hvorfor geostatistik?

- OBS: Direkte korrelation var jo ikke muligt
- Et skridt tilbage – konservativt
- XSD signaler konverteres til en tilstedeværelses/fraværs-indikator
 - Fjerner baggrundsstøj
 - Stoler ikke på *størrelsen* af udslaget, men derimod *om hvorvidt forurening er tilstede*
 - Variogram: Et geostatistisk værktøj → *sandsynligheden* for JA/NEJ væk fra sonderinger

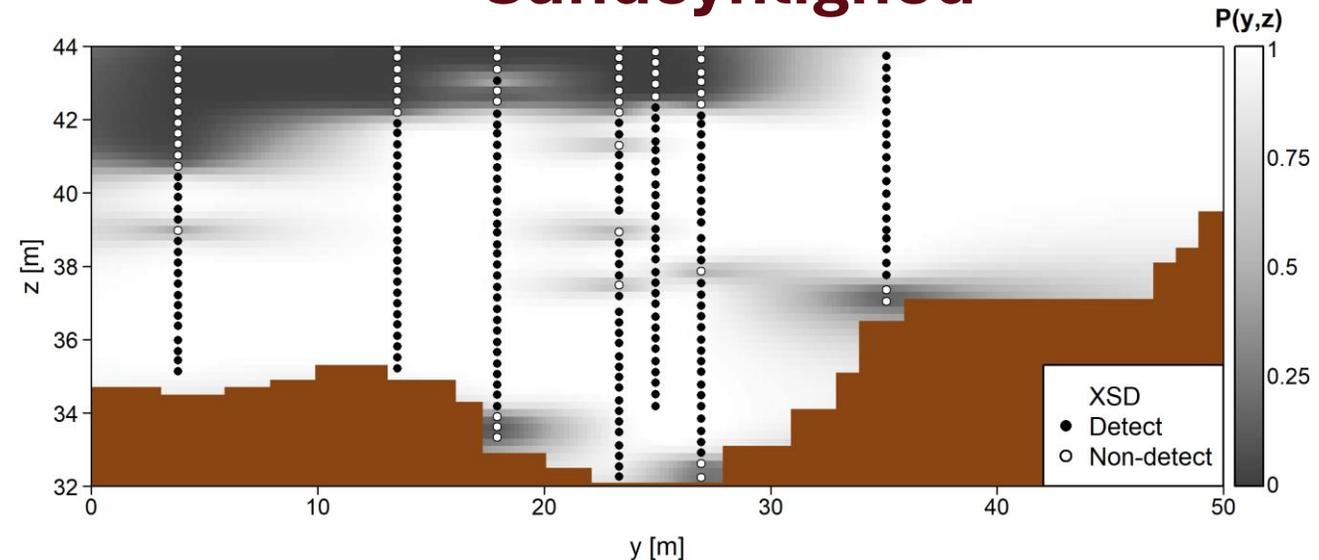
JA/NEJ



Indicator kriging



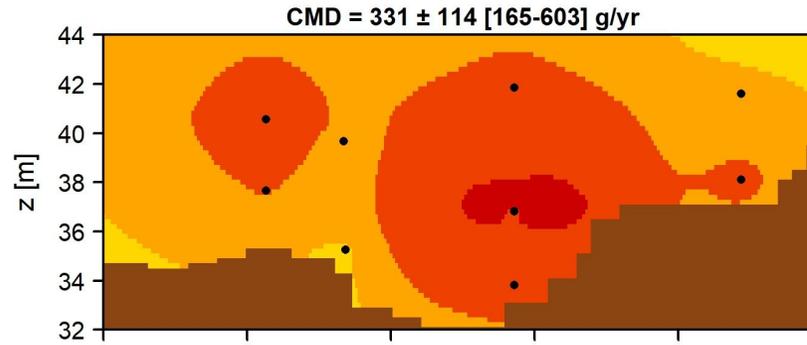
Sandsynlighed



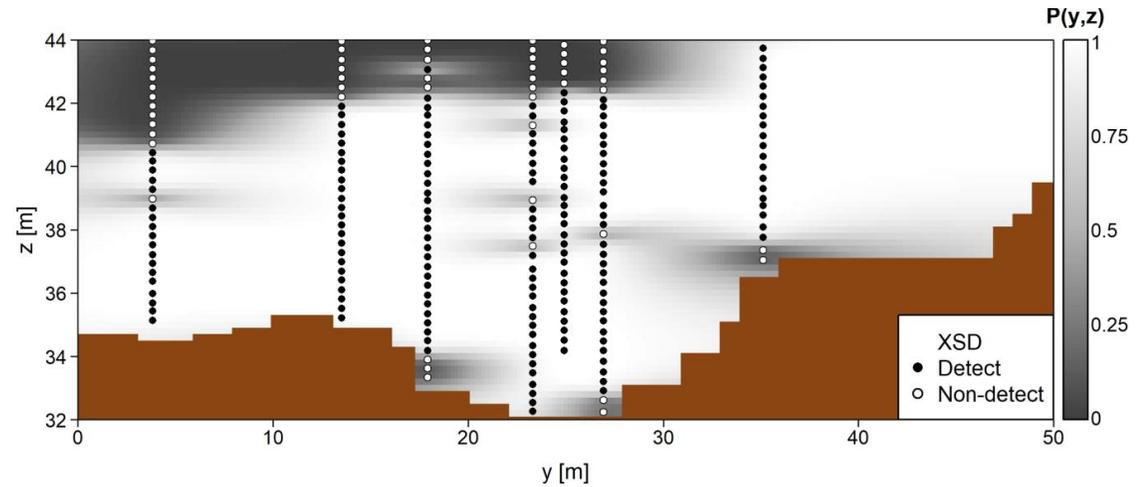
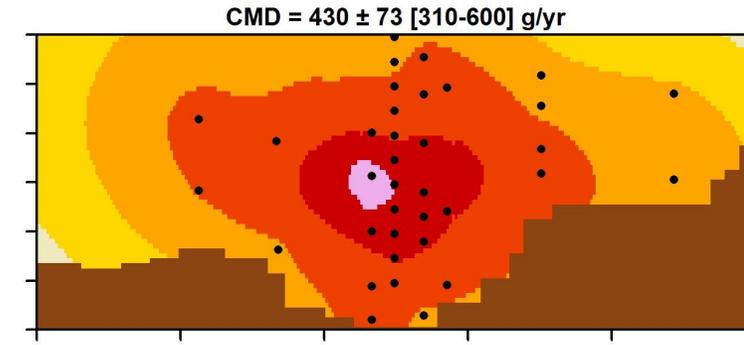
Resultater – XSD

- ‘Traditionel’ fane overlappes med sandsynlighed → en ‘maskering’
- Ingen blød data → interpoleret fane fastholdes
- Lighed ml. fane og XSD

Small Dataset



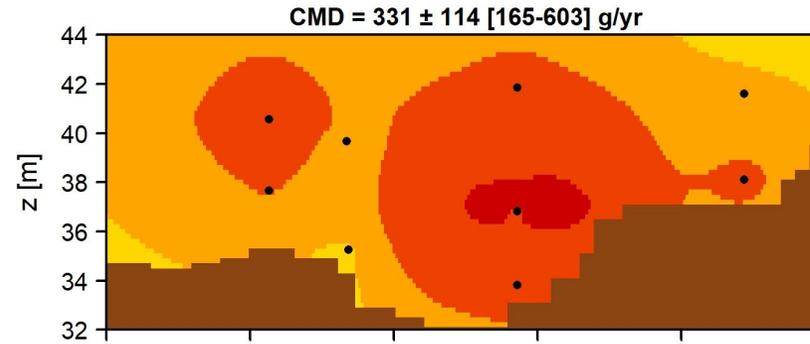
Large Dataset



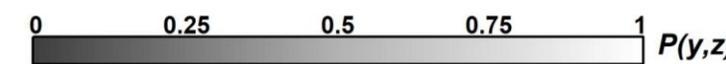
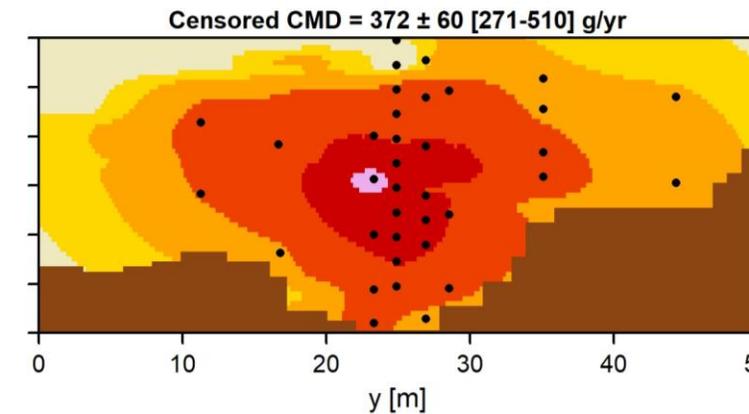
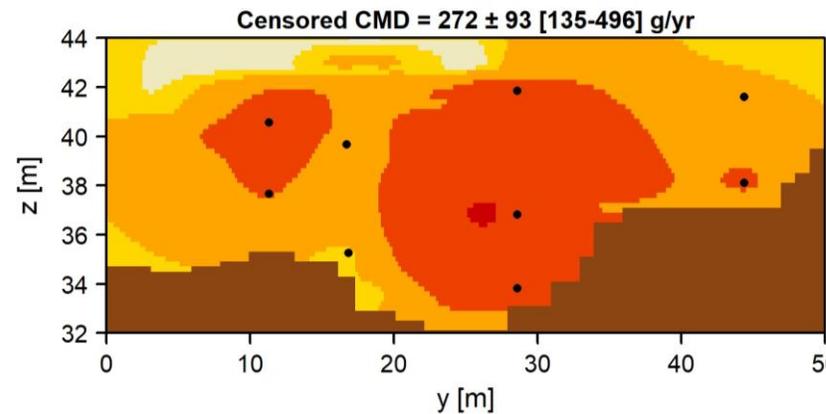
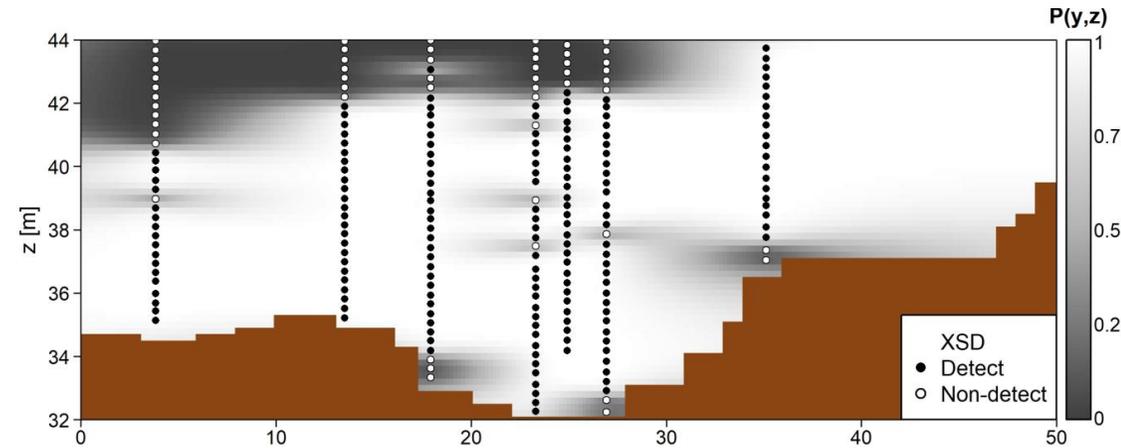
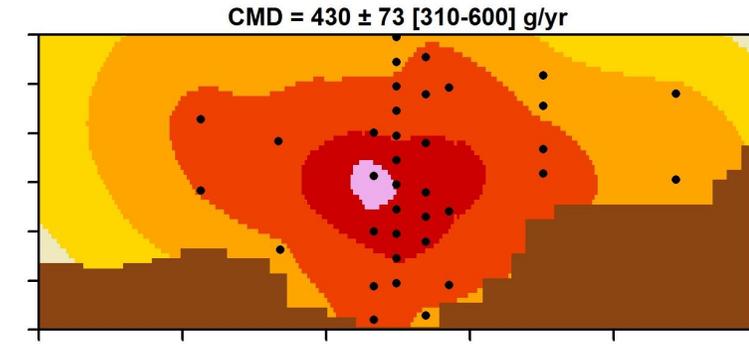
Resultater – XSD

- ‘Traditionel’ fane overlappes med sandsynlighed → en ‘maskering’
- Ingen blød data → interpoleret fane fastholdes
- Lighed ml. fane og XSD
- Fanen afgrænses og fluxen reduceres
- Mere detaljeret forureningsbillede
- Øger områder med lave koncentrationer (<10 µg/L)
- Reducerer ikke konfidensinterval
 - Usikkerhed styret af kilden!

Small Dataset

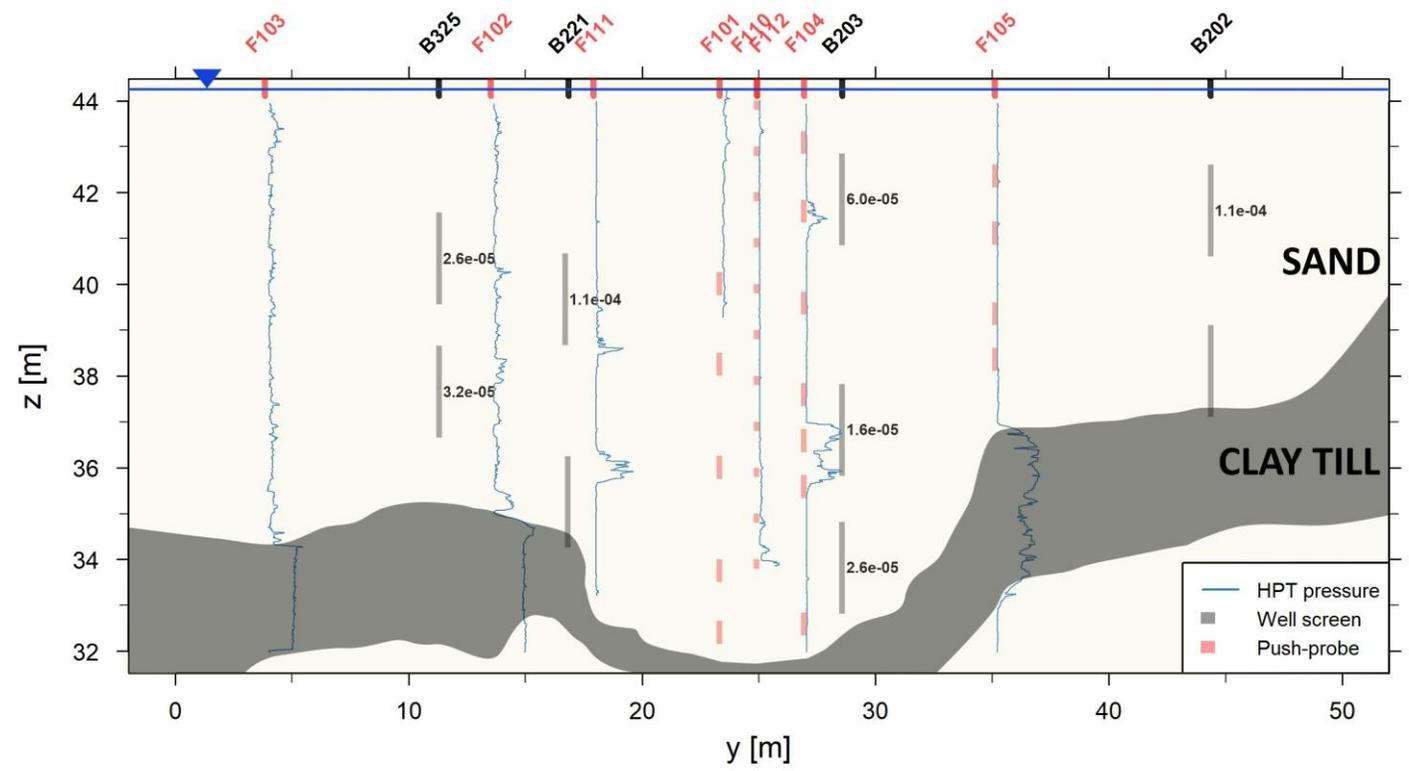


Large Dataset



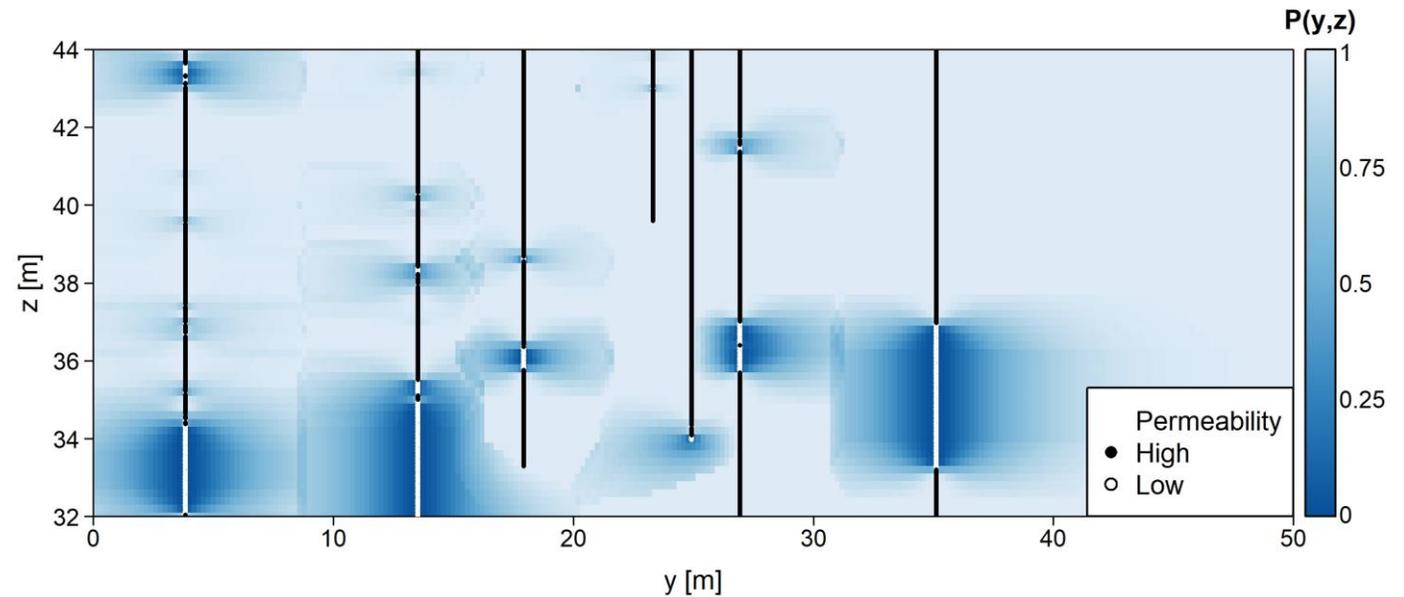
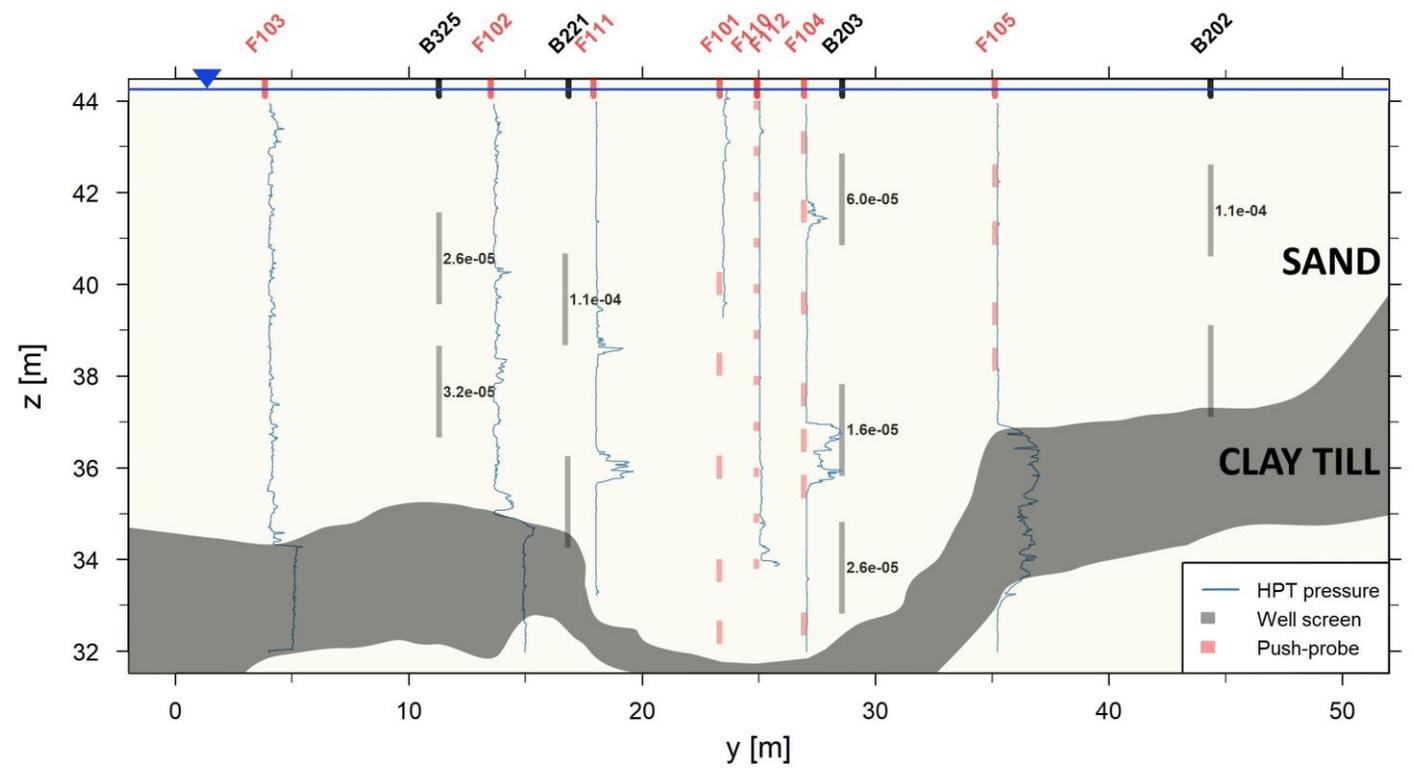
Resultater – HPT

- Virker også på HPT og K
- Det meget grove K-felt fra slugtest kan overlappes med den relative indikation af permeabiliteten givet HPT modtrykket



Resultater – HPT

- Virker også på HPT og K
- Det meget grove K-felt fra slugtest kan overlappes med den relative indikation af permeabiliteten givet HPT modtrykket
- Men i en *meget høj opløsning*
- Fanger lav-permeable zoner som der ikke ses fra slugtests



Semi-kvantitativ data *kan* udnyttes bedre

- Interpoleret fane forbedres ved at kombinere traditionelle grundvandsprøver med højopløselige, semikvantitative LL-MiHPT data
 - Data drevet
 - Udnytter rumlig information fra 'blød' data uden at overfortolke
 - Integreret direkte i optegning af fane
- Fokus her: forbedre fane og reducere flux
 - Overførbar til andre data og formål
- Testet og udviklet på en 'rigtig' lokalitet
- Styrke konceptuel model og risikovurdering



Nysgerrig?

Støttedokument

Geostatistisk metode

Flux og remediering

Monitoring & Remediation Research Article

Temporal Evolution of Contaminant Mass Discharge: Effect of Source Remediation at Contaminated Sites

by Anton Bøllingtoft, Mads Trolborg, Charlotte Riis, Nina Tuxen and Paul L. Bjerg

Abstract

Contaminant mass discharge (CMD) is a key metric for evaluating remediation performance at contaminated sites posing a risk to groundwater. This study assesses temporal CMD trends and associated uncertainties using a geostatistical approach at a chlorinated solvent contaminated site following source zone remediation, supported by two decades of groundwater monitoring data. The site serves as a case to derive learnings and recommendations for long-term monitoring at contaminated sites using the CMD approach. A significant reduction in mean CMD was observed from 2009 to 2023, 62% when using a reduced dataset of traditional monitoring wells and 72% when including data from five high-resolution multilevel samplers, reducing CMD uncertainty from CV=45 to 80% to ~35 to 40%. The timing and magnitude of CMD decline aligned with expected plume transport and reflected combined remediation effects. A temporary vinyl chloride (VC) increase in 2015–2016 suggested enhanced dechlorination, highlighting the need to monitor both parent compounds and degradation products. The study emphasizes the value of CMD uncertainty quantification in long-term monitoring, enabling robust interpretation of remediation effects, temporal trends, and risk. While the reduced dataset captured overall patterns, high-resolution data yielded lower uncertainty and clearer insights into plume dynamics. A hybrid monitoring approach—combining frequent lower-resolution sampling with periodic high-resolution campaigns—is recommended. Consistent monitoring of flow and attenuation processes downstream can further improve CMD quantifications without excessive resource demand. Overall, this study shows that long-term, consistent monitoring supports reliable evaluation of source zone remediation and interpretation of CMD response in downgradient groundwater.

Introduction

Point source contamination from industrial activities poses a risk to groundwater resources and downstream receptors worldwide. One important metric for groundwater management is contaminant mass discharge (CMD), defined as the total contaminant mass per unit time passing through a downgradient transect perpendicular to the contaminant plume (ITRC 2010; Finarson 2017; Horst et al. 2021). CMD is increasingly used to monitor the effectiveness of remediation efforts at contaminated sites (Horst et al. 2017; Halaska et al. 2019; Thaland-Hansen et al. 2023) and has been applied across a wide range of contaminants, includ-

ing chlorinated ethenes (Cai et al. 2012; Finarson 2017; Balbarini et al. 2018; Bøllingtoft et al. 2025a, 2025b), PFAS (Adamson et al. 2020; Quinnan et al. 2021), and pesticides (Frederiksen et al. 2023).

The temporal evolution of groundwater (CMD)—and its relationship with source mass reduction—has been explored in several studies. Brooks et al. (2018) combined long-term monitoring data with spatially distributed CMD measurements obtained at distinct points in time to estimate source strength functions over time. Fjorndal et al. (2012b) used temporal CMD measurements to evaluate the performance of a source zone remediation, capturing both initial reductions and rebound effects. Earlier studies have shown that the relationship between source mass depletion and CMD is often nonlinear and can be described using source strength functions (Pala et al. 2005; Hsu et al. 2008; DiStefano and Brusseau 2008). They highlight how mass removal may not immediately result in proportional CMD reductions. Similarly, Brusseau et al. (2011, 2013) and Mathies et al. (2014) characterized and linked temporal trends in CMD to source mass removal, emphasizing the importance of continuous monitoring for understanding contaminant behavior over time. These studies highlight the importance of CMD in informing remediation strategies and assessing the long-term effectiveness of this (Truxet et al. 2017).

Article impact statement: Long term CMD monitoring enables statistical evaluation of remediation performance and allows quantification of groundwater parameters.

© 2026 The Author(s). Groundwater Monitoring & Remediation published by Wiley Periodicals, LLC on behalf of National Ground Water Association. doi: 10.1111/gwmr.70043

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NGWA.org

Groundwater Monitoring & Remediation 1

Bøllingtoft, A., Trolborg, M., Riis, C., Tuxen, N., & Bjerg, P. L. (2026). Temporal Evolution of Contaminant Mass Discharge: Effect of Source Remediation at Contaminated Sites. *Groundwater Monitoring and Remediation*. <https://doi.org/10.1111/gwmr.70043>

Fluxparametre og usikkerhed

Valg af parametre til geostatistisk model

Anton Bøllingtoft, Mads Trolborg, Nina Tuxen & Paul L. Bjerg

DTU Sustain, September 2025.

Version 1.0



Bøllingtoft, A., Trolborg, M., Tuxen, N., & Bjerg, P. L. (2025). Fluxparametre og usikkerhed: Valg af parametre til geostatistisk model. DTU Sustain.

Kode til fluxberegning

Code for Contaminant Mass Discharge Quantification and Uncertainty Estimation in Groundwater

City Download all (88.73 kB) Share Embed Collect

Software posted on 2025-08-18, 13:14 authored by [Anton Bo Bøllingtoft](#)

25 views 10 downloads 0 citations

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 & Palocaiusa, 1982) to estimate the mean concentration field and generate concentration residuals which are then transformed using 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.

DTU Data

Bøllingtoft, A. (2025). *Code for Contaminant Mass Discharge Quantification and Uncertainty Estimation in Groundwater* (Version 1.0). Technical University of Denmark. Software. <https://doi.org/10.11583/DTU.29891264>

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journal homepage: www.elsevier.com/locate/jconhyd

Quantification of contaminant mass discharge and uncertainties: Method and challenges in application at contaminated sites

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ARTICLE INFO

Keywords: Contaminant mass discharge (CMD); Uncertainty estimation; Risk assessment; Groundwater contamination; Conceptual model

ABSTRACT

Contaminant mass discharge (CMD) estimation involves combining multilevel concentration and flow measurements to quantify the contaminant mass passing through a control plane downgradient of a point source. However, geological interpretation and limited data introduce uncertainties that complicate CMD estimation and risk assessment. Although CMD is increasingly used in groundwater management, methods for quantifying and handling these uncertainties are still needed. This study develops and tests a CMD estimation method based on Bayesian geostatistics to quantify CMD uncertainties using data from a control plane perpendicular to the contaminant plume. By combining geostatistical conditional simulations of the spatial concentration distribution with the flow, an ensemble of CMD realizations is generated, from which a cumulative distribution function is derived. A key element of this approach is the use of a nondegenerative transport model to simulate the spatial concentration trend. This ensures that the estimated concentration reflects the expected physical behavior of the contaminant plume while also allowing the integration of site-specific conceptual information. The method is applicable to plumes with dissolved contaminants, such as chlorinated solvents, petroleum hydrocarbons, Per- and polyfluoroalkyl substances (PFAS) and pesticides. Site-specific conceptual understanding is used to inform the prior probability density functions of the structural model parameters and to define acceptable simulated concentration limits. We applied the method at three sites contaminated with chlorinated ethenes, demonstrating its robustness across varying information levels and data availability. Our results show that strong site-specific conceptual knowledge and high sampling density constrains the CMD uncertainty (CV = 21 %) and results in estimated model parameters and a spatial concentration distribution that agrees well with the conceptual model. For a site with low data and limited conceptual knowledge, CMD and concentration distribution estimates are still feasible, though with higher uncertainty (CV = 41 %). Extending the method to account for multiple source zones and complex plume migration improved parameter identification and reduced the 95 % CMD confidence interval by 11 % (4096–8790) to (3096–8468) g yr⁻¹, while also providing a spatial concentration distribution in better agreement with the plume conceptualization. This study highlights the importance of integrating site-specific conceptual knowledge in CMD estimation, particularly for less-sampled sites. The method can furthermore assist in identifying remediation targets, evaluating remedial effectiveness, and optimizing sampling strategies.

1. Introduction

Contaminated sites originating from former historic industrial activities pose a risk to the environment and human health worldwide. Chlorinated solvents are among the most omnipresent and persistent subsurface contaminants in the world (Stroevius et al., 2020), but also contaminants such as per- and polyfluoroalkyl substances (PFAS) are becoming an increasing concern in soil and groundwater (Sims et al., 2023).

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Bøllingtoft, A., Bjerg, P. L., Rønde, V., Tuxen, N., Nowak, W., & Trolborg, M. (2025). Quantification of contaminant mass discharge and uncertainties: Method and challenges in application at contaminated sites. *Journal of Contaminant Hydrology*, 268, 104453. <https://doi.org/10.1016/j.jconhyd.2024.104453>

Semi-kvantitativ data

Groundwater

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

by Anton Bøllingtoft^{1,2}, Wolfgang Nowak³, Paul L. Bjerg⁴, Gro Lilbek⁴, Anders G. Christensen⁴, and Mads Trolborg⁵

Abstract

Reliable mapping and delineation of contaminant plumes and accurate estimation of contaminant mass discharge (CMD) are critical for groundwater risk assessment and planning of remedial actions at contaminated sites. However, traditional interpolation methods are often challenged by low-density sampling resulting in improper plume delineation. This study introduces a probabilistic censoring method that enhances geostatistical interpolation by incorporating comparably cheap, high-resolution, but semi-quantitative data collected from direct push-probes in the subsurface. The method converts halogen-specific detector signals into binary presence-absence indicators, which are interpolated using indicator kriging to generate a probability field of contaminant distribution. The probability field is then used to censor a spatial concentration field derived from traditional groundwater sampling, retaining interpolated concentration values only in areas where contamination is likely. We apply the method to a site contaminated with chlorinated solvents using two datasets with different sampling densities. Results show that, using our new method, plume fringes became more clearly defined and the total area with low concentrations (<10 µg L⁻¹) increased by 41–85%. CMD estimates were reduced by 13–18%, while relative uncertainty remained largely unchanged. The method integrates seamlessly with traditional interpolation methods and our censoring workflow can be applied to other forms of direct-push data (e.g., relative permeability). As such, the framework offers a useful method for incorporating semi-quantitative field measurements into concentration interpolation and CMD estimation at contaminated sites.

Introduction

Contaminant mass discharge (CMD), the mass of contaminant passing through a control plane per unit time, is increasingly recognized as a key metric in groundwater risk assessment and contaminated site management (e.g., ITRC 2010; Koch and Nowak 2015; Anderson 2021;

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