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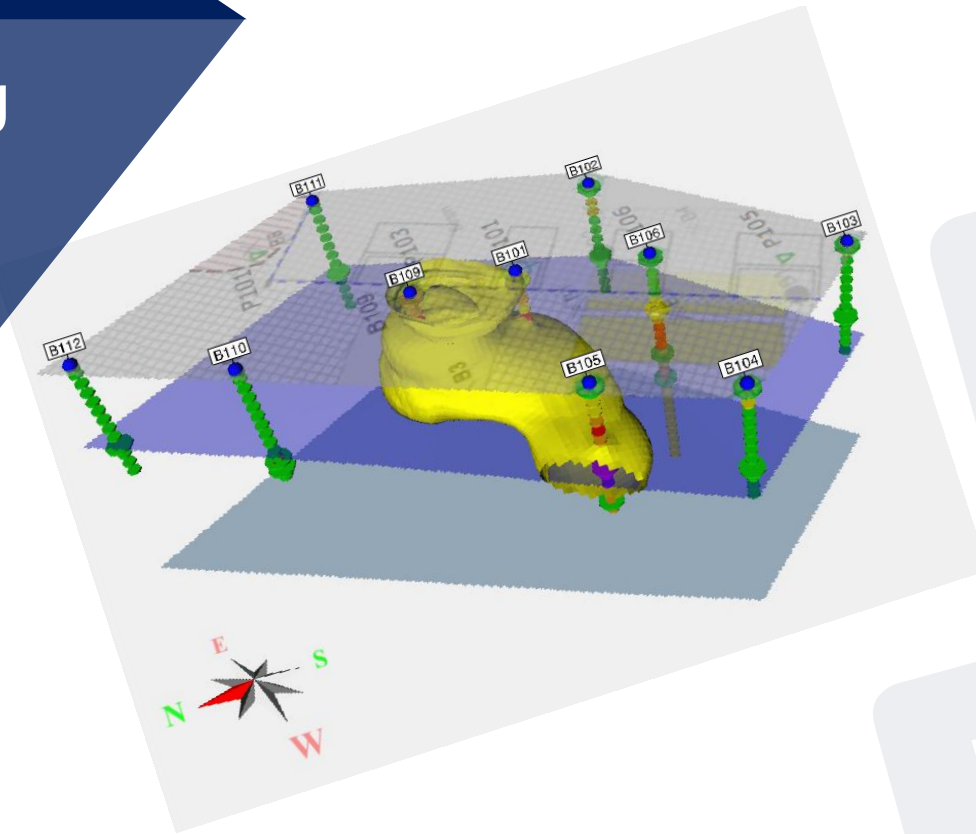
Use of geostatistical modelling in investigation of soil contamination – working toward a better definition of remedial mass and volume



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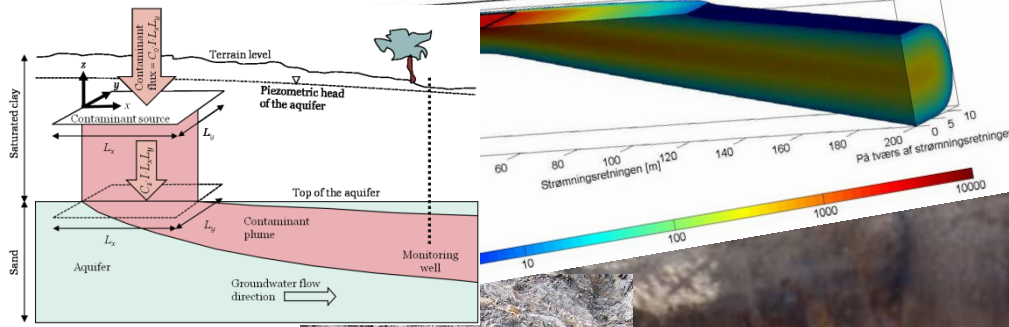
Background for application of geostats

- A lot of resources are spent on investigating and remediating contaminated sites, especially chlorinated solvent sites (DK).
- Remediation is the game of reducing mass flux/exposure
  - Flux is related to concentration and volume
  - Which again is related to mass



- And the game becomes: Find the mass!

- Inherent inhomogeneities in geology and contaminant concentrations lead to uncertainty.
  - How can we deal with uncertainty?
- In recent years, we have seen a dramatic drop in sample prices, and an increase in data density.

=> Geostatistical modelling

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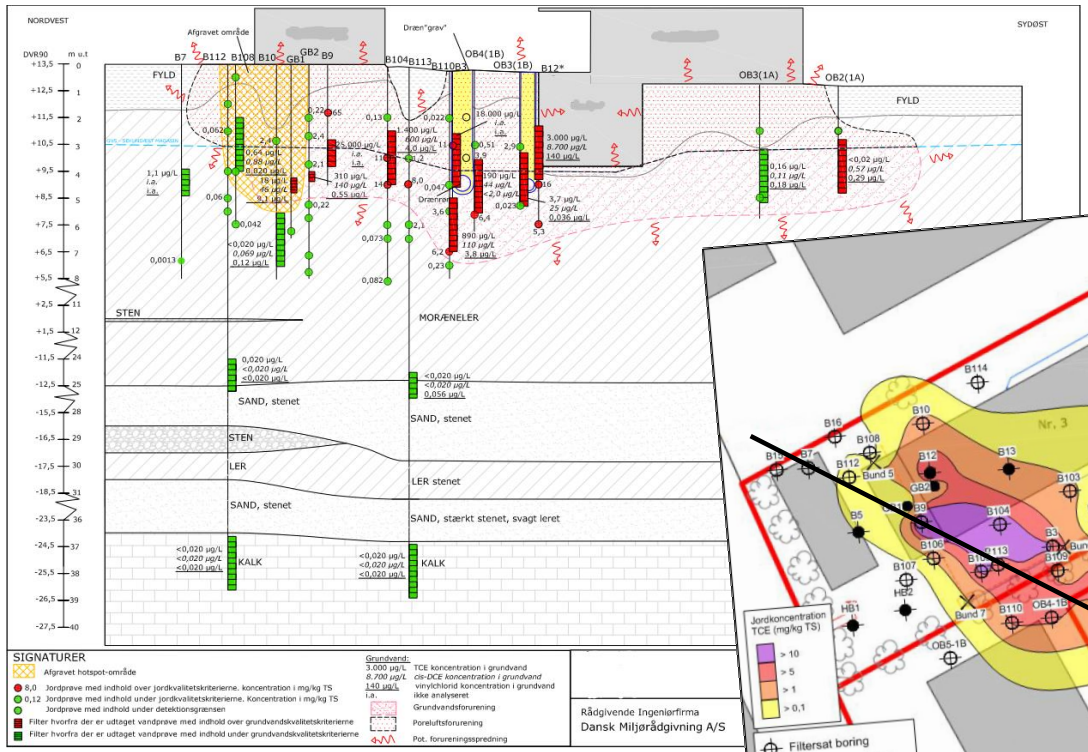
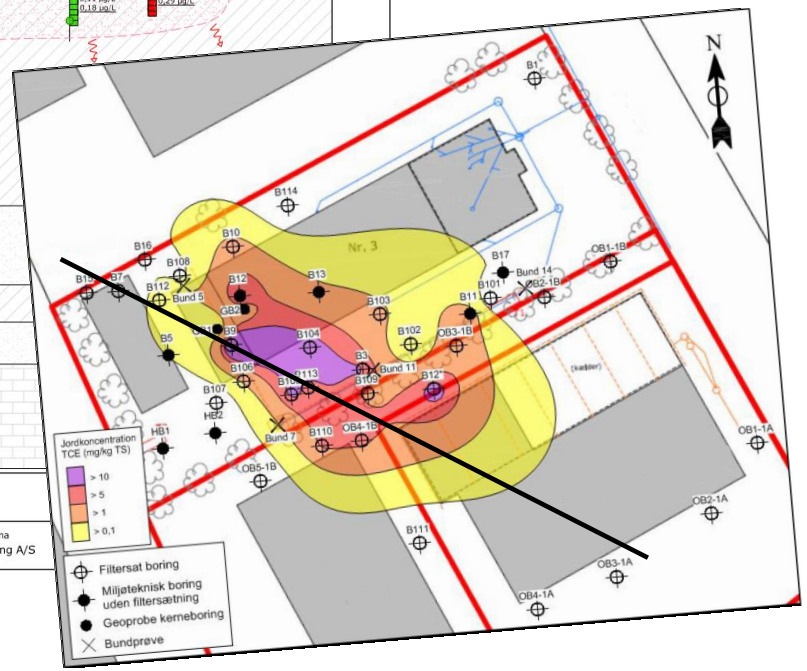
Lots of data vs. data presentation and communication

- How should we present our data and communicate with clients and authorities? (one of my reports from 2014)





Jordanalyser, oliekomponenter og chlorerede opløsningsmidler.

Boring	Rapport årstal	Dybde	Chlorerede opløsningsmidler (mg/kg TS) TCM	1,1,1-TCA	TeCM	TCE	PCE
B112	2014	1,5	0,014	<0,010	<0,010	<0,010	<0,010
		2,5	<0,010	<0,010	<0,010	0,062	<0,010
		4,0	<0,010	<0,010	<0,010	<0,010	<0,010
		5,0	<0,010	<0,010	<0,010	0,60	<0,010
		5,5	<0,010	<0,010	<0,010	<0,010	<0,010
B113	2014	3,5	<0,010	<0,010	<0,010	1,2	<0,010
		4,5	<0,010	<0,010	<0,010	8,0	<0,010
		6,0	<0,010	<0,010	<0,010	2,1	<0,010
		6,5	<0,010	<0,010	<0,010	<0,010	<0,010
B114	2014	0,2	<0,010	<0,010	<0,010	<0,010	<0,010
		1,0	<0,010	<0,010	<0,010	<0,010	<0,010
		2,5	<0,010	<0,010	<0,010	<0,010	<0,010
		4,0	<0,010	<0,010	<0,010	<0,010	<0,010
		5,5	<0,010	<0,010	<0,010	<0,010	<0,010
GB1	2014	2,5-3,0	<0,010	<0,010	<0,010	<0,010	<0,010
		3,0-4,0	<0,010	<0,010	<0,010	0,075	<0,010
		5,0-6,0	<0,010	<0,010	<0,010	0,27	<0,010
		6,0-6,5	<0,010	<0,010	<0,010	<0,010	<0,010
GB2	2014	2,0	<0,010	<0,010	<0,010	0,22	<0,010
		2,75	0,013	<0,010	<0,010	2,4	<0,010
		3,75	<0,010	<0,010	<0,010	2,1	<0,010
		5,25	<0,010	<0,010	<0,010	0,22	<0,010
		5,75	<0,010	<0,010	<0,010	<0,010	<0,010
		7,25	<0,010	<0,010	<0,010	<0,010	<0,010
		7,75	<0,010	<0,010	<0,010	<0,010	<0,010
HB2	2014	1,0					
Prøve 2	1993	1,1					
Prøve 4	1993	1,0					
Prøve 8	1993	2,0					
B1	1996	17					
		27					
		39					
		4,5					
B3	1996	3,0					
B5	1996	2,0					
		4,5					
B6	1996	1,5					
B7	1996	7,5					
B8	1996	4,5					
B9	1996	2,0					
B10	1996	3,0					
B11	1996	3,0					
H1	1996	0,5					
Jordkvalitetskriterium			50				

Boring	Rapport årstal	Dybde	Chlorerede opløsningsmidler (mg/kg TS) TCM	1,1,1-TCA	TeCM	TCE	PCE
B12	1997	2,0	-	-	-	10	-
B13	1997	3,5	-	-	-	1,0	-
Bund 5	1998	5,4	<0,001	<0,001	<0,001	0,88	<0,001
Bund 7	1998	4,0	<0,001	<0,001	<0,001	0,91	<0,001
Bund 11	1998	4,0	<0,001	<0,001	<0,001	0,007	<0,001
Bund 14	1998	6,0	<0,001	<0,001	<0,001	0,005	<0,0005
B12	2002	4,5	-	-	-	16	-
		6,0	-	-	-	5,3	-
OB1-1A	2013	2,5	<0,010	<0,010	<0,010	<0,010	<0,010
		4,0	<0,010	<0,010	<0,010	<0,010	<0,010
OB2-1A	2013	2,5	<0,010	<0,010	<0,010	<0,010	<0,010
OB3-1A	2013	2,5	<0,010	<0,010	<0,010	<0,010	<0,010
		5,0	<0,010	<0,010	<0,010	<0,010	<0,010
OB4-1A	2013	2,0	<0,010	<0,010	<0,010	<0,010	<0,010
		4,0	<0,010	<0,010	<0,010	<0,010	<0,010
OB1-1B	2013	3,5	<0,010	<0,010	<0,010	<0,010	<0,010
OB2-1B	2013	3,5	<0,010	<0,010	<0,010	0,46	<0,010
OB3-1B	2013	3,0	0,028	<0,010	<0,010	2,9	<0,010
		5,0	<0,010	<0,010	<0,010	0,023	<0,010
OB4-1B	2013	3,0	<0,010	<0,010	<0,010	0,51	<0,010
		5,5	0,074	<0,010	<0,010	6,4	<0,010
OB5-1B	2013	3,0	<0,010	<0,010	<0,010	0,010	<0,010
		5,0	<0,010	<0,010	<0,010	<0,010	<0,010
Jordkvalitetskriterium			50	200	5	5	5

Boring	Rapport årstal	Dybde	Chlorerede opløsningsmidler (mg/kg TS) TCM	1,1,1-TCA	TeCM	TCE	PCE
OB1-1A	2014	2,0	0,036	<0,010	<0,010	<0,010	<0,010
		4,0	0,026	<0,010	<0,010	0,019	<0,010
		6,5	0,036	<0,010	<0,010	0,14	<0,010
OB2-1A	2014	3,0	0,043	<0,010	<0,010	0,058	<0,010
		4,0	0,040	<0,010	<0,010	<0,010	<0,010
		5,5	0,040	<0,010	<0,010	<0,010	<0,010
OB3-1A	2014	0,5	<0,010	<0,010	<0,010	0,67	<0,010
		2,5	0,029	<0,010	<0,010	0,80	<0,010
		3,5	<0,010	<0,010	<0,010	1,5	<0,010
		4,0	<0,010	<0,010	<0,010	<0,010	<0,010
		5,0	<0,010	<0,010	<0,010	0,13	<0,010
OB4-1A	2014	2,0	<0,010	<0,010	<0,010	11	<0,010
		3,5	<0,010	<0,010	<0,010	14	<0,010
		4,5	0,091	<0,010	<0,010	<0,010	<0,010
		6,0	<0,010	<0,010	<0,010	0,073	<0,010
		6,5	<0,010	<0,010	<0,010	0,082	<0,010
OB1-1B	2014	8,0	0,078	<0,010	<0,010	0,24	<0,010
		3,0	0,071	<0,010	<0,010	1,1	<0,010
		3,5	0,098	<0,010	<0,010	12	<0,010
OB2-1B	2014	4,5	0,086	<0,010	<0,010	7,7	<0,010
		4,5[2]	0,096	<0,010	<0,010	<0,010	<0,010
		6,0	0,10	<0,010	<0,010	0,015	<0,010
OB3-1B	2014	6,5	0,10	<0,010	<0,010	<0,010	<0,010
		1,5	0,076	<0,010	<0,010	0,17	<0,010
		2,5	<0,010	<0,010	<0,010	1,2	<0,010
				<0,010	<0,010	0,025	<0,010
				<0,010	<0,010	<0,010	<0,010
				<0,010	<0,010	<0,010	<0,010
				<0,010	<0,010	<0,010	<0,010
				<0,010	<0,010	<0,010	<0,010
				<0,010	<0,010	<0,010	<0,010
				<0,010	<0,010	<0,010	<0,010
				<0,010	<0,010	<0,010	<0,010
				<0,010	<0,010	0,042	<0,010
				<0,010	<0,010	<0,010	<0,010
				<0,010	<0,010	3,9	<0,010
				<0,010	<0,010	3,8	<0,010
				<0,010	<0,010	0,013	<0,010
				<0,010	<0,010	0,022	<0,010
				<0,010	<0,010	0,022	<0,010
				<0,010	<0,010	0,047	<0,010
				<0,010	<0,010	3,6	<0,010
				<0,010	<0,010	6,2	0,015
				<0,010	<0,010	0,23	<0,010
				<0,010	<0,010	<0,010	<0,010
				<0,010	<0,010	<0,010	<0,010
				<0,010	<0,010	<0,010	<0,010
				<0,010	<0,010	<0,010	<0,010
				<0,010	<0,010	<0,010	<0,010
Jordkvalitetskriterium			50	200	5	5	5

- Key points:
  - It takes a lot of effort to get a good feel for the data
  - Geostatistical software/modelling can help us compile and visualize the data

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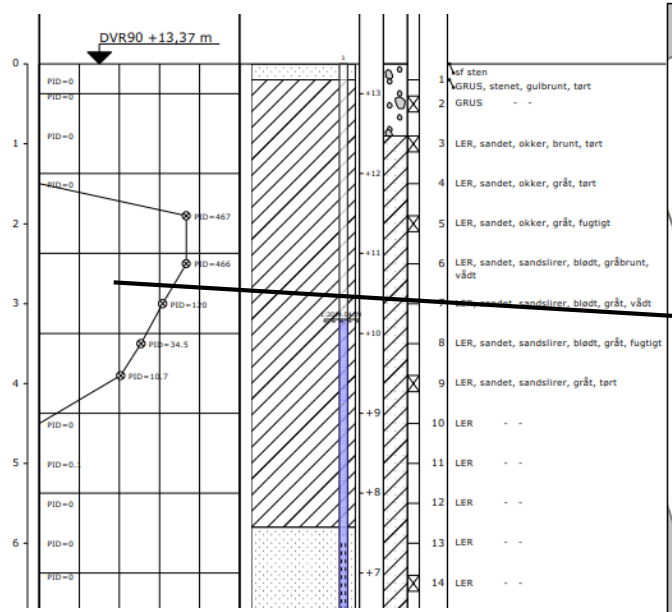
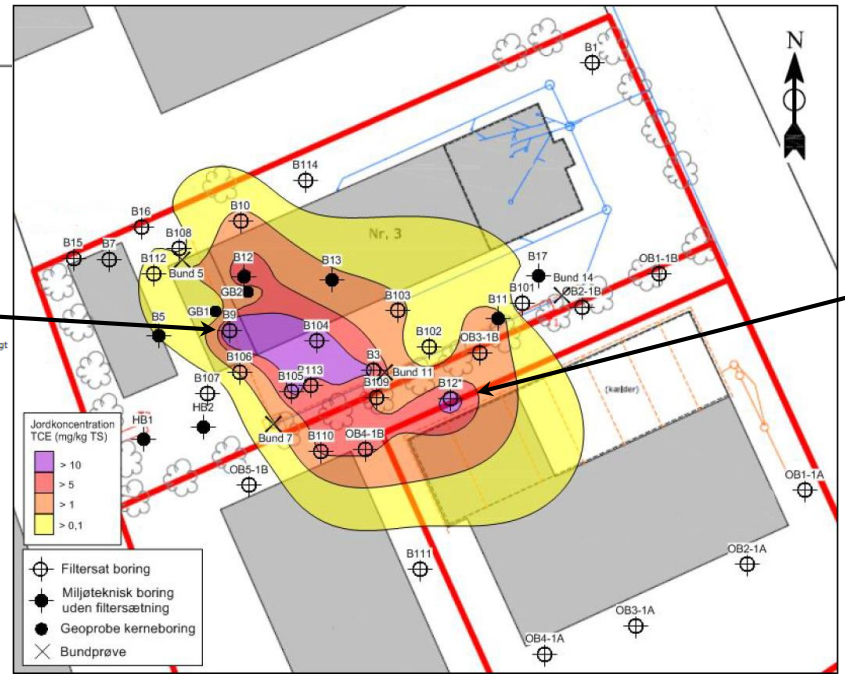
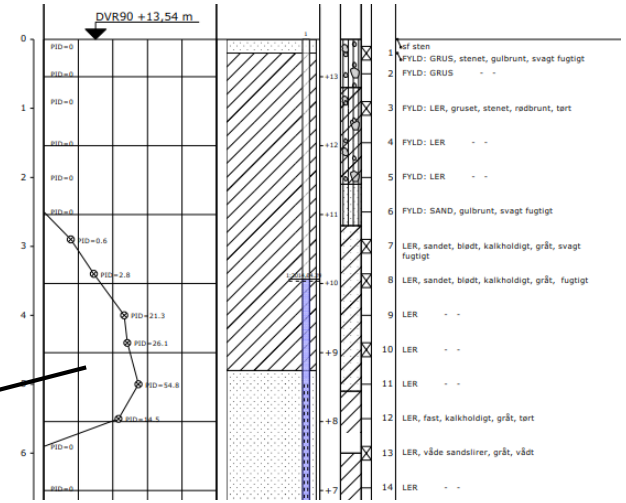
Mass estimate – including uncertainties

- How do we estimate contaminant mass?







TCE-konc. (mg/kg TS)	Areal (m^2)	Antaget lagtykkelse (m)	Volumen (m^3)	Heraf kælder (m^3)	Effektivt jordvolumen (m^3)
> 0,1	1285	5,0	6.425	595	5.830
> 1,0	617	3,0	1.851	210	1.641
> 5,0	258	2,5	645	-	645
> 10	81	1,25	101	-	101

- Area · depth · ρ_b · avg. conc. = 30 kg TCE
- Added uncertainty on layer thickness ± 0,5 m
- Key points:
  - It's time consuming and associated with low "confidence"
  - Geostatistical software/modelling can help us

TCE-konc. (mg/kg TS)	Effektivt jordvolumen (m^3)	Gns. TCE-konc. (mg/kg TS)	TCE-masse (kg)
0,1 – 1,0	4.189	0,37	2,6
1,0 – 5,0	996	2,53	4,3
5,0 – 10	544	7,12	6,6
> 10	101	13,91	2,4
		SUM:	Ca. 16

13-19 kg TCE

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Advantages of applying geostatistical modelling

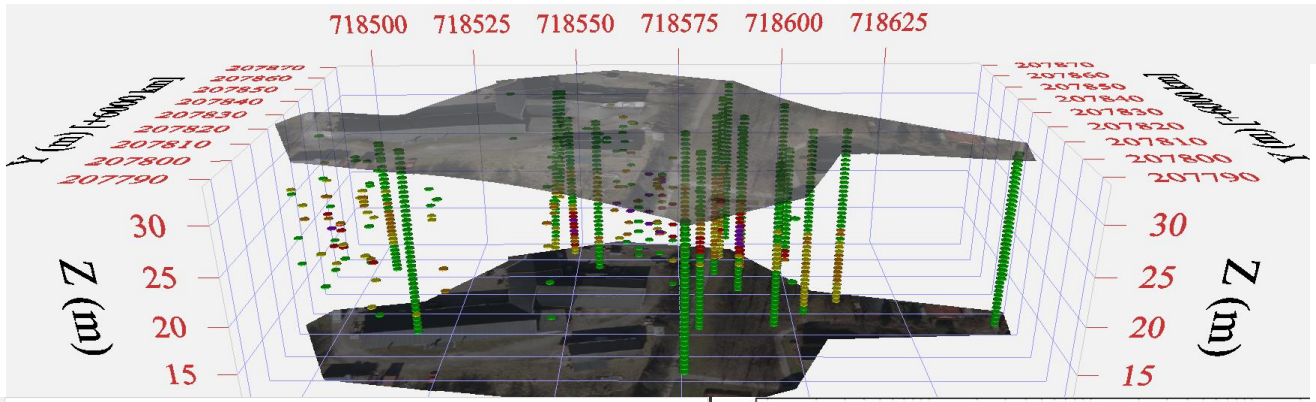
- I have applied a software package (Kartotrak) at ~10 cases now.
- So I want to relay to you some of the things I really like about geostatistical modelling.

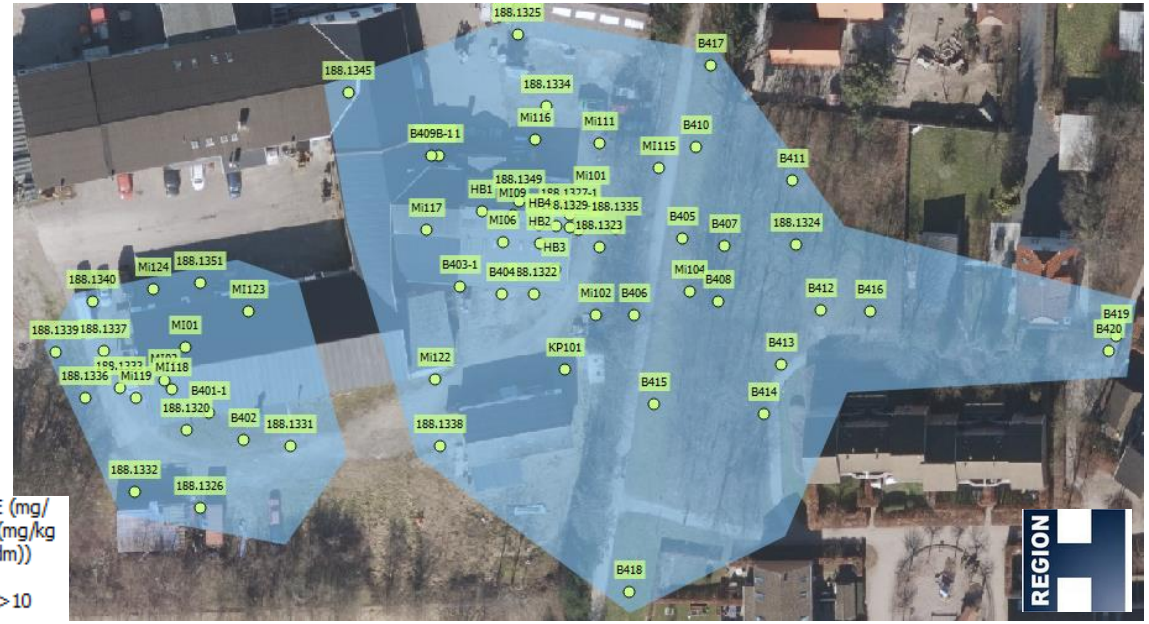
- I feel like I get more out of my data:
  - I can include semi-quantitative data (like PID),
  - A best estimate less influenced by "expert judgement" (kriging),
  - Uncertainty estimates of mass and volume (conditional simulation).

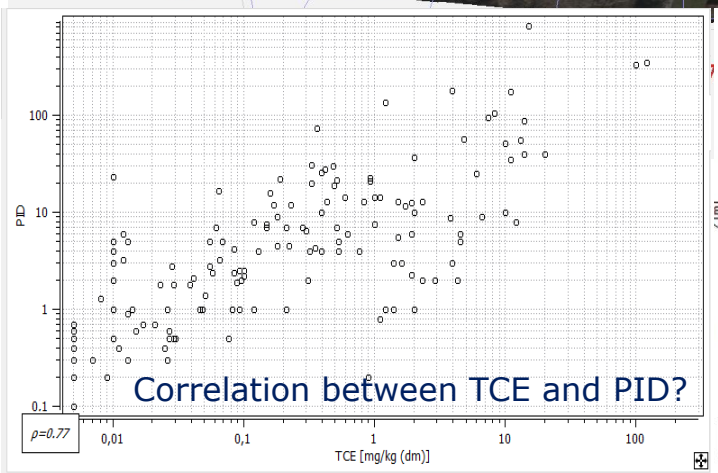
- I get integrated 2D and 3D visualization of my data and results:
  - Even of where to collect more data to reduce uncertainty.

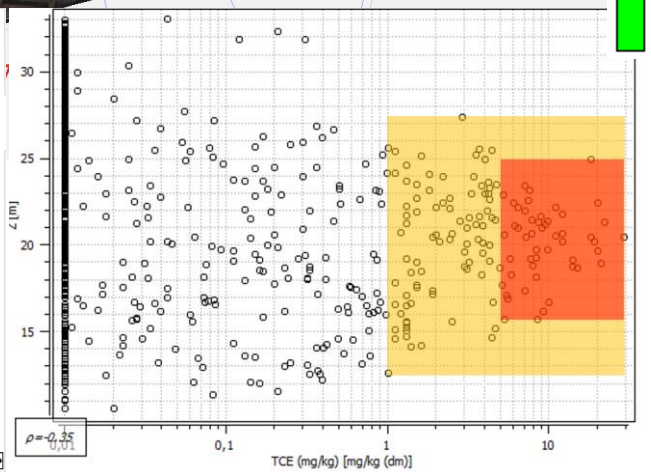
How do we do it? (part 1)

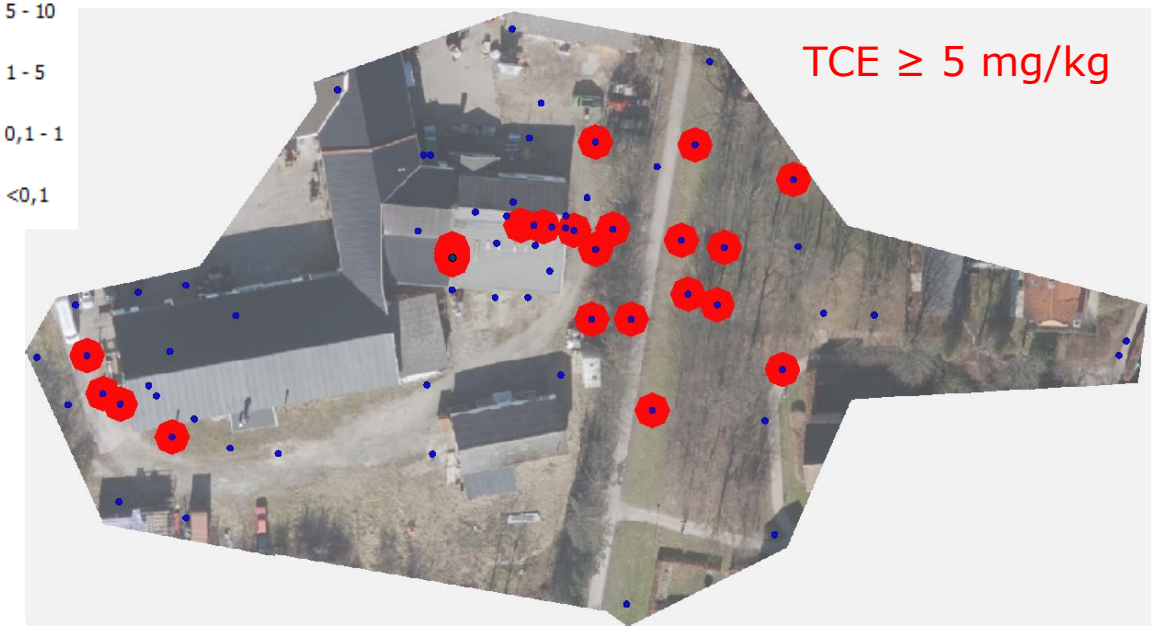
A. Collect georeferenced data (X, Y, Z)
B. Do a thorough data check/wash
C. Explore the data –check vs. CSM









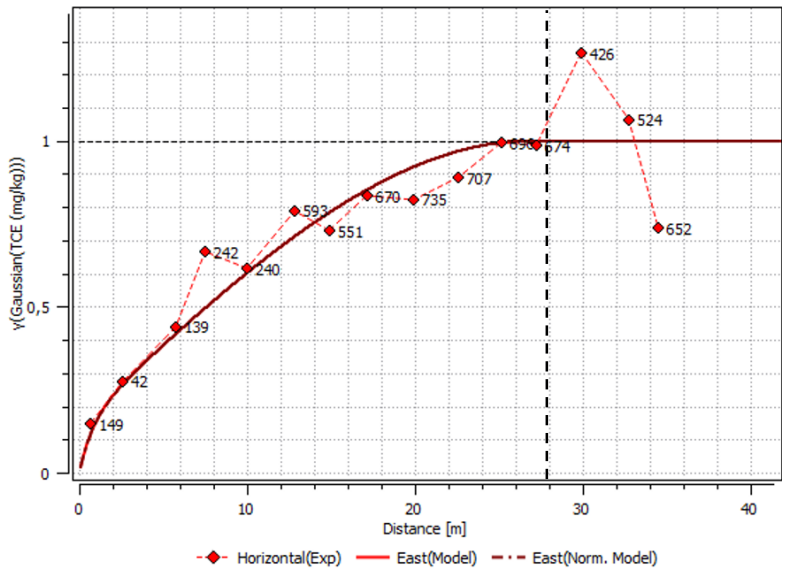


TCE ≥ 5 mg/kg (8-17,2 m bgs.)
TCE ≥ 1 mg/kg (5,5-20,5 m bgs.)

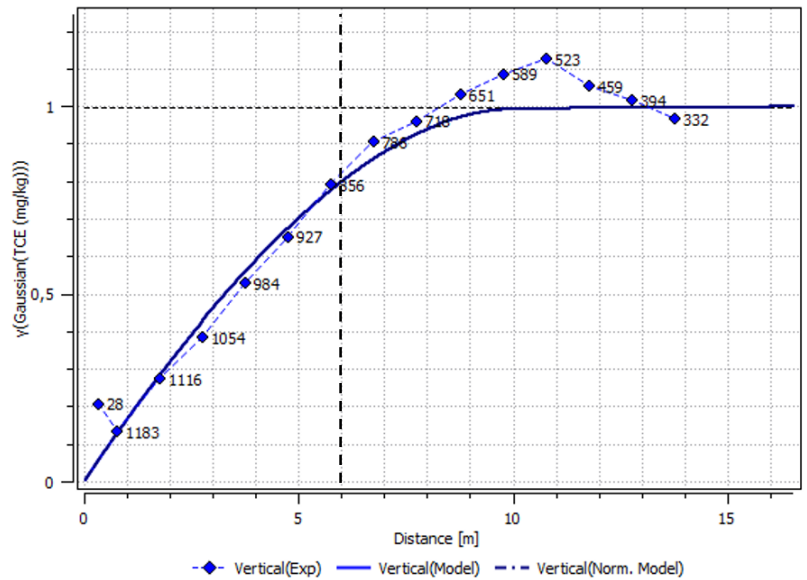
How do we do it? (part 2)

D. Analyze the spatial structure of the data

Horizontal structure (TCE) <28 m

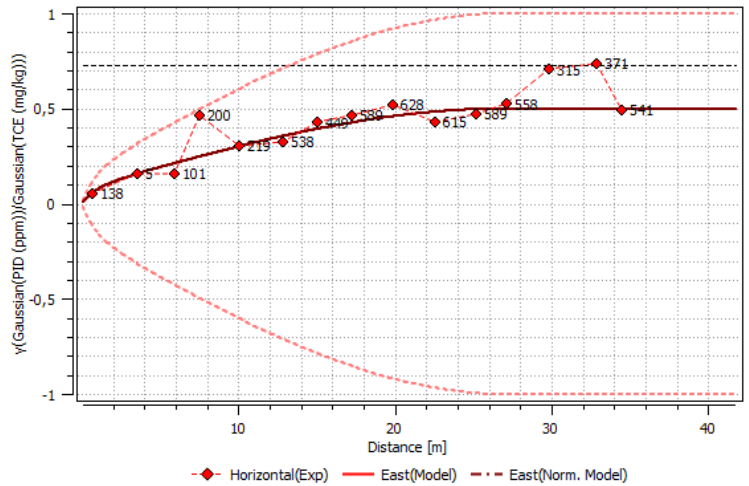


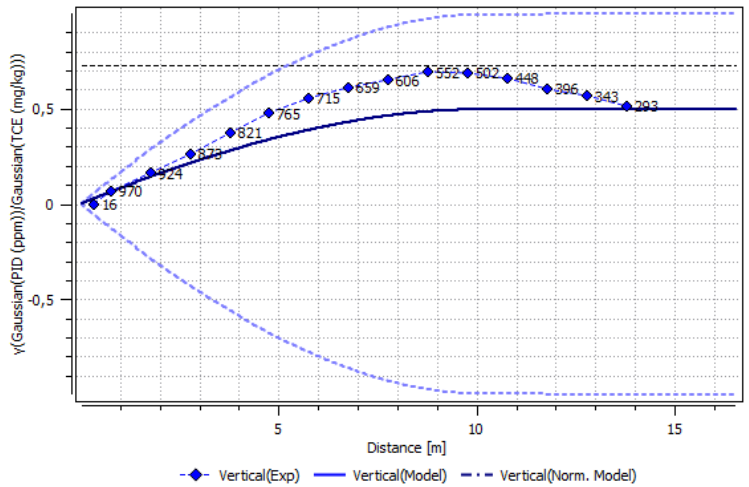
Vertical structure (TCE) <6 m



More variance/difference between TCE concentrations collected further apart

Cross-variograms PID-TCE





- We run the model based on these structures

E. Define objectives up front - results should support decision-making

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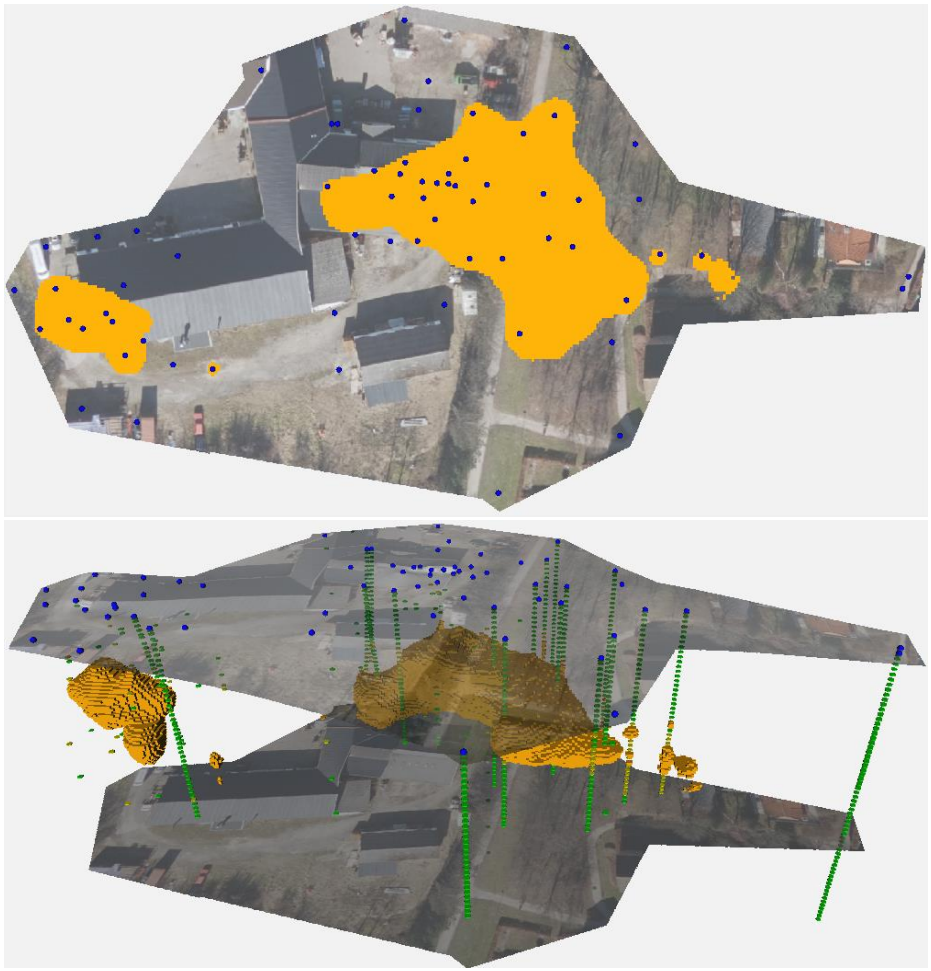
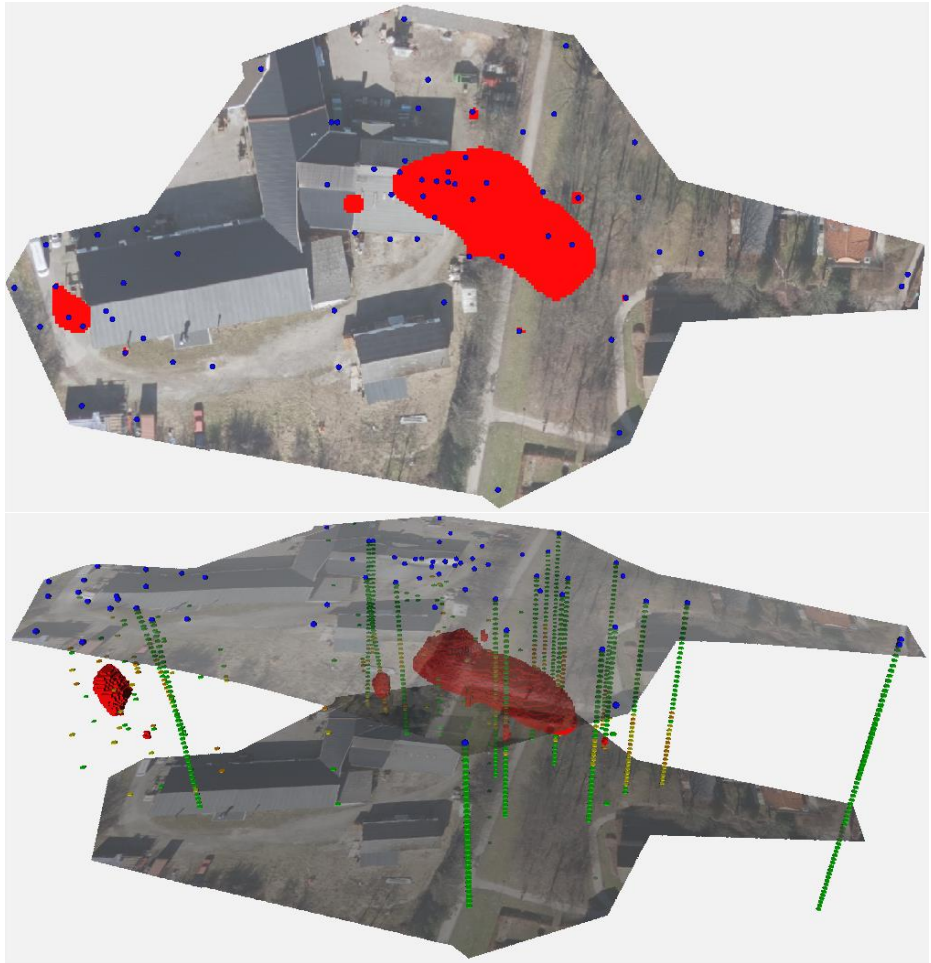
How do we do it? (part 3)

F. Perform kriging (obtain best estimate)

TCE ≥ 1 mg/kg



TCE ≥ 5 mg/kg



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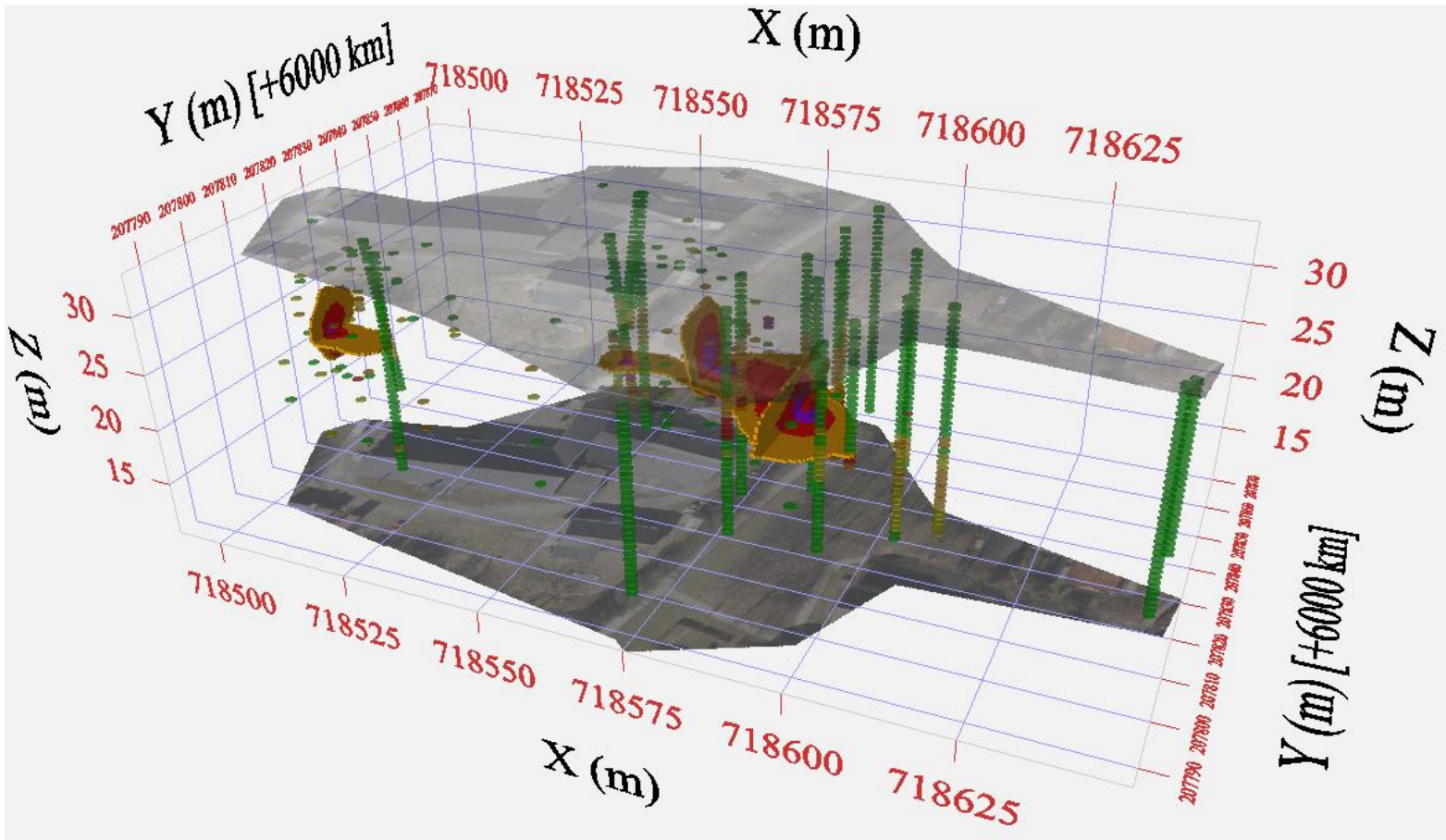
How do we do it? (part 3)

F. Perform kriging (obtain best estimate)



Mass estimate: 183 kg TCE in two hot-spots
~64% in volumes with TCE > 5 mg/kg
~86% in eastern hot-spot

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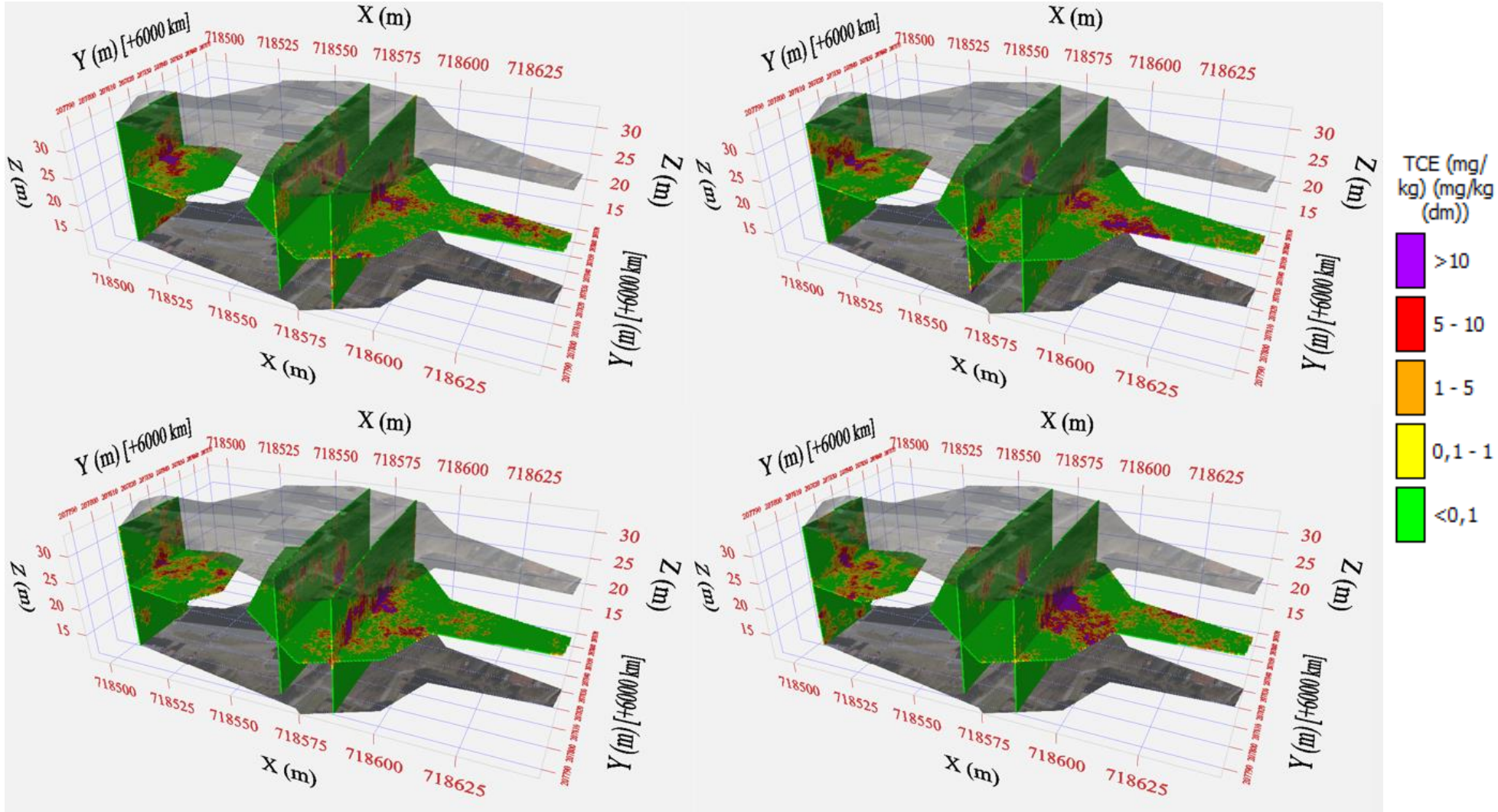
How do we do it? (part 4)

G. Perform conditional simulation (Monte Carlo simulation)

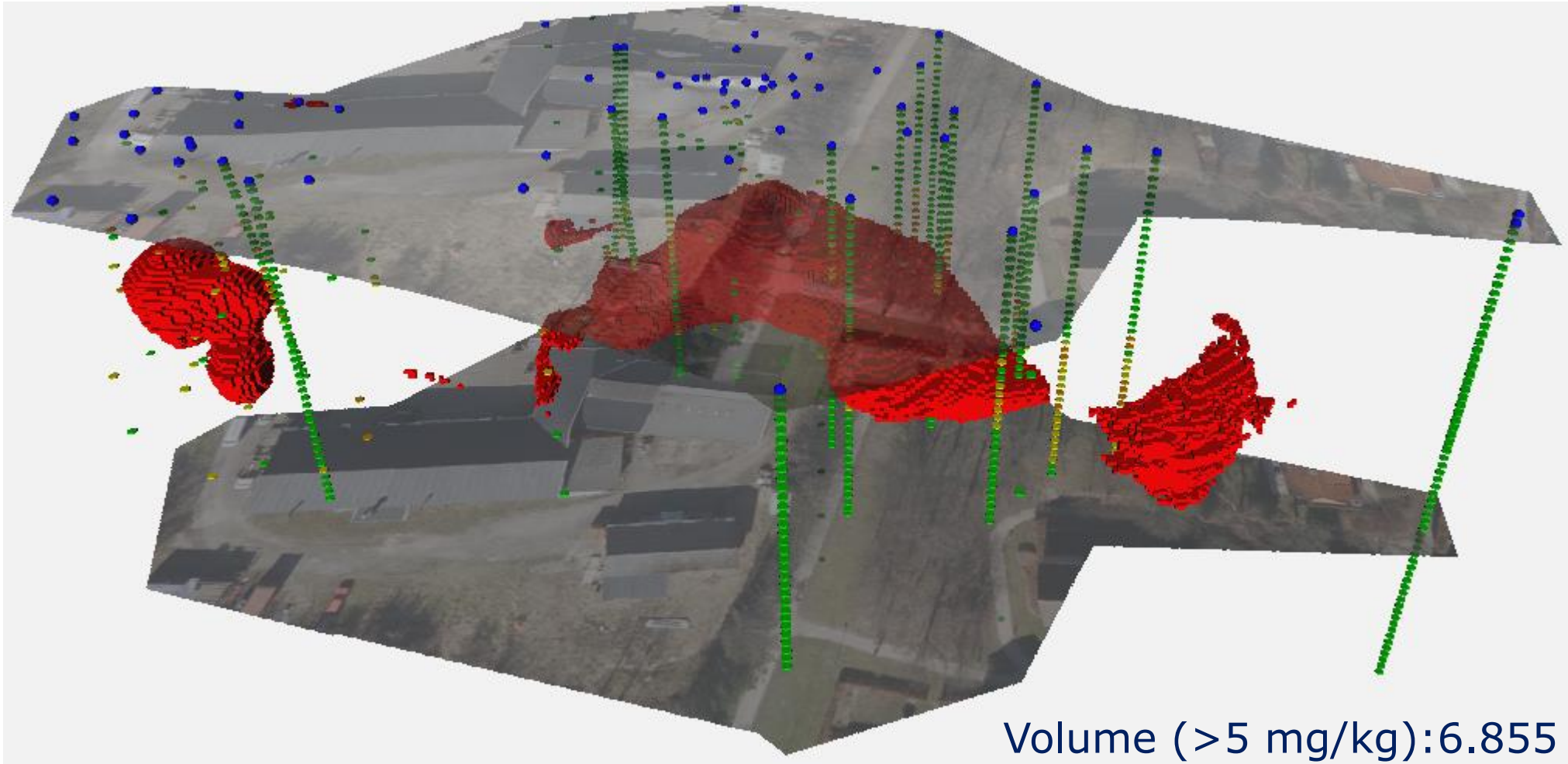


Mass estimate: 183 kg TCE @ 90% [137-266 kg]

How do we do it? (part 4)

G. Perform conditional simulation (Monte Carlo simulation)

- The data allows to work at the 17,5% risk level (5 mg/kg) for remediation



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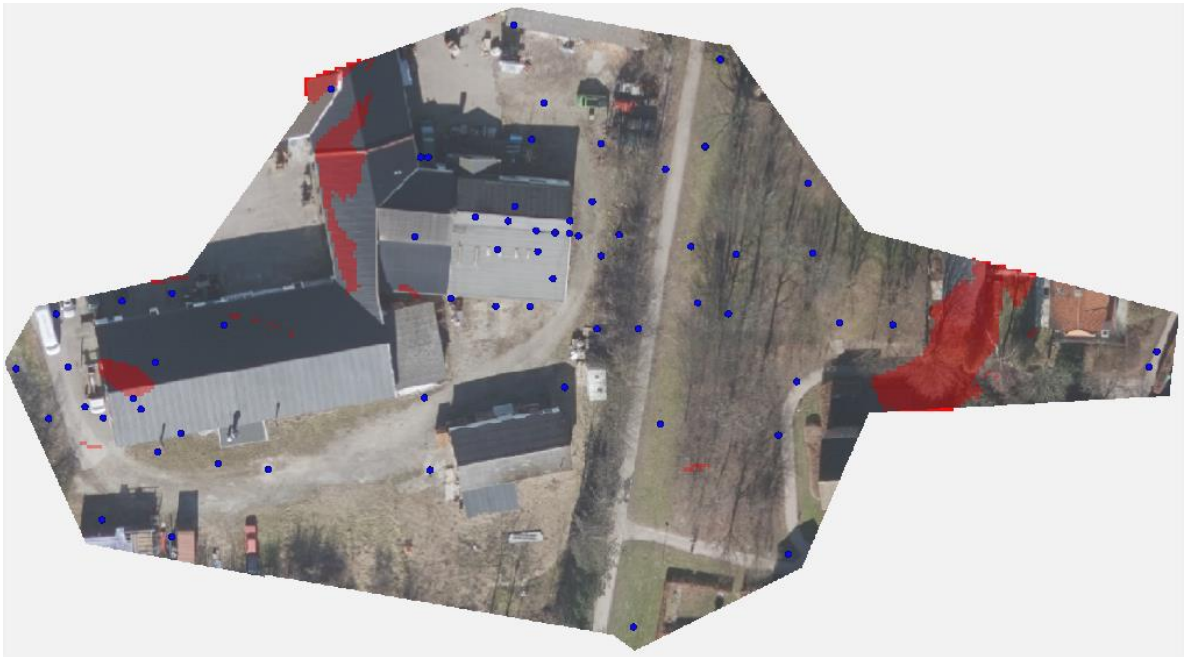
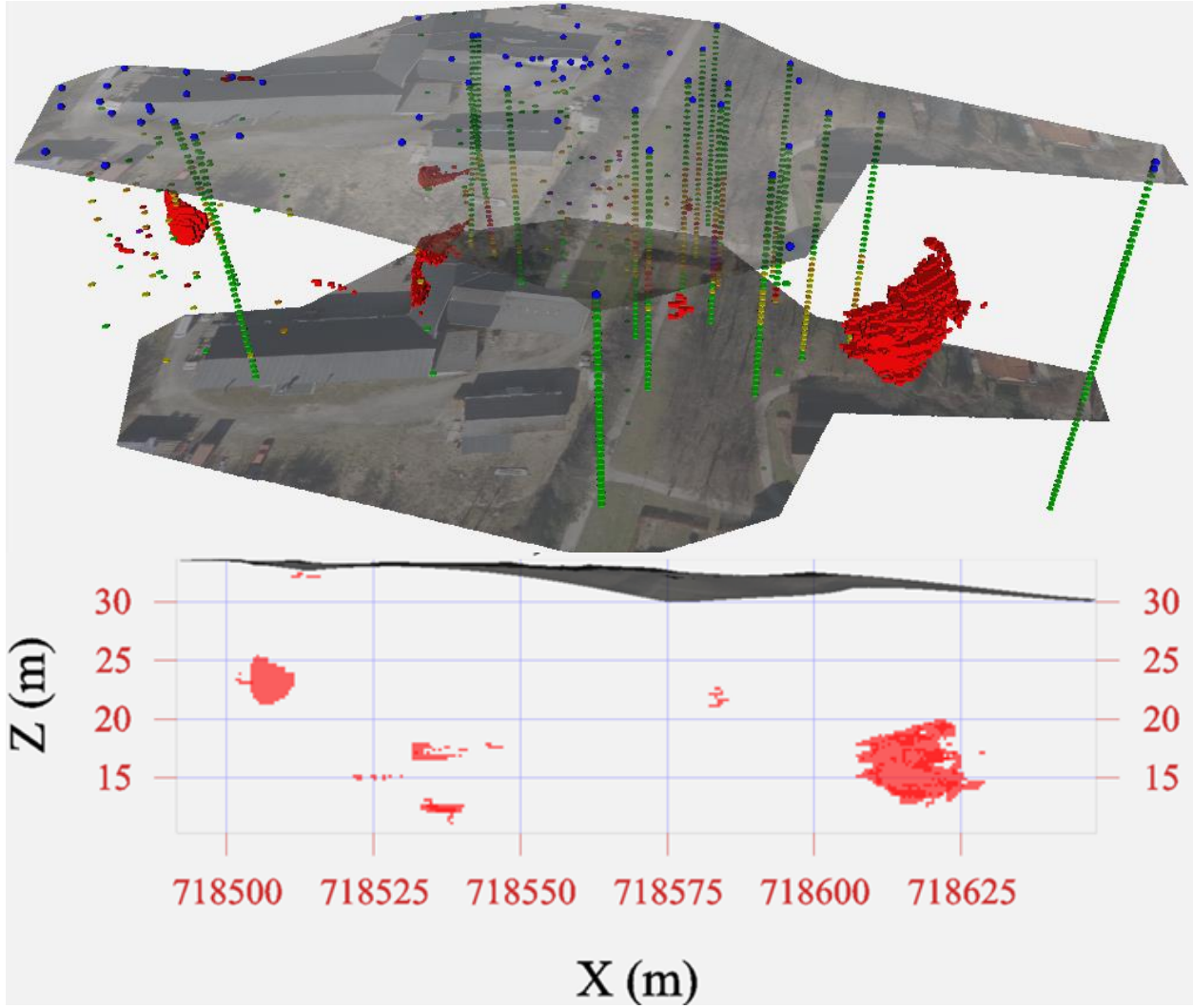
How do we do it? (part 4)

G. Perform conditional simulation (Monte Carlo simulation)

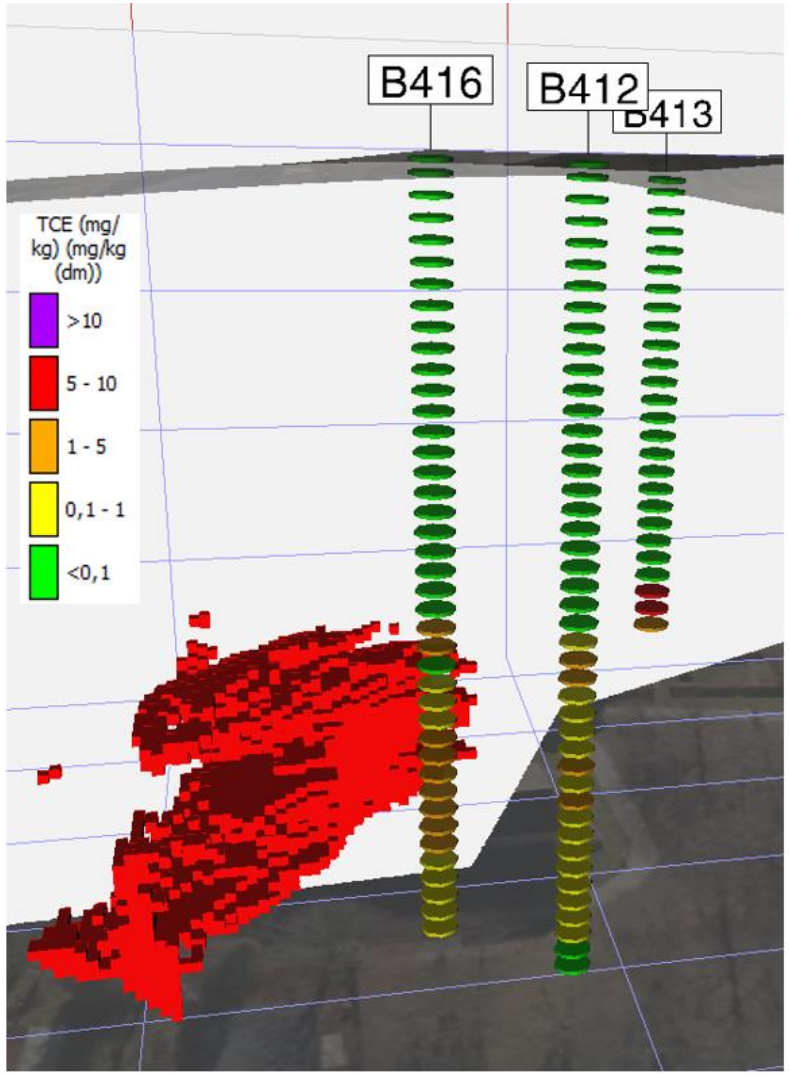
- The most uncertain parts of the data at the 17,5% risk level (5 mg/kg)

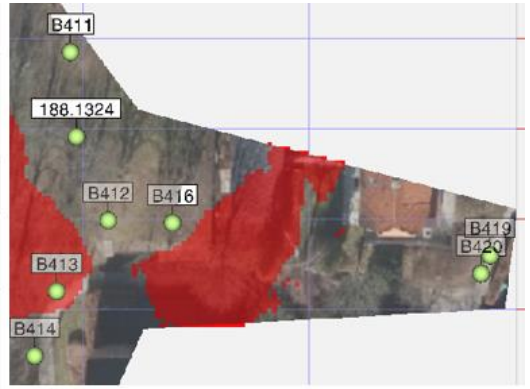




Uncertain volumes with a risk of having high concentrations (>5 mg/kg) can now be targeted for further sampling.

Discussion about uncertainties





Dybde	B416	B412	B413
(m u.t.)	(mg/kg TS)		
10,0	<0,01	<0,01	<0,01
10,5	<0,01	<0,01	<0,01
11,0	<0,01	<0,01	<0,01
11,5	2,0	<0,01	8,3
12,0	3,1	0,18	8,3
12,5	<0,01	3,9	3,0
13,0	0,11	3,2	
13,5	0,33	0,16	
14,0	0,32	0,32	
14,5	1,5	0,59	
15,0	1,3	0,69	
15,5	1,1	1,3	
16,0	1,2	0,76	
16,5	1,3	1,3	
17,0	1,3	0,76	
17,5	1,1	0,61	
18,0	0,40	0,36	
18,5	0,13	0,15	
19,0	0,32	0,23	
19,5	0,33	0,38	
20,0	0,14	0,16	

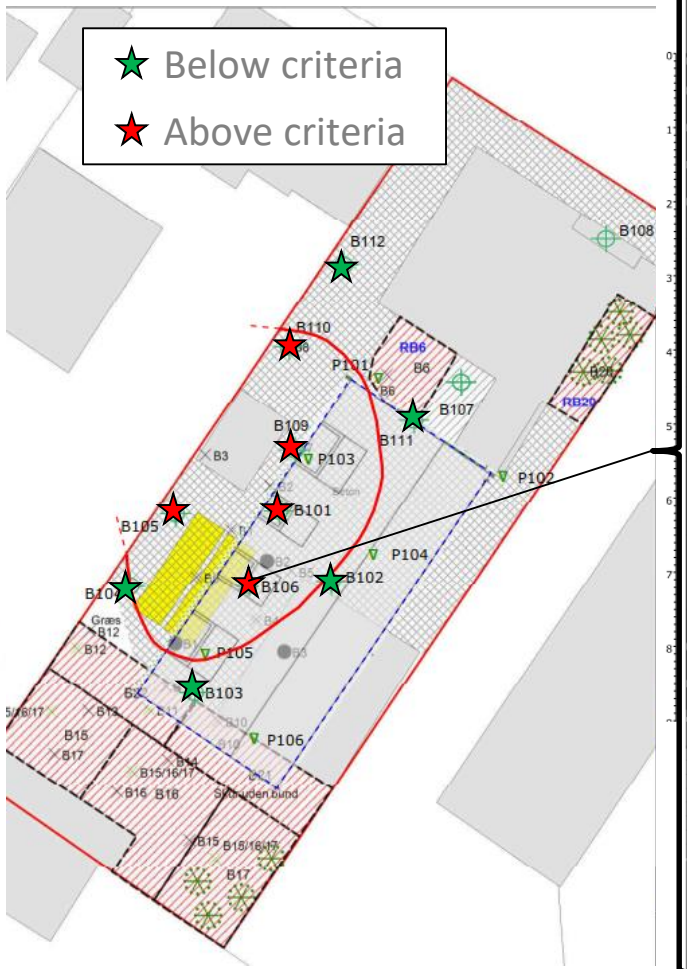
- We have to redefine our strategy when working with uncertainty!

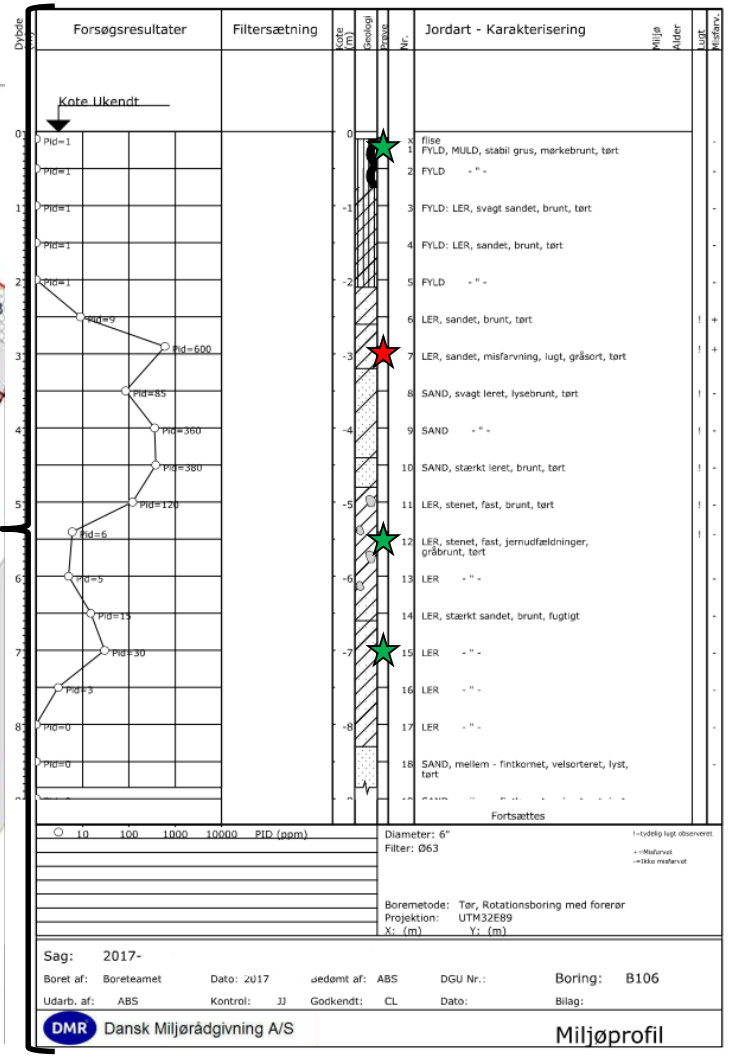
Can we do more with less data, too?

- Geostatistical software can make it easy to visualize our data.
- Kriging provides an unbiased estimate of contaminate mass and location – less based on "expert judgement".
- Something like this:

Boring	Dybde	Benzen	C_6-C_{10}	C_{10}-C_{15}	C_{15}-C_{20}	C_{20}-C_{35}	THC
	m.u.t.	mg/kg TS	mg/kg TS	mg/kg TS	mg/kg TS	mg/kg TS	mg/kg TS
B101	0,5	i.p.	**30**	**260**	**13**	i.p.	**300**
B101	4,0	i.p.	**150**	**1.100**	**65**	i.p.	**1.400**
B101	6,0	i.p.	i.p.	i.p.	i.p.	i.p.	i.p.
B102	0,2	i.p.	i.p.	i.p.	i.p.	i.p.	i.p.
B102	4,0	i.p.	i.p.	i.p.	i.p.	i.p.	i.p.
B103	0,2	i.p.	i.p.	i.p.	i.p.	44	44
B103	4,0	i.p.	i.p.	i.p.	i.p.	i.p.	i.p.
B104	0,2	i.p.	i.p.	15	i.p.	i.p.	15
B104	4,5	i.p.	i.p.	i.p.	i.p.	i.p.	i.p.
B105	0,2	i.p.	i.p.	i.p.	i.p.	i.p.	i.p.
B105	4,5	i.p.	**860**	**4.700**	**730**	160	**6.400**
B105	6,5	i.p.	i.p.	i.p.	i.p.	i.p.	i.p.
B106	0,2	i.p.	i.p.	i.p.	i.p.	i.p.	i.p.
B106	3,0	i.p.	**62**	**390**	41	i.p.	**490**
B106	5,5	i.p.	i.p.	i.p.	i.p.	i.p.	i.p.
B106	7,0	i.p.	i.p.	i.p.	i.p.	i.p.	i.p.
B109	0,2	i.p.	**35**	**350**	41	88	**510**
B109	3,5	i.p.	**77**	**540**	21	i.p.	**640**
B109	5,5	i.p.	**97**	**850**	27	i.p.	**980**
B109	6,0	i.p.	i.p.	i.p.	i.p.	i.p.	i.p.
B110	5,0	i.p.	i.p.	**65**	i.p.	i.p.	65
B110	5,5	i.p.	i.p.	i.p.	i.p.	i.p.	i.p.
B111	4,0	i.p.	i.p.	i.p.	i.p.	i.p.	i.p.
B112	4,5	i.p.	i.p.	i.p.	i.p.	i.p.	i.p.
Jordkvalitetskriterier		1,5	25	40	55	100	100
Afskæringskriterium		-	-	-	-	300	-

- 10 boreholes
- 24 soil samples
- 144 PID measurements





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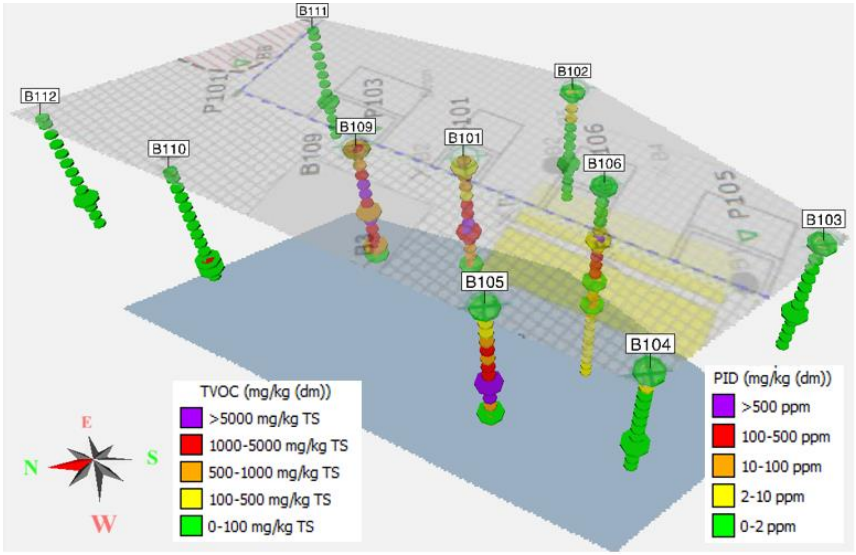
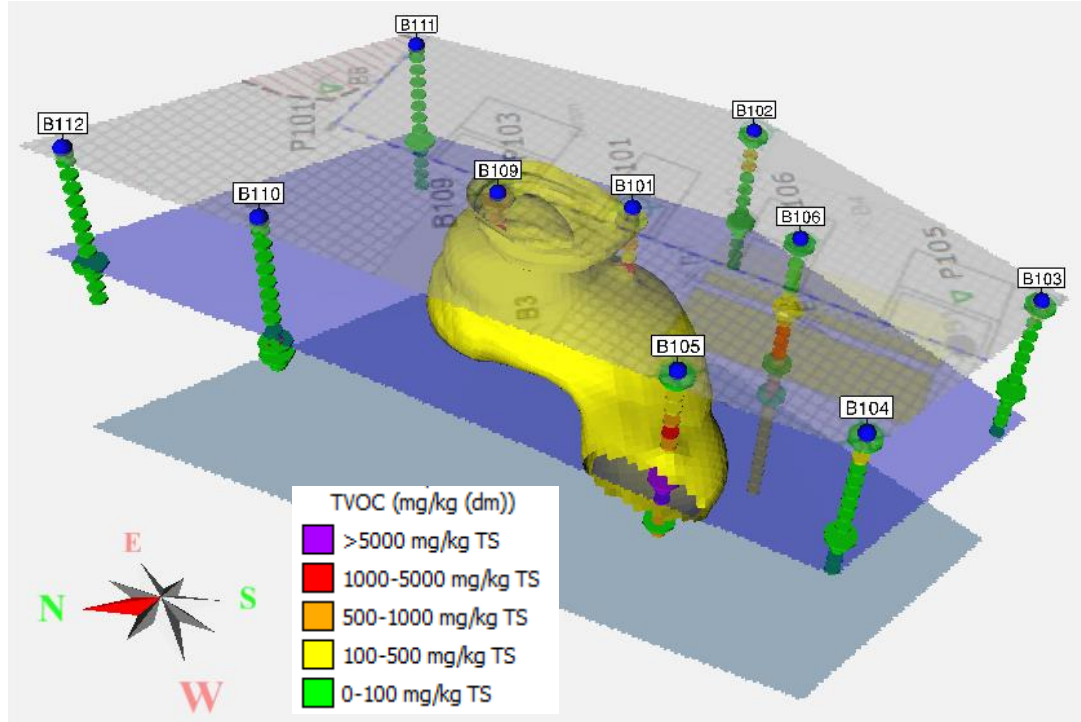
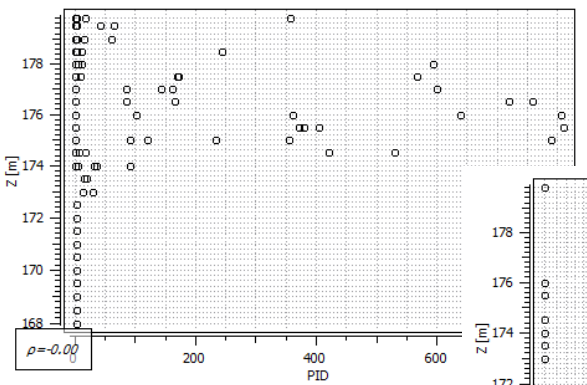
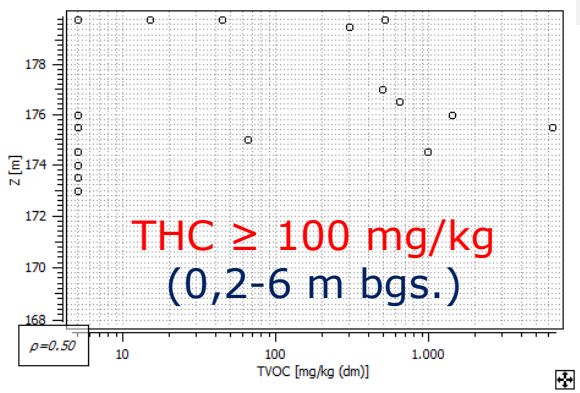
Can we do more with less data, too?

- Can turn into this (kriging THC > 100 mg/kg):



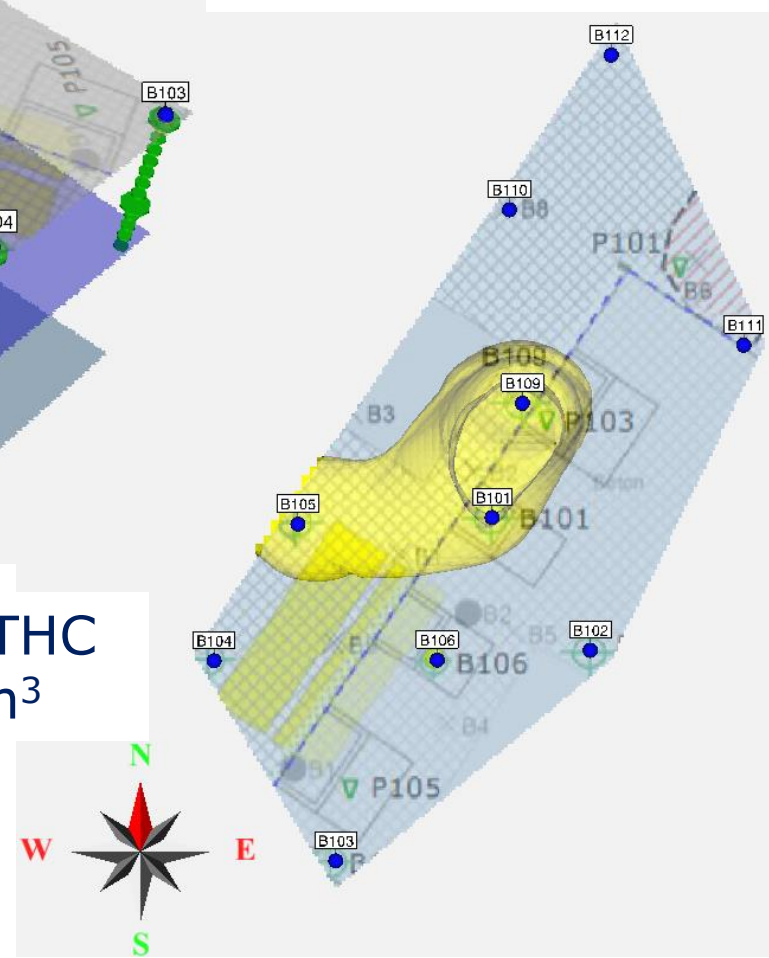






THC ≥ 100 mg/kg
(0,2-6 m bgs.)

Mass estimate = 890 kg THC
Volume estimate = 450 m³



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Summary

- Geostatistical modelling can help us get the most out of our money.
- With today's data density, we need only to apply the right tools.

Thank you ?