

Møde i ATV Jord og Grundvand om PFAS i jord og grundvand - hvad har vi lært?

# Monitering og modellering af PFAS skæbne i umættet zone

## SCENARIOS

Knud Erik Klint<sup>1</sup>, John Bastrup<sup>1</sup>, Samuel Kolade<sup>2</sup>, Ofer Dahan<sup>2</sup> Nadia Bali<sup>3</sup>, Christos Tsakiroglou<sup>3</sup>

<sup>1</sup>GEO, Copenhagen, Denmark

<sup>2</sup>Zuckerberg Institute for Water Research, Ben-Gurion University of the Negev, Israel

<sup>3</sup>Foundation for Research and Technology Hellas, Institute of Chemical Engineering Sciences, 26504 Patras, Greece

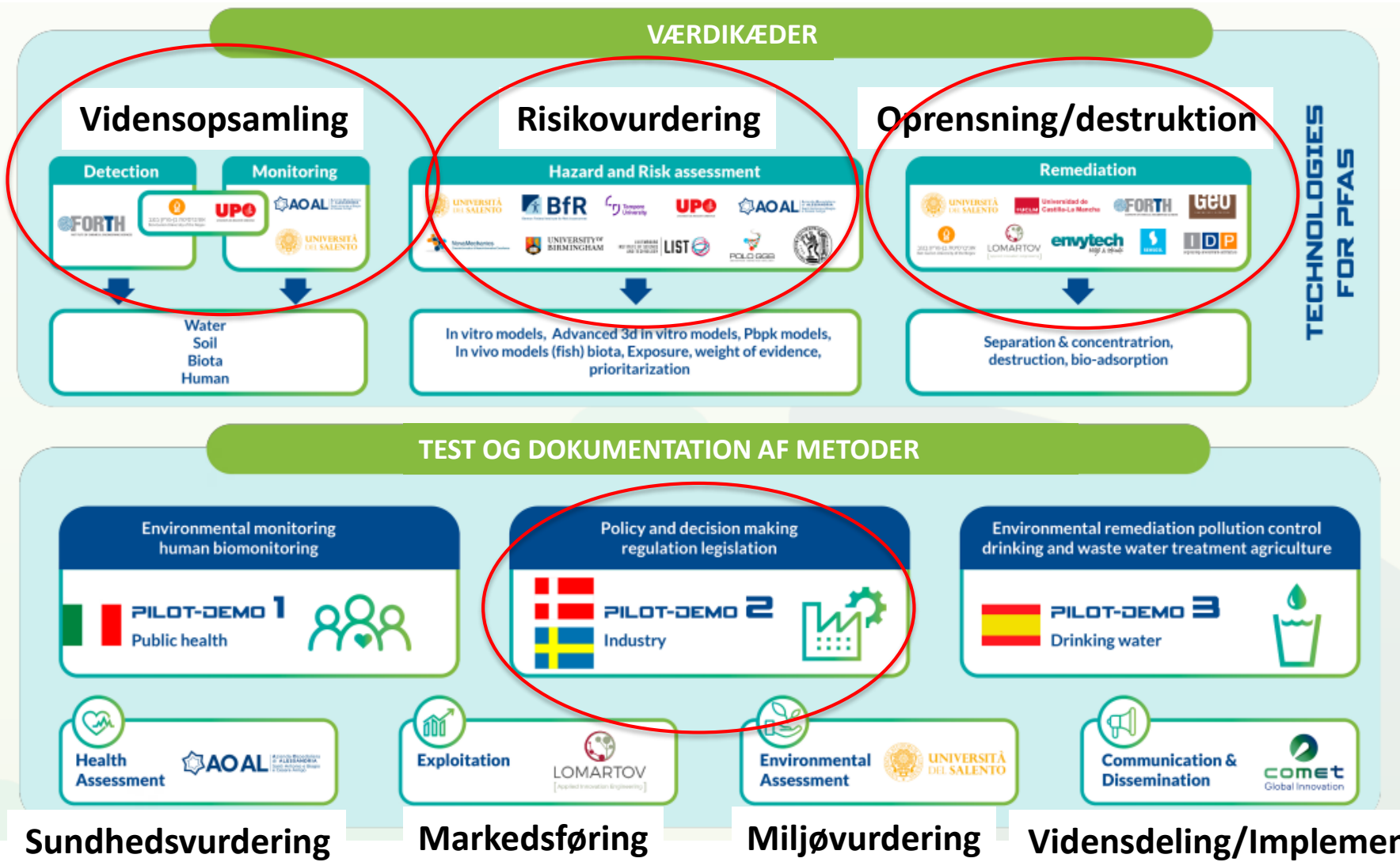


This project has received funding from the H2020 programme under Grant Agreement No. 101037509



# Baggrund: PFAS undersøgelser

## SCENARIOS Horizon 2020 projekt



- **Korsør Rescue center (Danmark)**  
smeltevandssand/silt/ler  
morænesand, i issøbakke
- **Trelleborg brandøvelses plads (Sverige)**  
Losseplads på moræneler og  
smeltevandssand i ådal

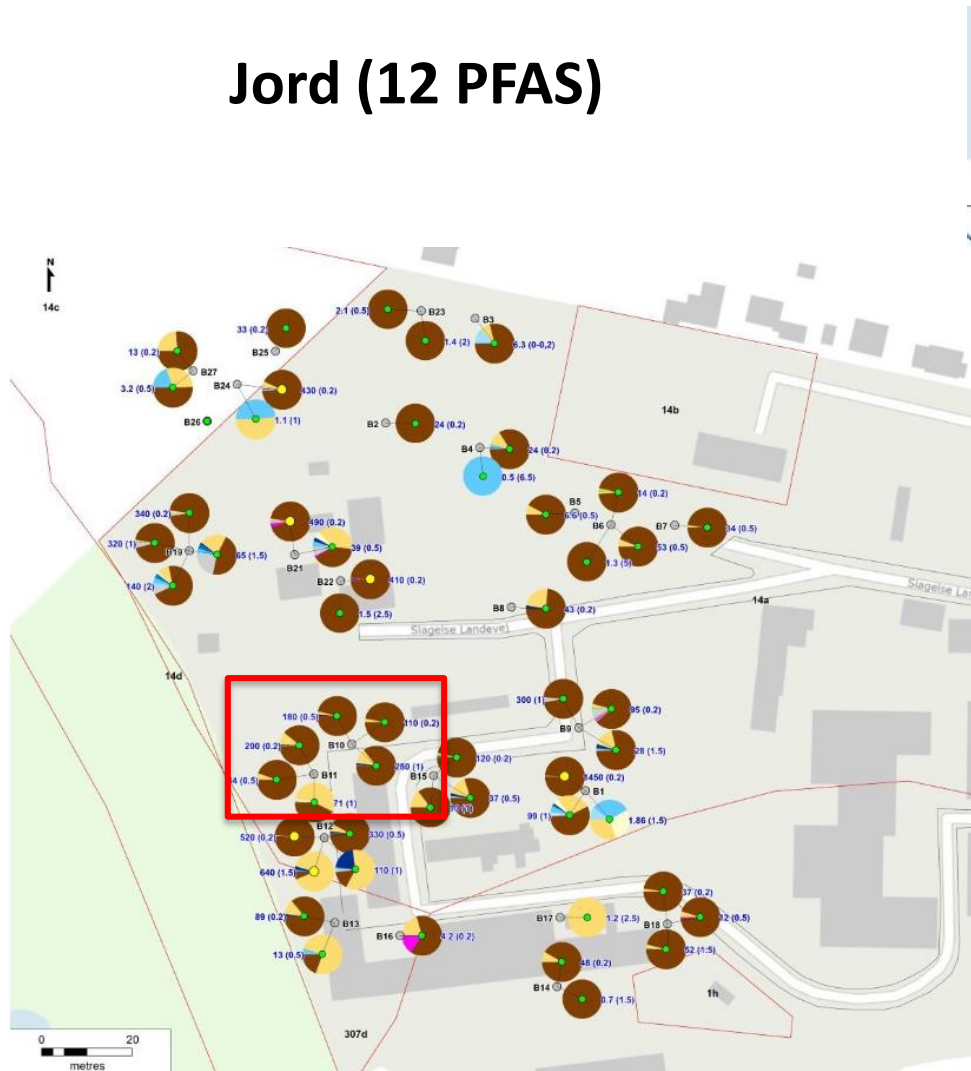




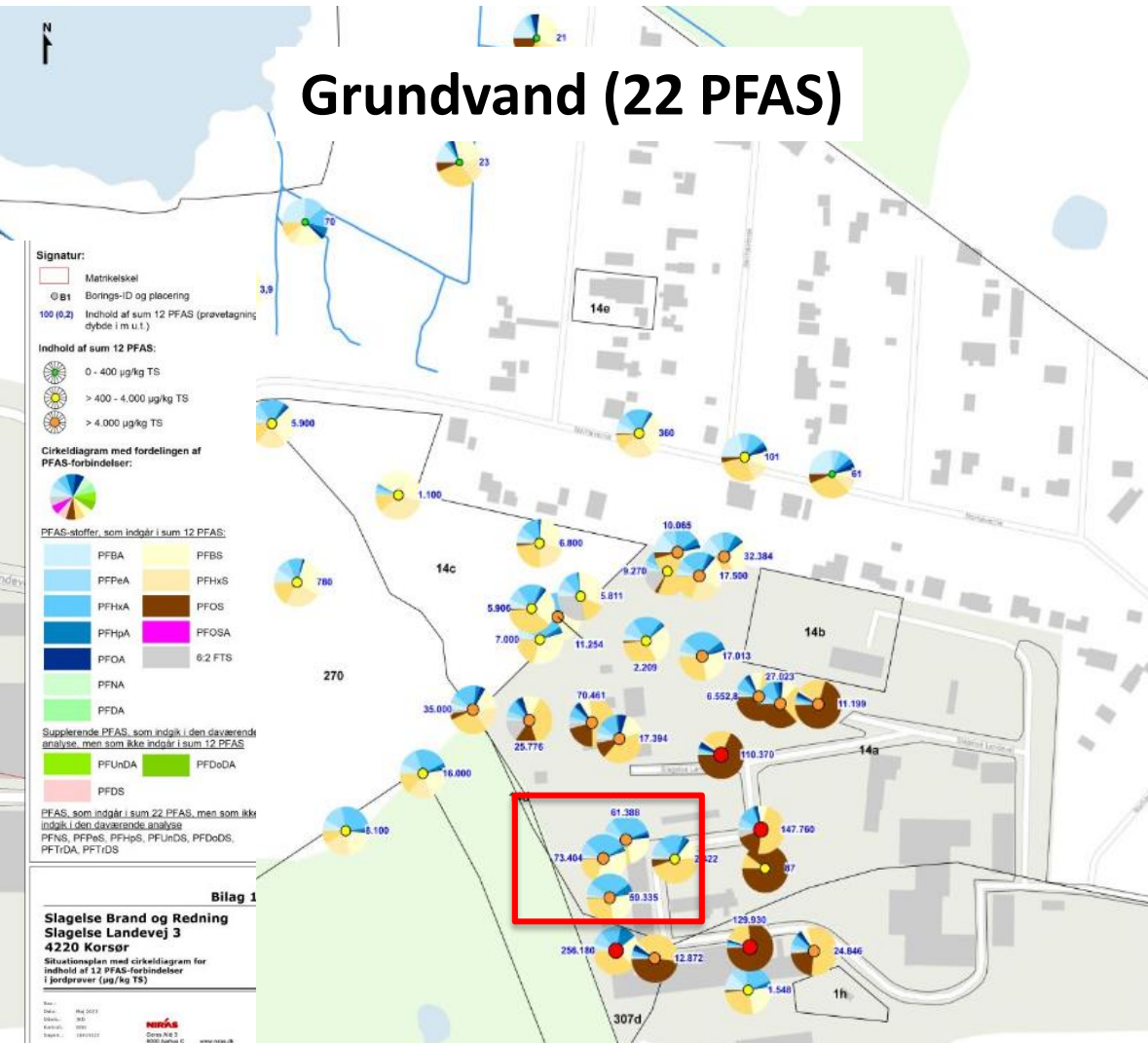




## Jord (12 PFAS)



## Grundvand (22 PFAS)



**Signatur:**

- Matrikelskel
- 1.500 Indhold af sum 12 / 22 PFAS [ng/l]

**Indhold af sum 12 / 22 PFAS:**

- > 0 - 100 ng/l
- > 100 - 10.000 ng/l
- > 10.000 - 100.000 ng/l
- > 100.000 ng/l

**Cirkeldiagram med procentfordelingen af 12 / 22 PFAS-forbindelser:**

PFBA	PFBS
PFPeA	PFPeS
PFHxA	PFHxS
PFHpA	PFHpS
PFOA	PFOS
PFNA	PFOSA
PFDA	6:2 FTS
PFUnDA	PFNS
PFDoDA	PFDS
PFTDA	PFUnDS
	PFDoDS
	PFTDS
	PFOSA

**Bilag 1**

**Slagelse Brand og Redning**  
**Slagelse Landevej 3**  
**4220 Korsør**

Situationsplan med cirkeldiagram for indhold af 12 PFAS-forbindelser i jordprøver (µg/kg TS)

Scale: 1:1.400

**Bilag 1**

**Slagelse Brand og Redning**  
**Slagelse Landevej 3**  
**4220 Korsør**

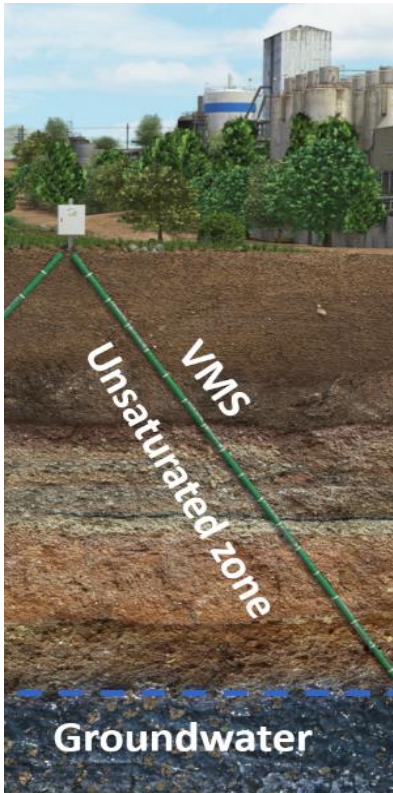
Situationsplan med cirkeldiagram for indhold af 12/22 PFAS-forbindelser i grundvand (ng/l)

NOVA  
 Dato: 14.03.2023  
 Udarbejdet af: 1409  
 Godkendt af: 2003  
 Tegnet af: 1042/419

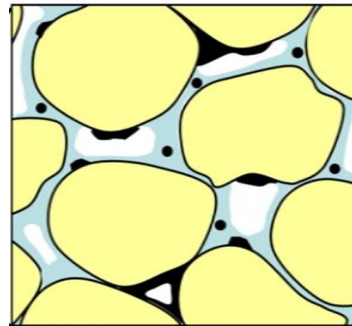
NOVA  
 CVR: 28050  
 BOKS A/S  
 www.nova.dk

## Pilot område:

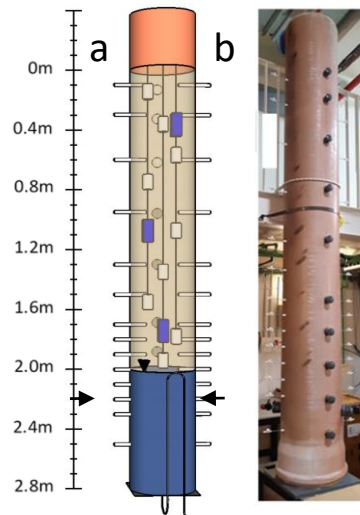
Prøvetagning og Monitoring  
Tidsserier af nedbør, vand og jord data i 2 år



## Pore scale study

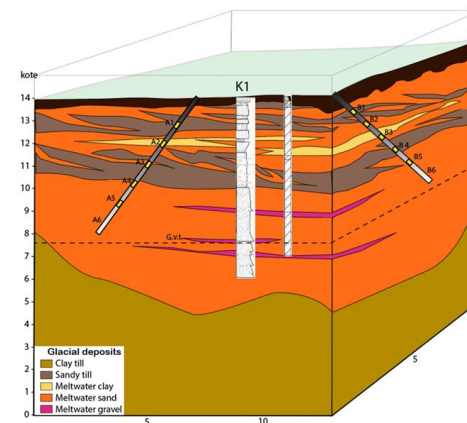


## Lab scale study

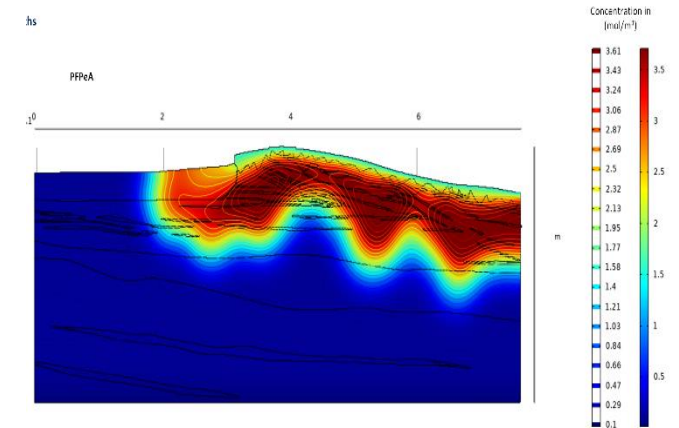
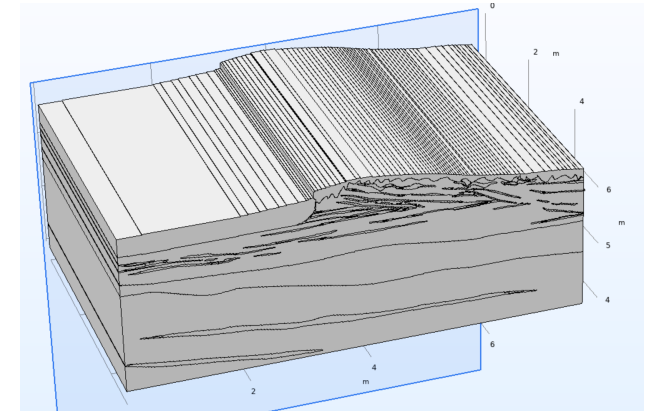


## Parameterestimering

- Konceptuel model
- jordparametre
- Nedbør
- Infiltration
- PFAS koncentration
- Udvaskning/binding
- Transport i matrix og makropore



## Modellering/Risikovurdering



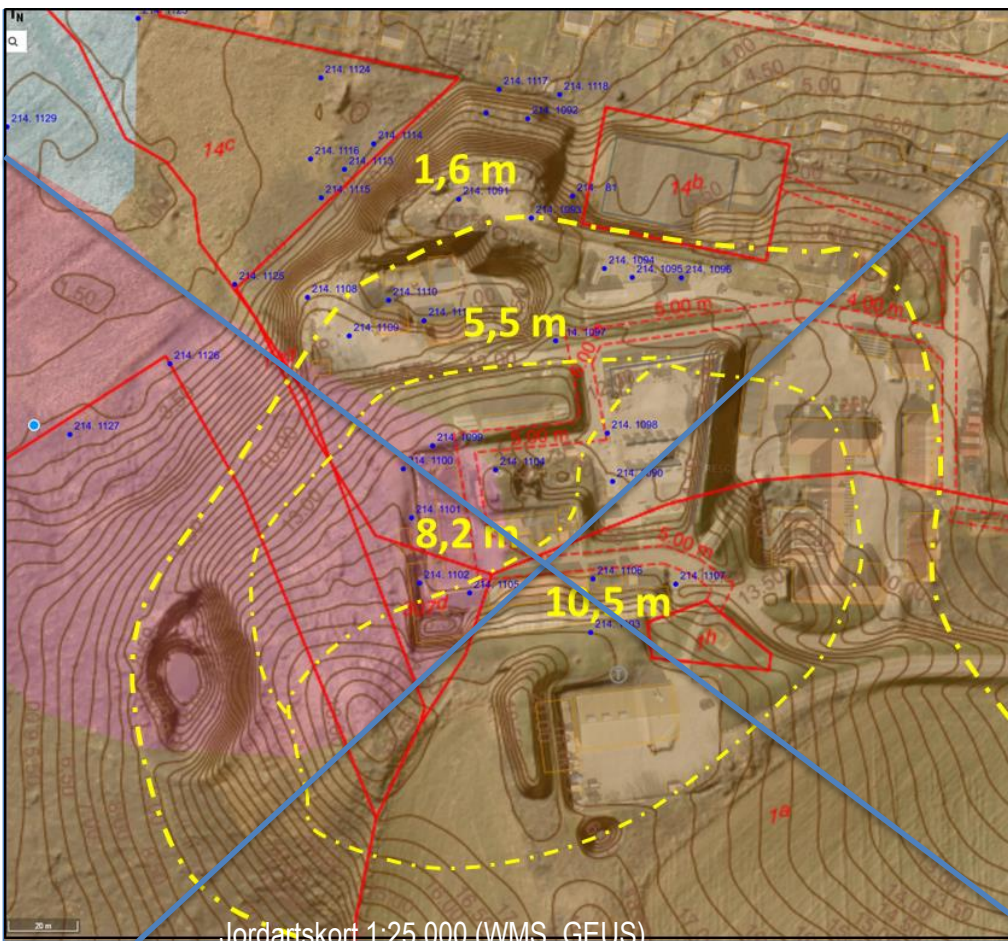


# Multi skala 3-D geologisk modellering og monitoring

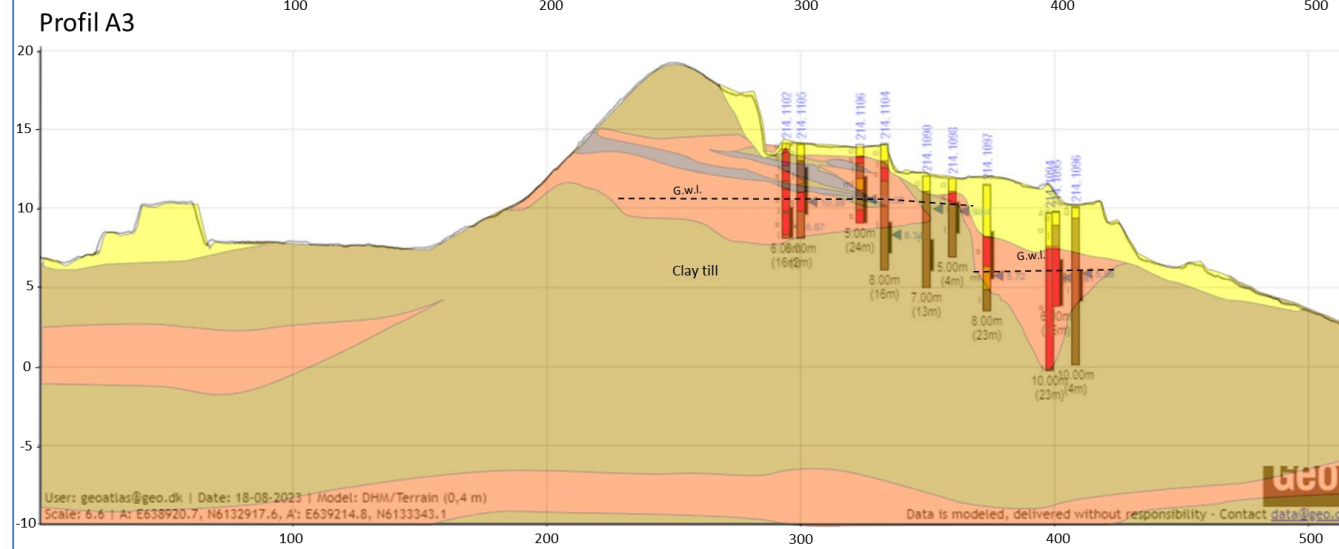
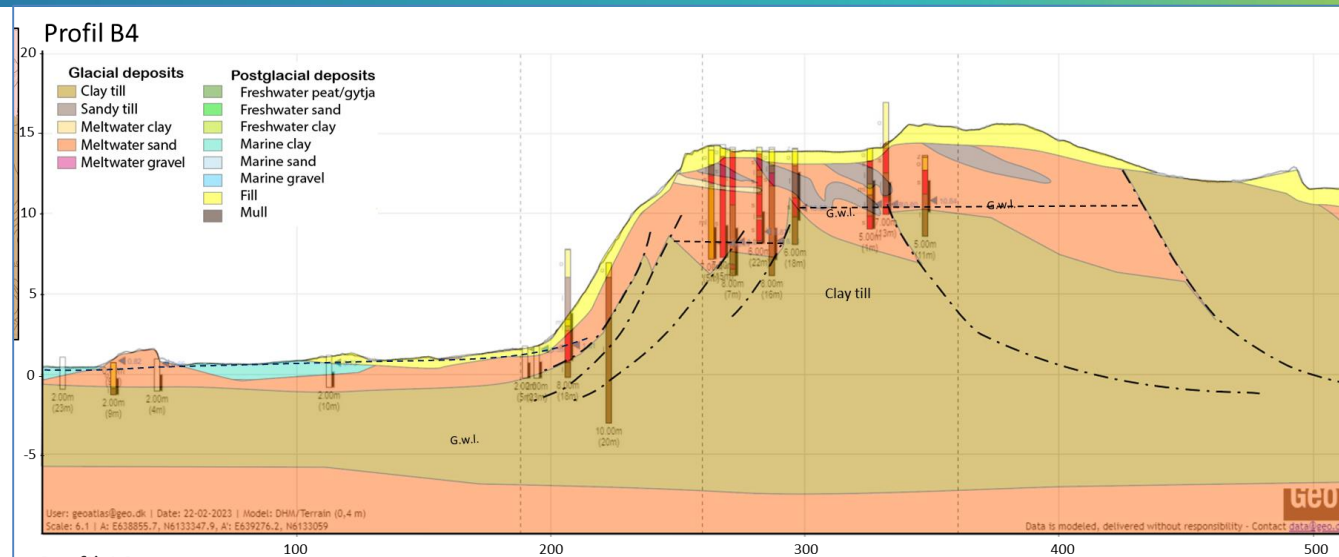




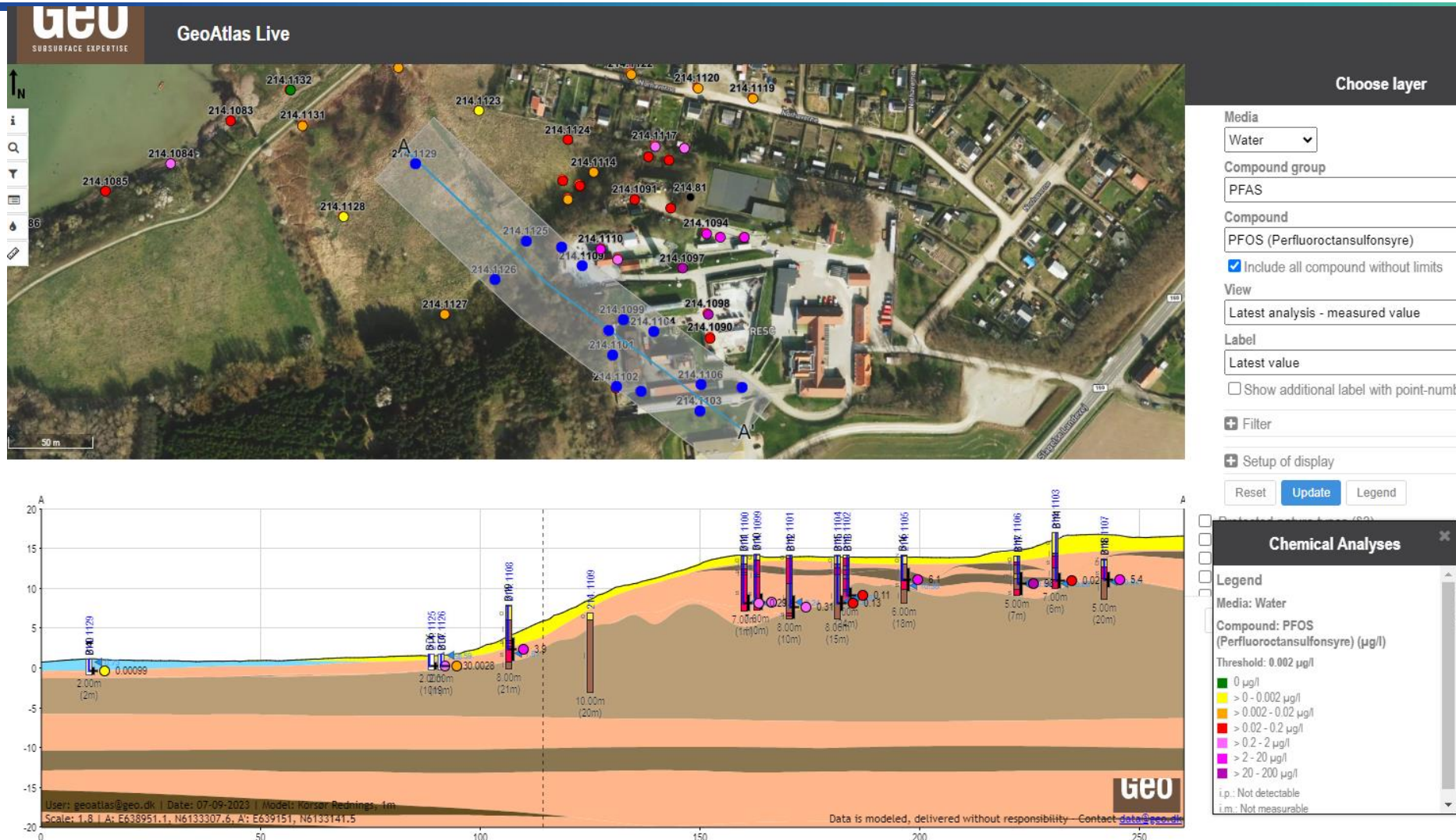
Flere separate grundvandsmagasiner med individuel gv.sp.



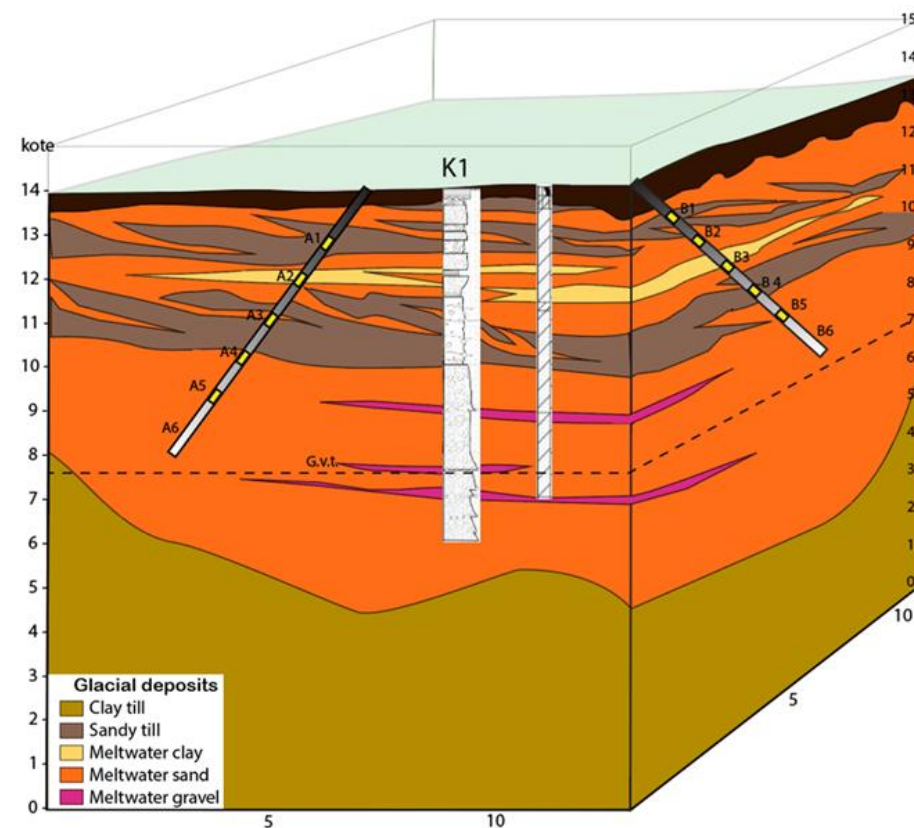
Jordartskort 1:25.000 (WMS, GEUS)





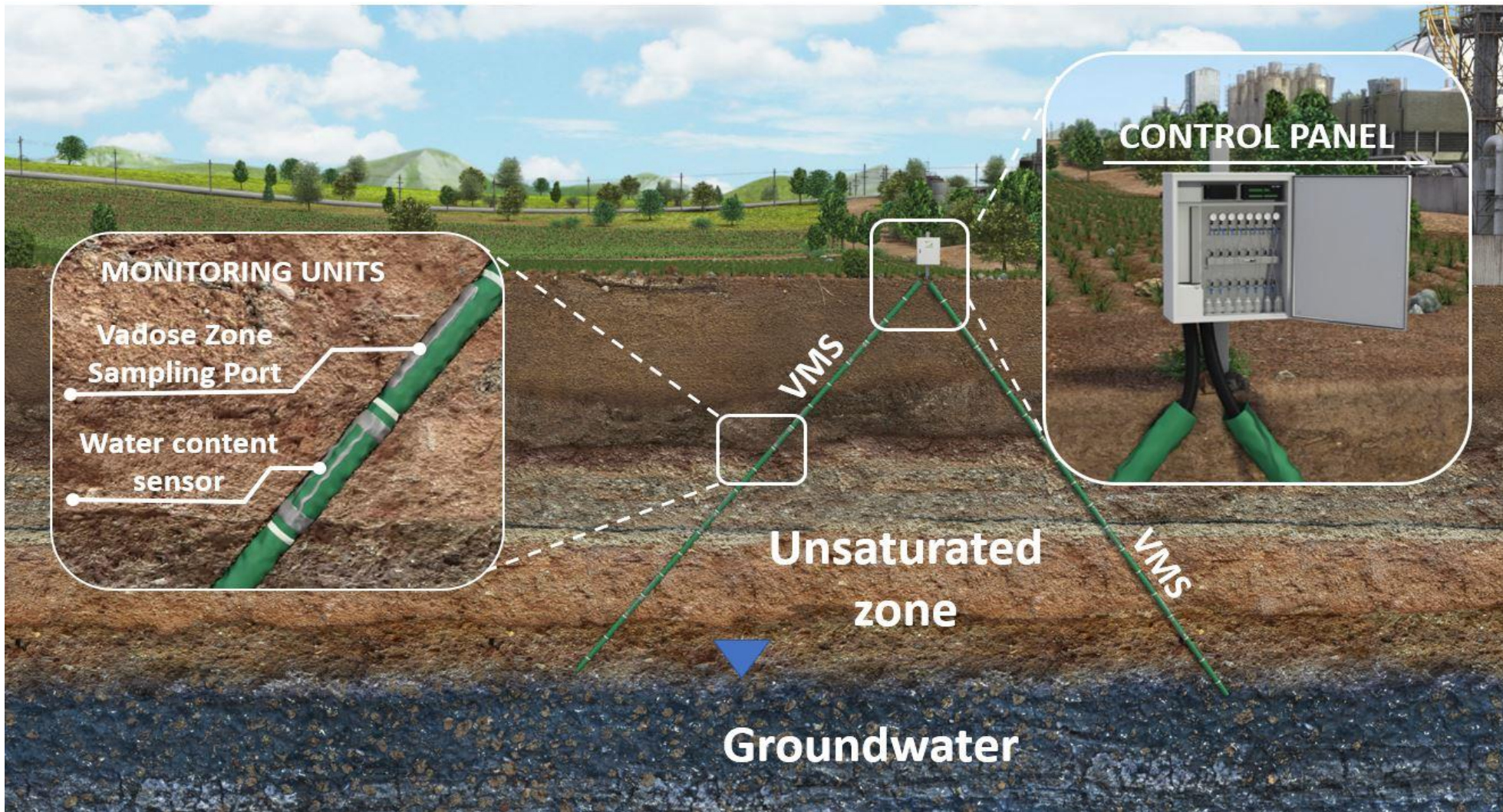




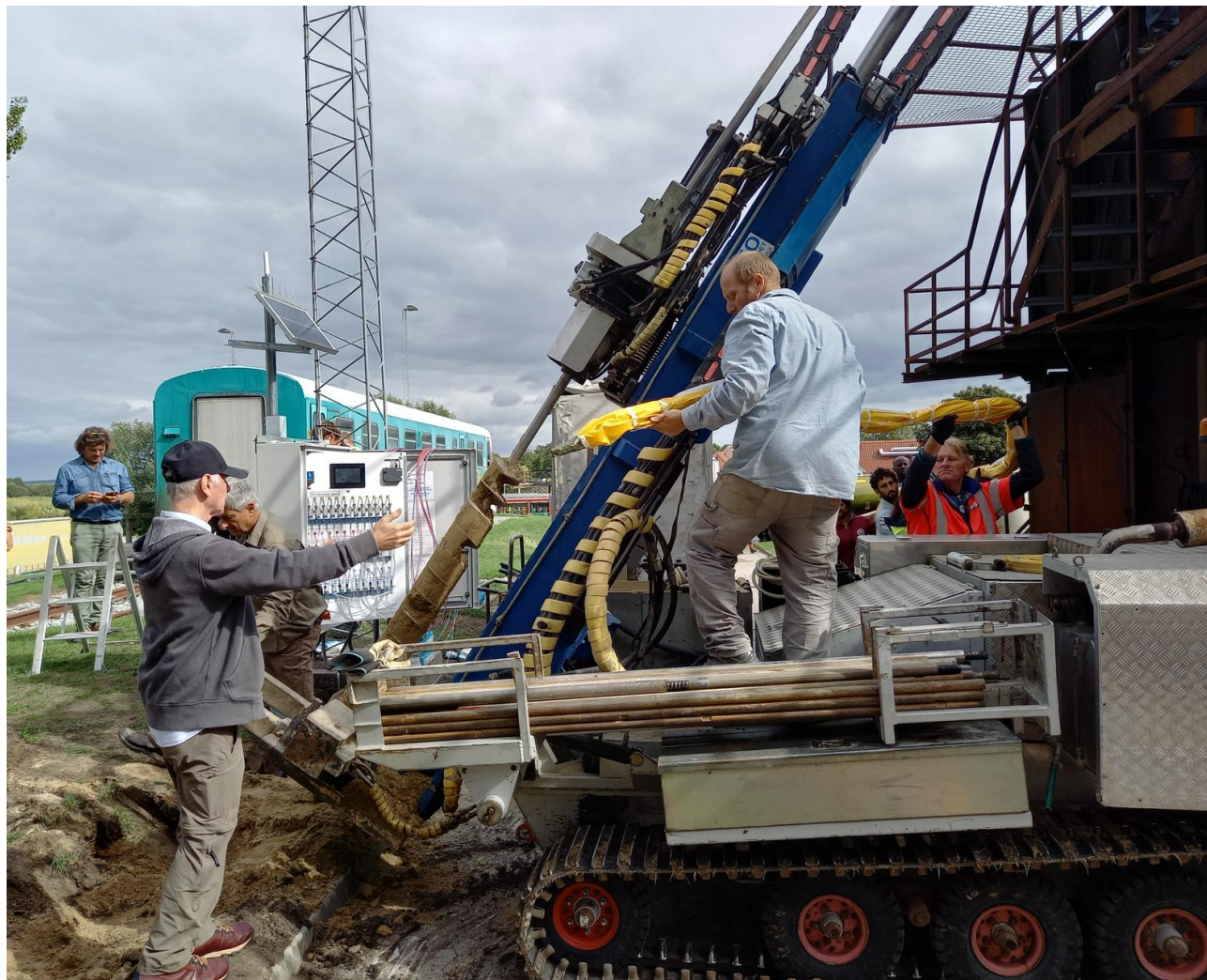




# Installering af VMS-anlæg til at monitorere transport af vand og PFAS i den umættede zone.





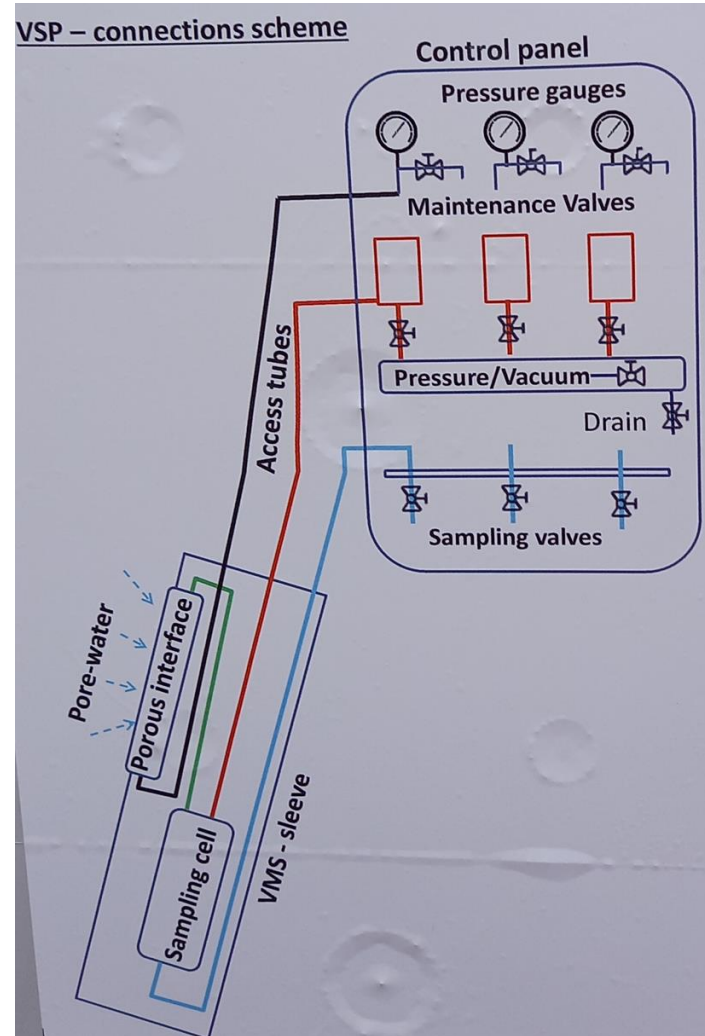




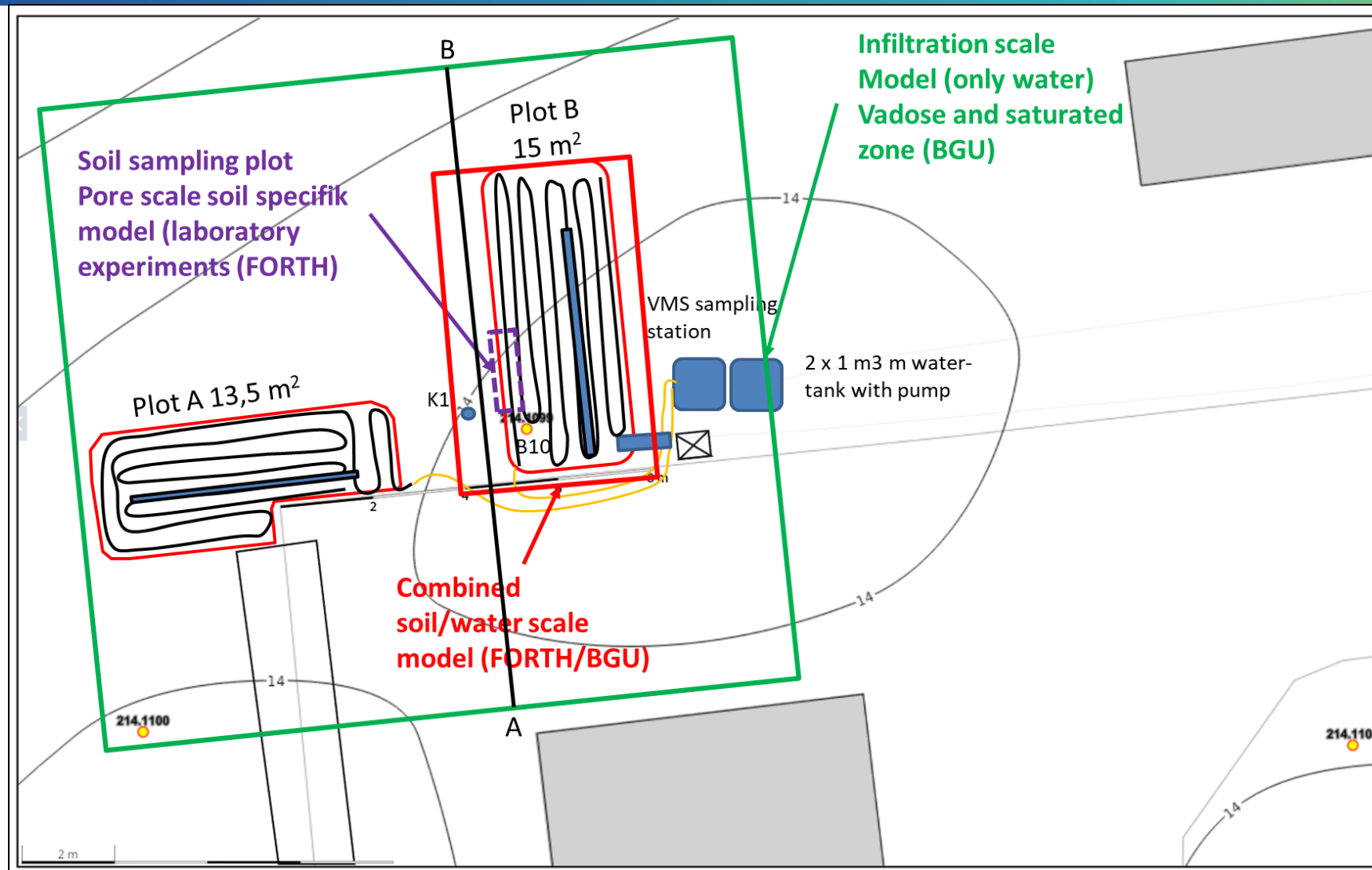




”anakondaen” pumpes op (fyldes med cement) så den forsegler kontakten til indersiden af borehullet dernæst forbindes alle slanger og ledninger til prøvetagningspanelet









# Prøvetagning af jordprøver

0-1



1-2



2-3



3-4



4-5



5-6

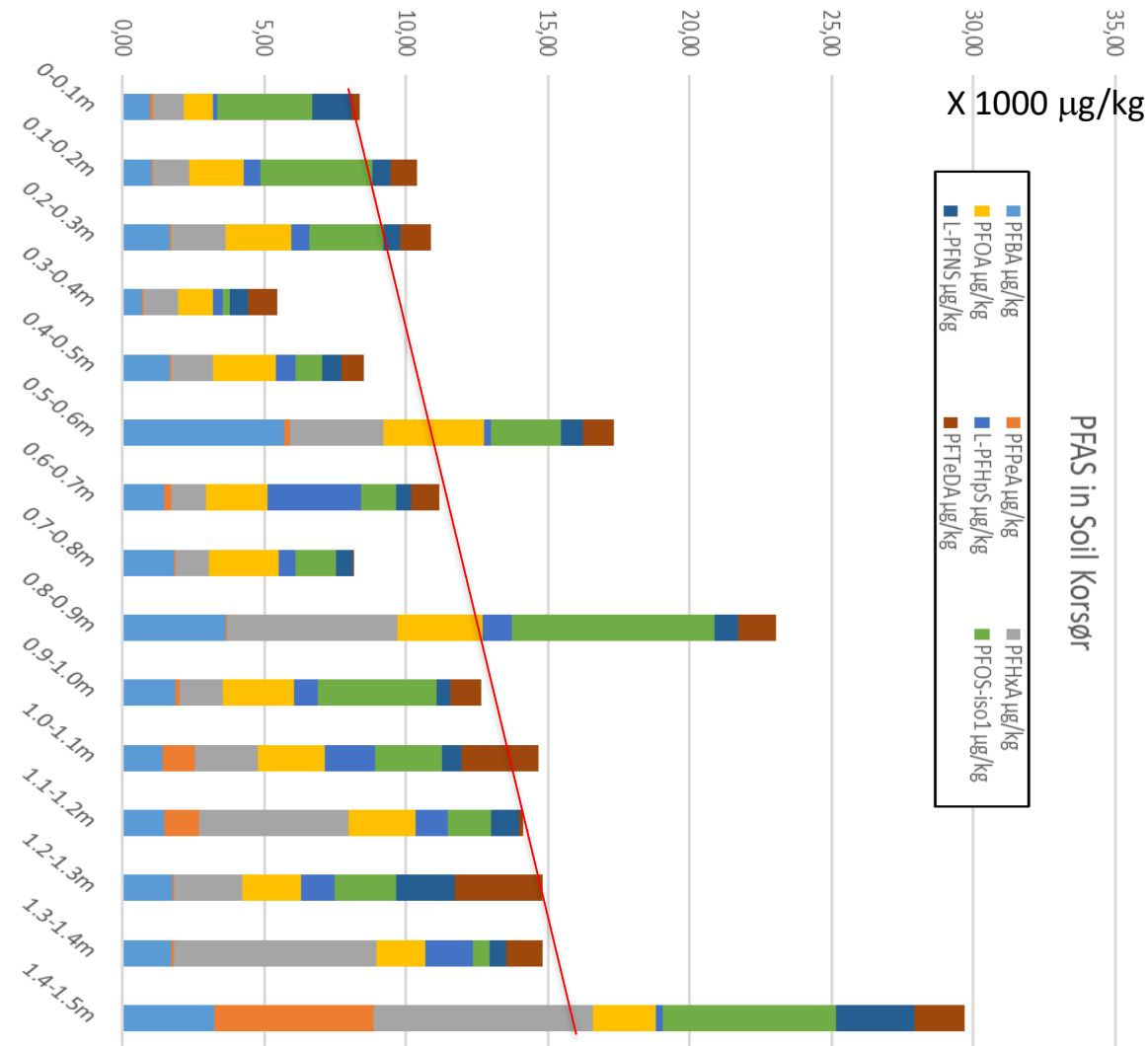


Drill log page 1/1		Borehole no: K1	Pl: KEK	<b>GEO</b>			
Project 205579		Driller id: Mats	Coordinat:				
Borehole: Korsoer		Start date:	Gw. table m b.g.s.:				
		End date:	kote, terrain: ROK:				
Depth m.	Filter	Drilling method Transitions	Lithology	Grainsize clay silt fine sand Medium sand coarse sand gravel stone	Description and geological setting	soil sample	Watersample
0,5			Rotary Auger		Mull, sandy topsoil brown CaCO <sub>3</sub> poor Sandy till, clayey, silty, few stones, yellowish brown CaCO <sub>3</sub> poor Sand, medium, light yellowish brown CaCO <sub>3</sub> poor "meltwatersand"	242	
1,0					Sandy till, w. clayey, silty, some gravel, brown CaCO <sub>3</sub> poor Sand, medium, light reddish brown CaCO <sub>3</sub> poor "meltwatersand"	245	
1,5					Sandy till, w. clayey, silty, some gravel, reddish brown CaCO <sub>3</sub> poor Sand, medium, light yellowish brown CaCO <sub>3</sub> rich "meltwatersand"		
2,0					Clay silty, massive, brown, CaCO <sub>3</sub> rich "meltwater-clay"	244	
2,5					Sand, fine, medium, coarse, laminated, light yellowish brown CaCO <sub>3</sub> rich "meltwatersand"	243	
3,0					Sandy till, w. clayey, silty, some gravel, few stones, sandstringer, brown, CaCO <sub>3</sub> rich, "flowtill"		
3,5					Sandy till, w. clayey, silty, some gravel, few stones, sandstringer, brown, CaCO <sub>3</sub> rich, "flowtill"	227	
4,0							
4,5					Sand, medium, coarse, gravelly, light yellowish brown, CaCO <sub>3</sub> rich "meltwatersand"		
5,0					Sand, medium, coarse, light yellowish brown CaCO <sub>3</sub> rich "meltwatersand"	223	
5,5					Sand, medium, coarse, gravelly, light yellowish brown, CaCO <sub>3</sub> rich "meltwatersand"		
6,0							
6,5					Sand, medium, coarse, gravelly, few stones, light yellowish brown, CaCO <sub>3</sub> rich "meltwatersand"		
7,0							
7,5					Sand, medium, coarse, gravelly, few stones, light yellowish brown, CaCO <sub>3</sub> rich "meltwatersand"	224	
8,0							
					Sand, medium, coarse, gravelly, few stones, light yellowish brown, CaCO <sub>3</sub> rich "meltwatersand"	222	





10	1.1	2.1	3.1	4.1
15	1.2	2.2	3.2	4.2
20	1.3	2.3	3.3	4.3
25	1.4	2.4	3.4	4.4
30	1.5	2.5	3.5	4.5
35	1.6	2.6	3.6	4.6
40	1.7	2.7	3.7	4.7
45	1.8	2.8	3.8	4.8
50	1.9	2.9	3.9	4.9
55	1.10	2.10	3.10	4.10
60	1.11	2.11	3.11	4.11
65	1.12	2.12	3.12	4.12
70	1.13	2.13	3.13	4.13
75	1.14	2.14	3.14	4.14
80	1.15	2.15	3.15	4.15
85	1.16	2.16	3.16	4.16





- Nedbør
- Nedsivning/vandindhold
- PFAS indhold i vandprøver

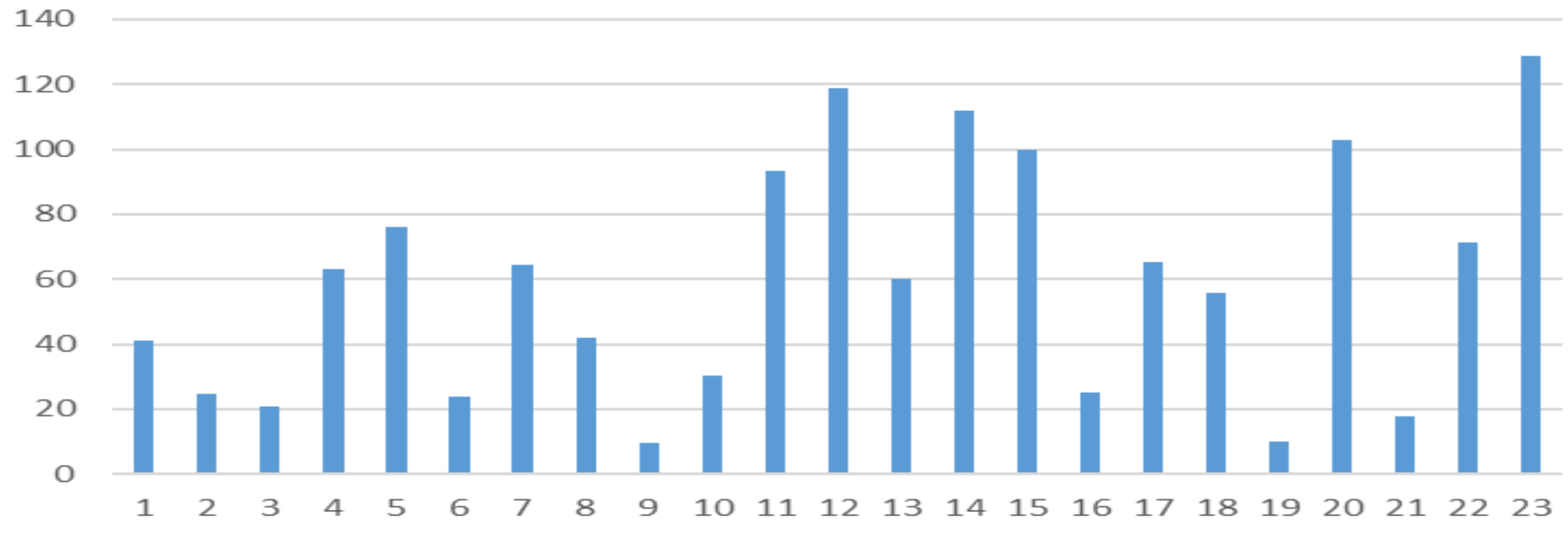


# Nedbør 28 Sep 2022 til Aug 2024 i målt i ved RESC Korsør



mm Regn

Samlet nedbør pr måned

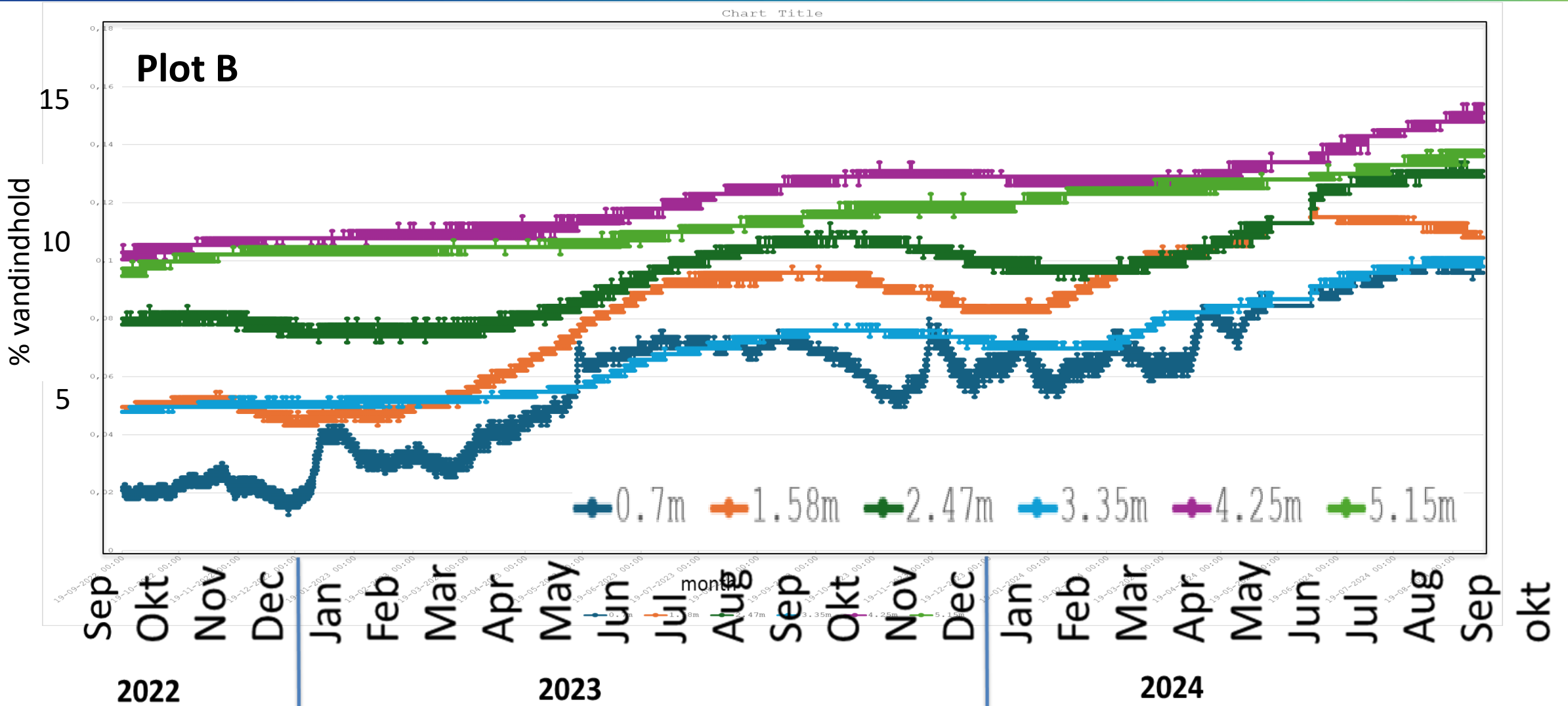


	Precipitation mm
	mm/month
10	41
11	25
12	21
1	63
2	76
3	24
4	65
5	42
6	10
7	31
8	93
9	119
10	60
11	112
12	100
1	25
2	65
3	56
4	10
5	103
6	18
7	71
8	129
9	141

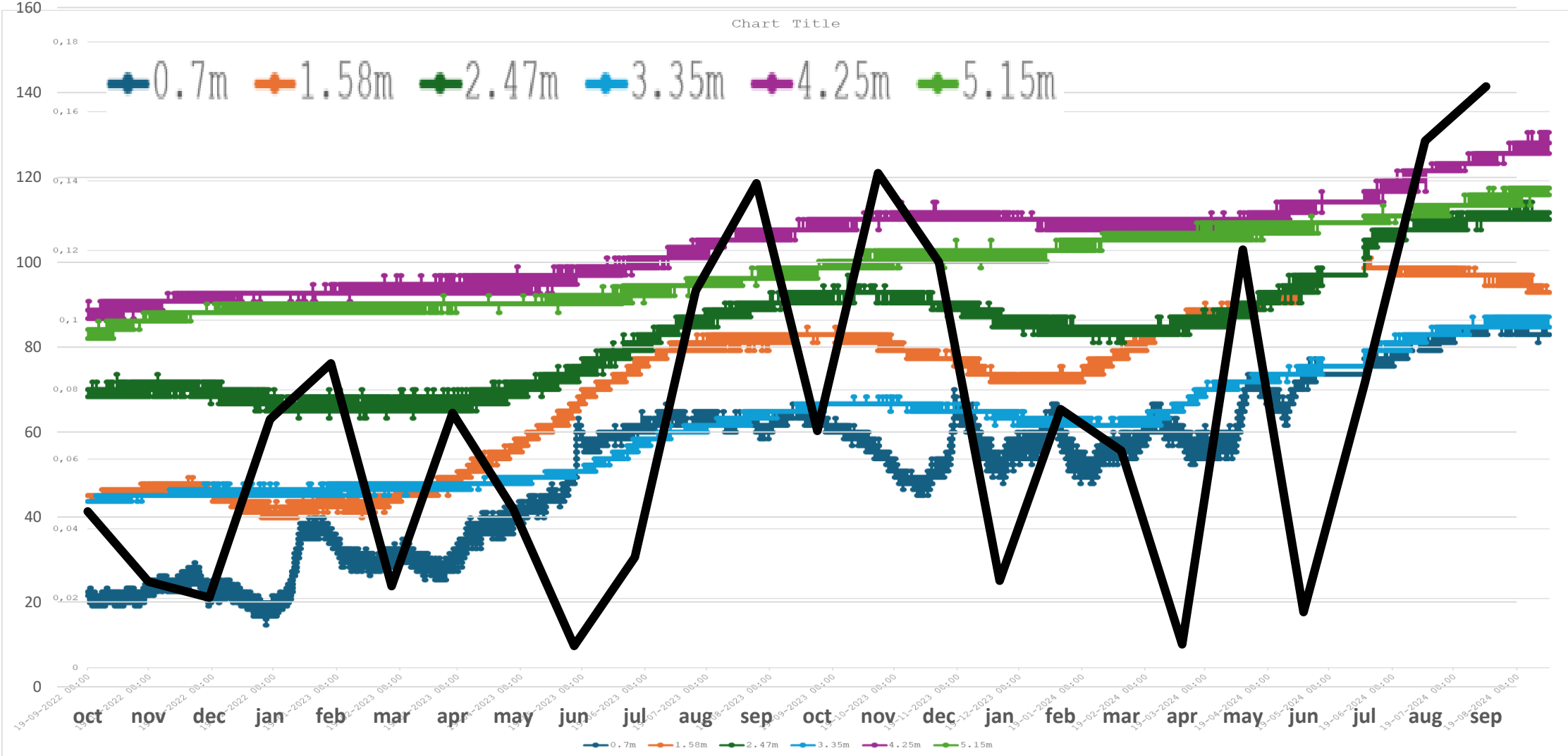
Sep 2022 | Okt 2022 | Nov 2022 | Dec 2022 | Jan 2023 | Feb 2023 | Mar 2023 | Apr 2023 | May 2023 | Jun 2023 | Jul 2023 | Aug 2023 | Sep 2023 | Okt 2023 | Nov 2023 | Dec 2023 | Jan 2024 | Feb 2024 | Mar 2024 | Apr 2024 | May 2024 | Jun 2024 | Jul 2024 | Aug 2024



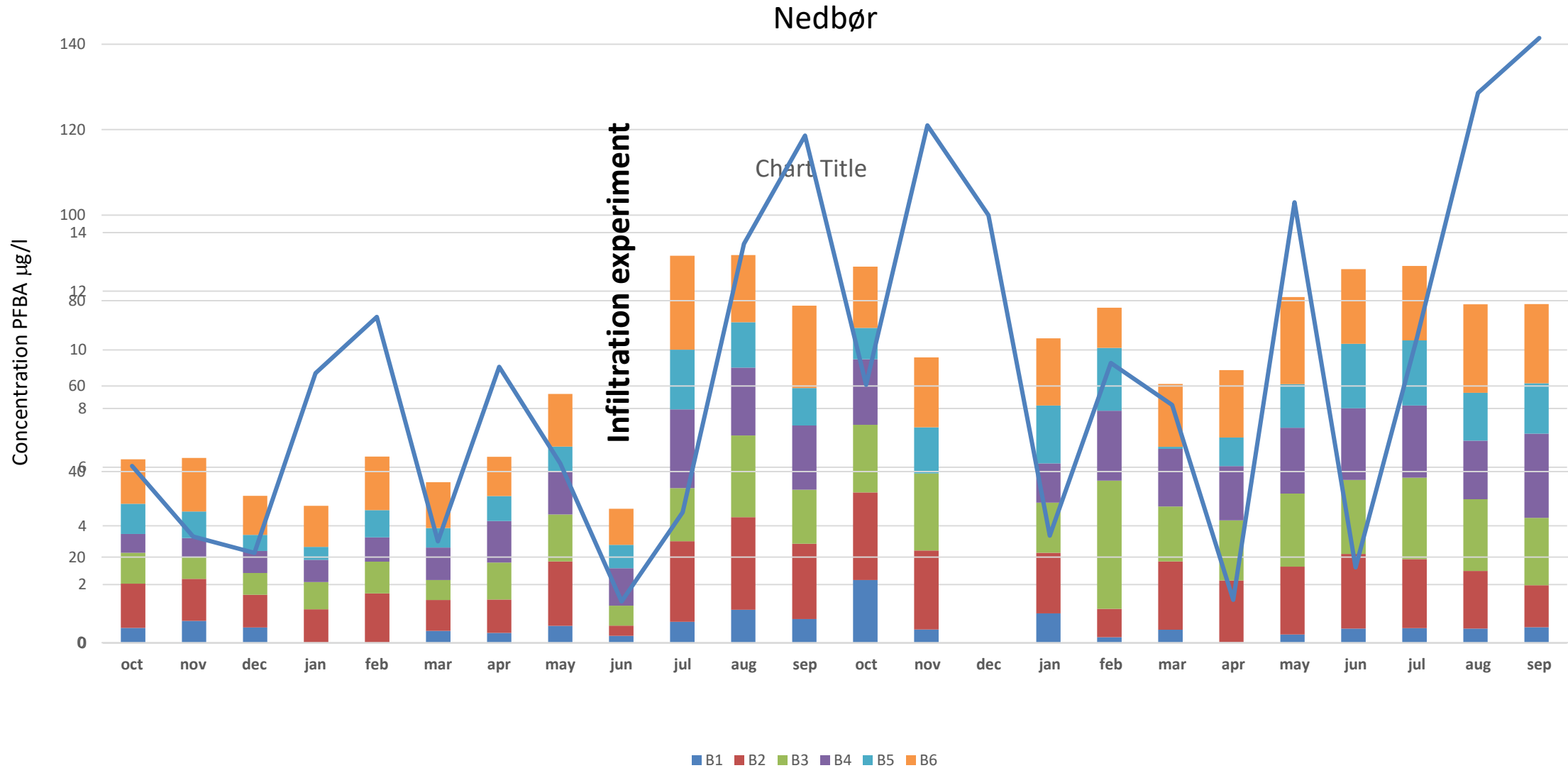
# Vandindhold i 6 dybder 28 Sep 2022 til Aug 2024









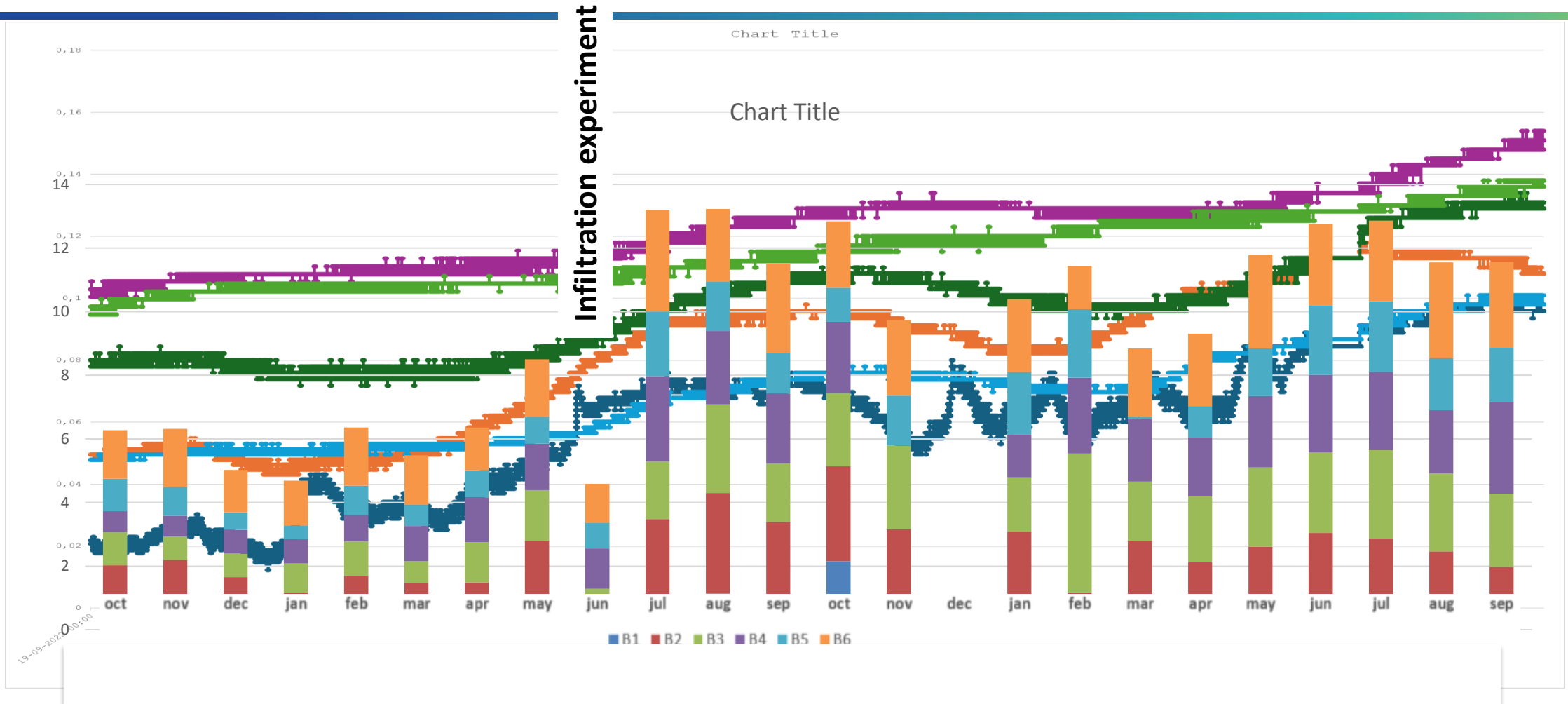




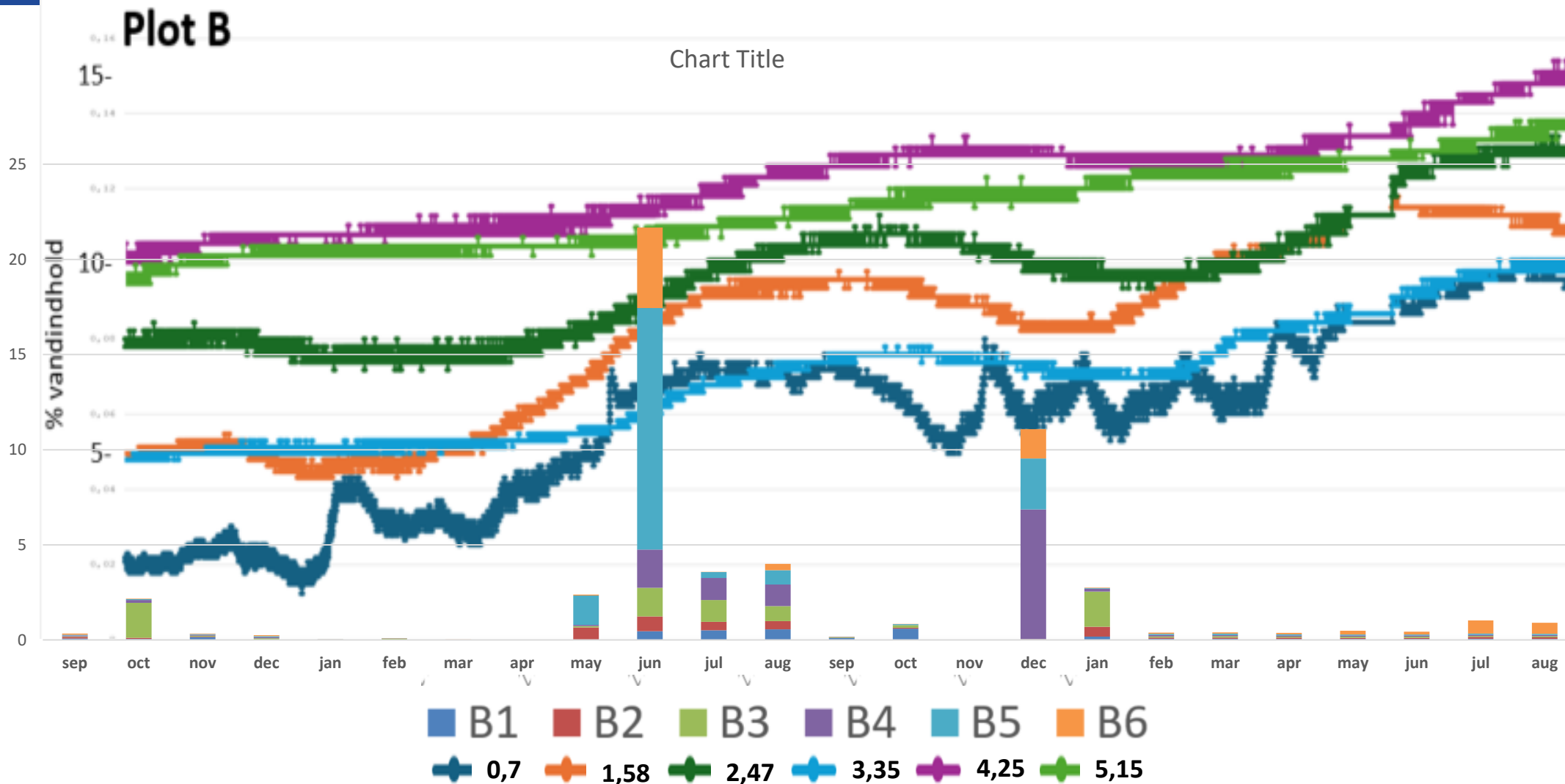




# Koncentration af PFBA som funktion af vandmætning i jorden

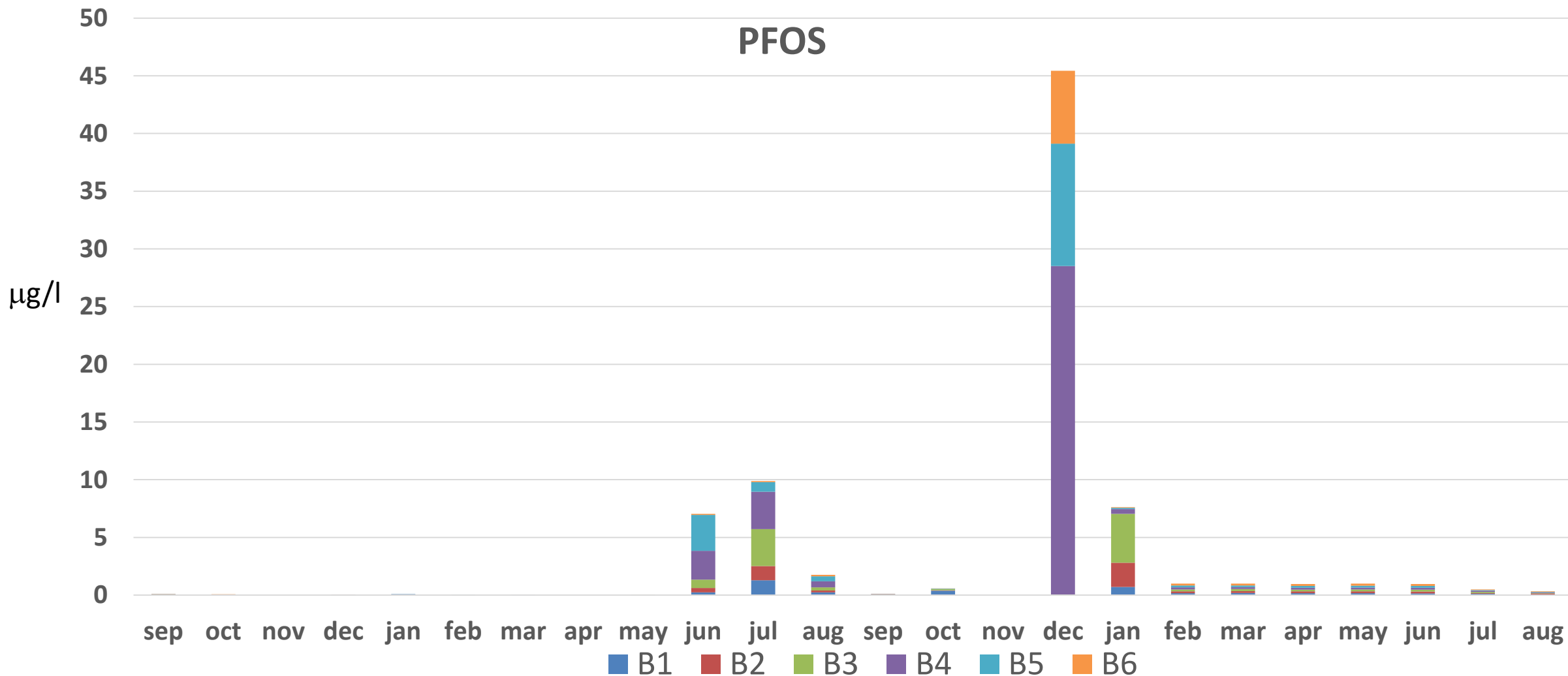


# Koncentration af PFOA som funktion af vandmætning i jorden

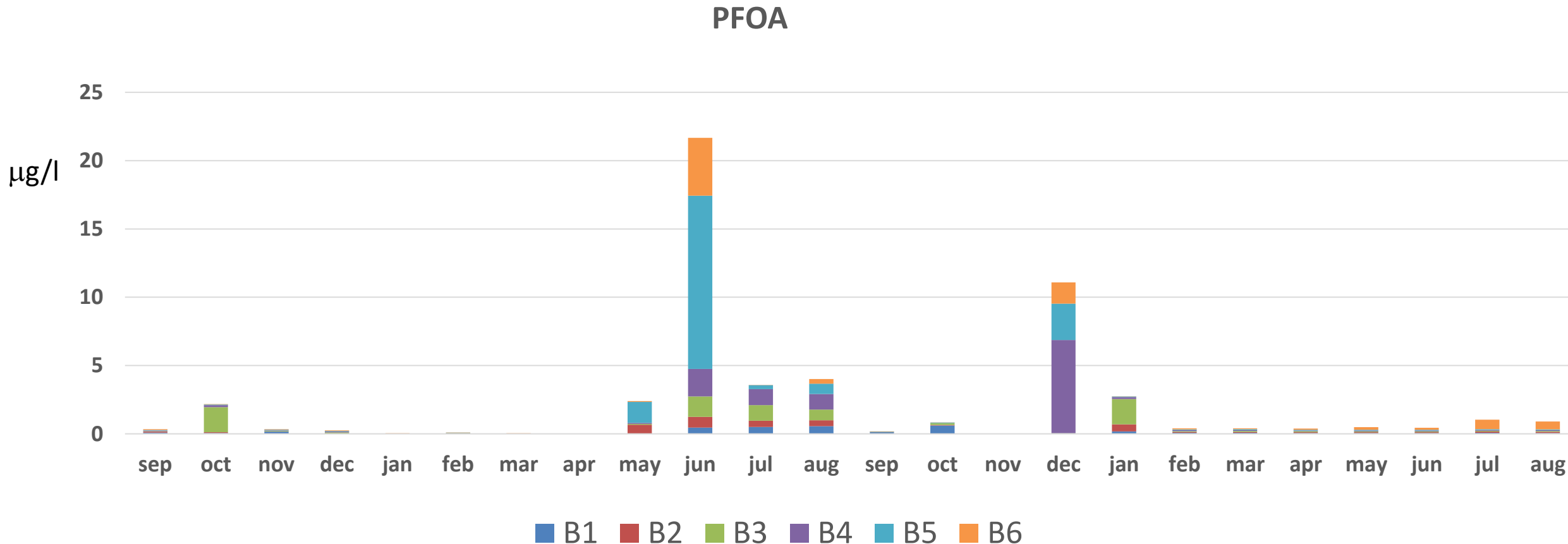




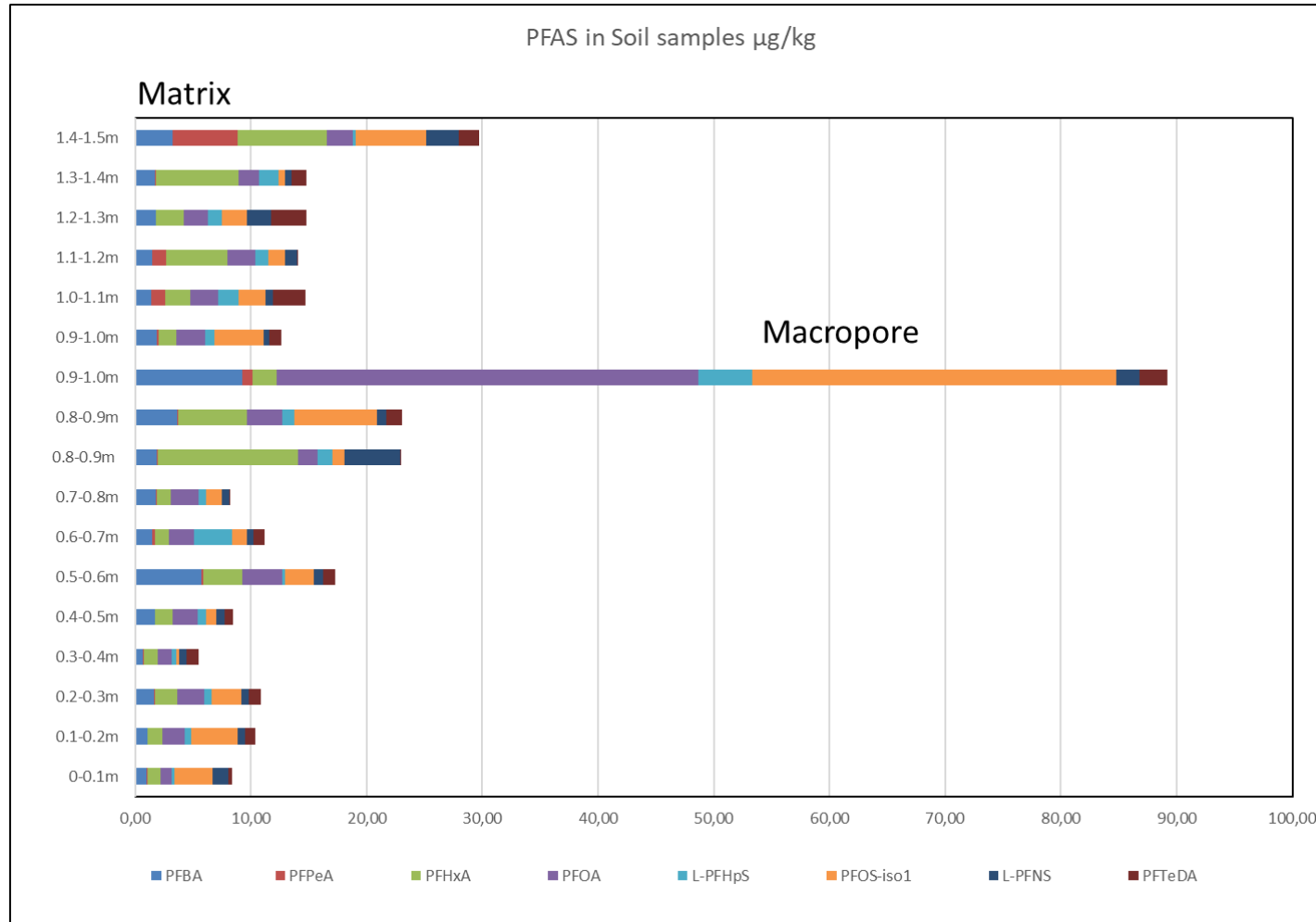
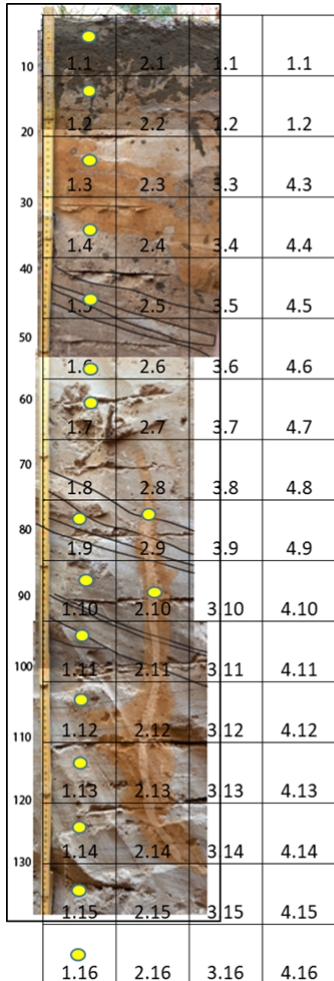
# Udvaskning af PFOS og PFOA sker kun ved høj vandmætning



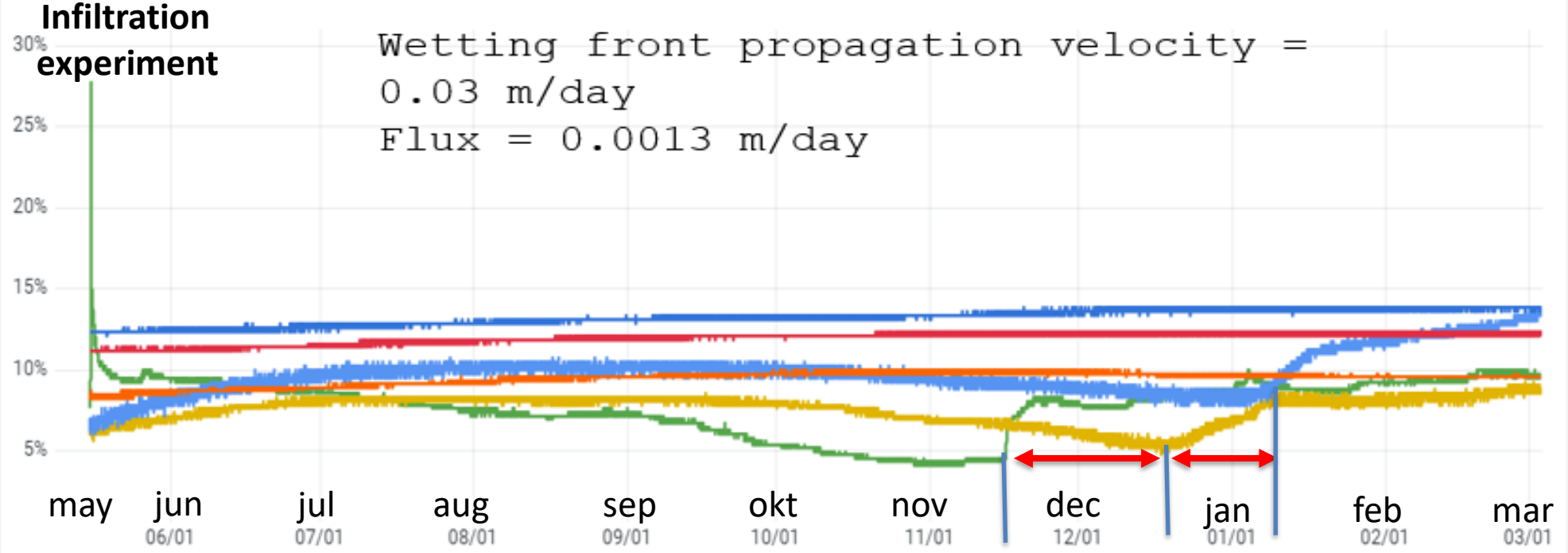
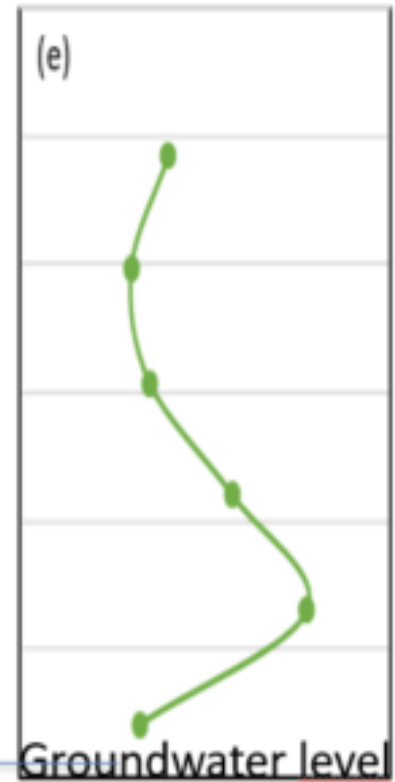
# Nye spørgsmål: Hvorfor er koncentrationen af PFOA højest i B5 og B4 dybere nede?







Br (mg/l)  
0 0.2 0.4



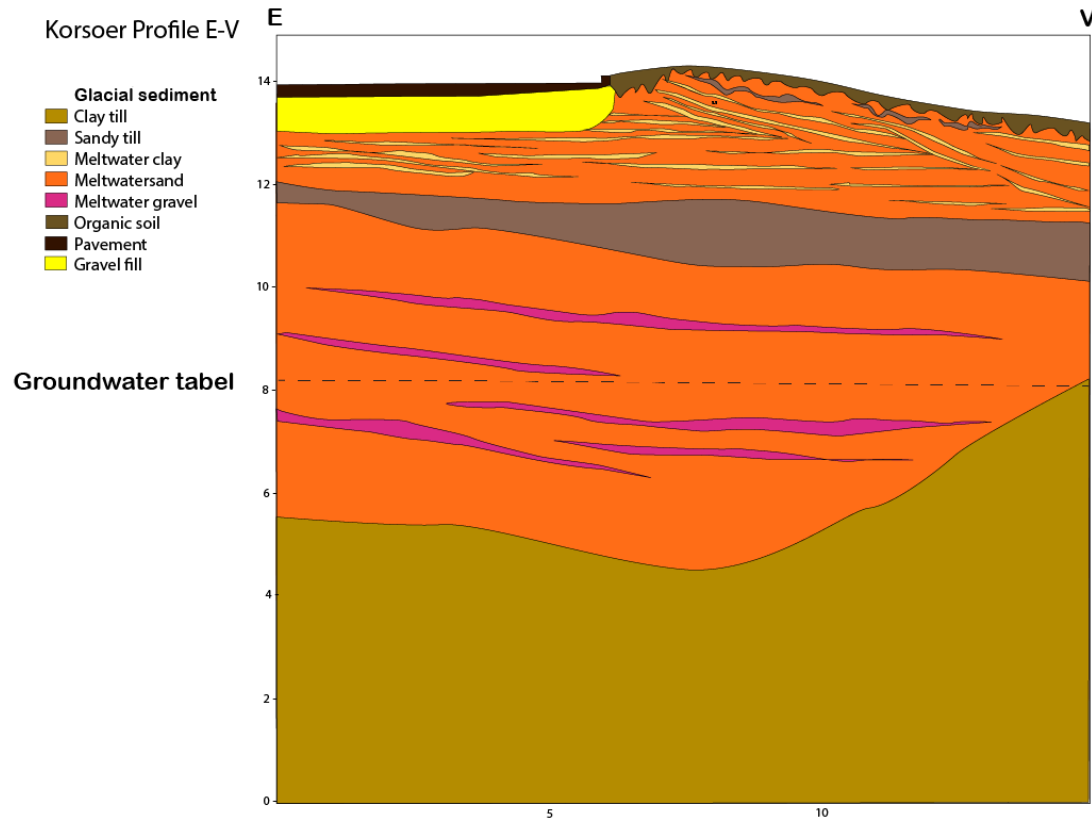
	Mean	Last *
A1_VWC_78cm	7.69%	9.48%
A2_VWC_166cm	7.54%	8.76%
A3_VWC_255cm	9.81%	13.3%
A4_VWC_343cm	9.42%	9.53%
A5_VWC_432cm	12.0%	12.1%
A6_VWC_522cm	13.2%	13.9%

**Bromide migrerer 6 m på mindre end 3 uger**

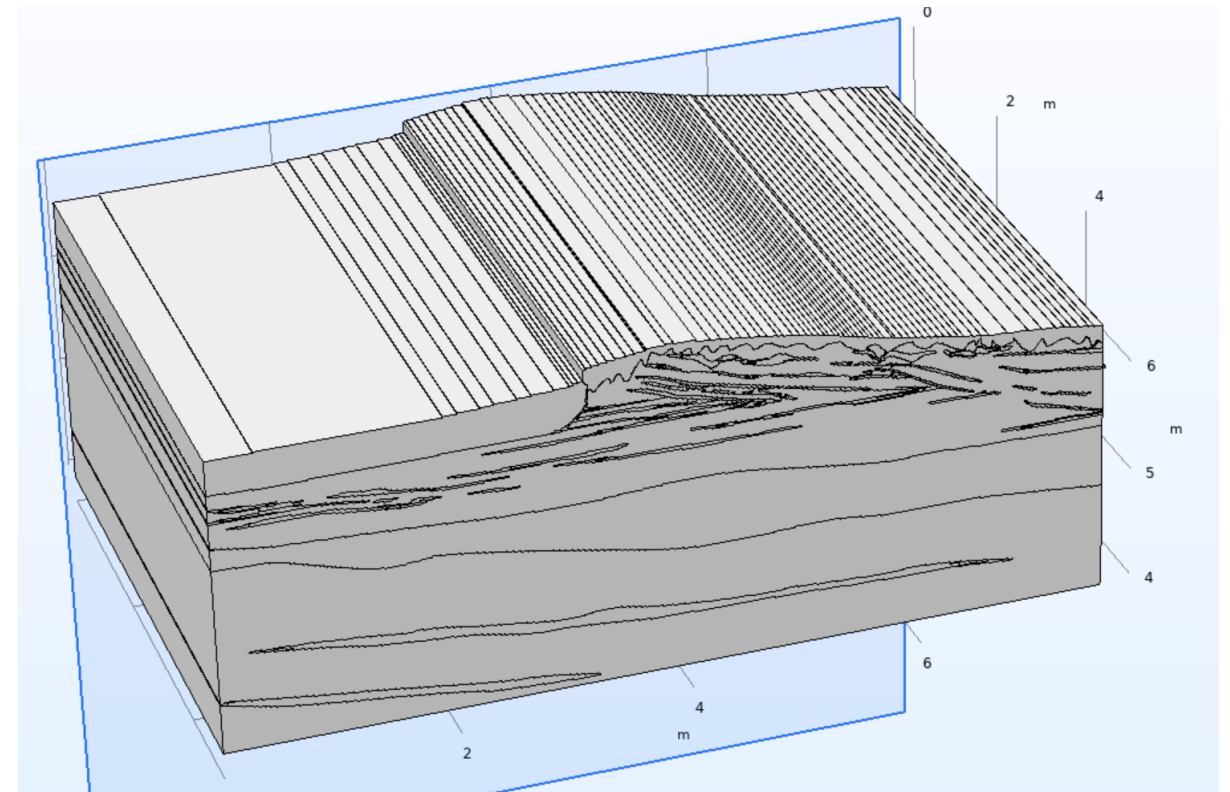
**"Wetting front" migrerer 90 cm på 4 uger hen over vinteren 2023/2024.**



## Geological conceptual model



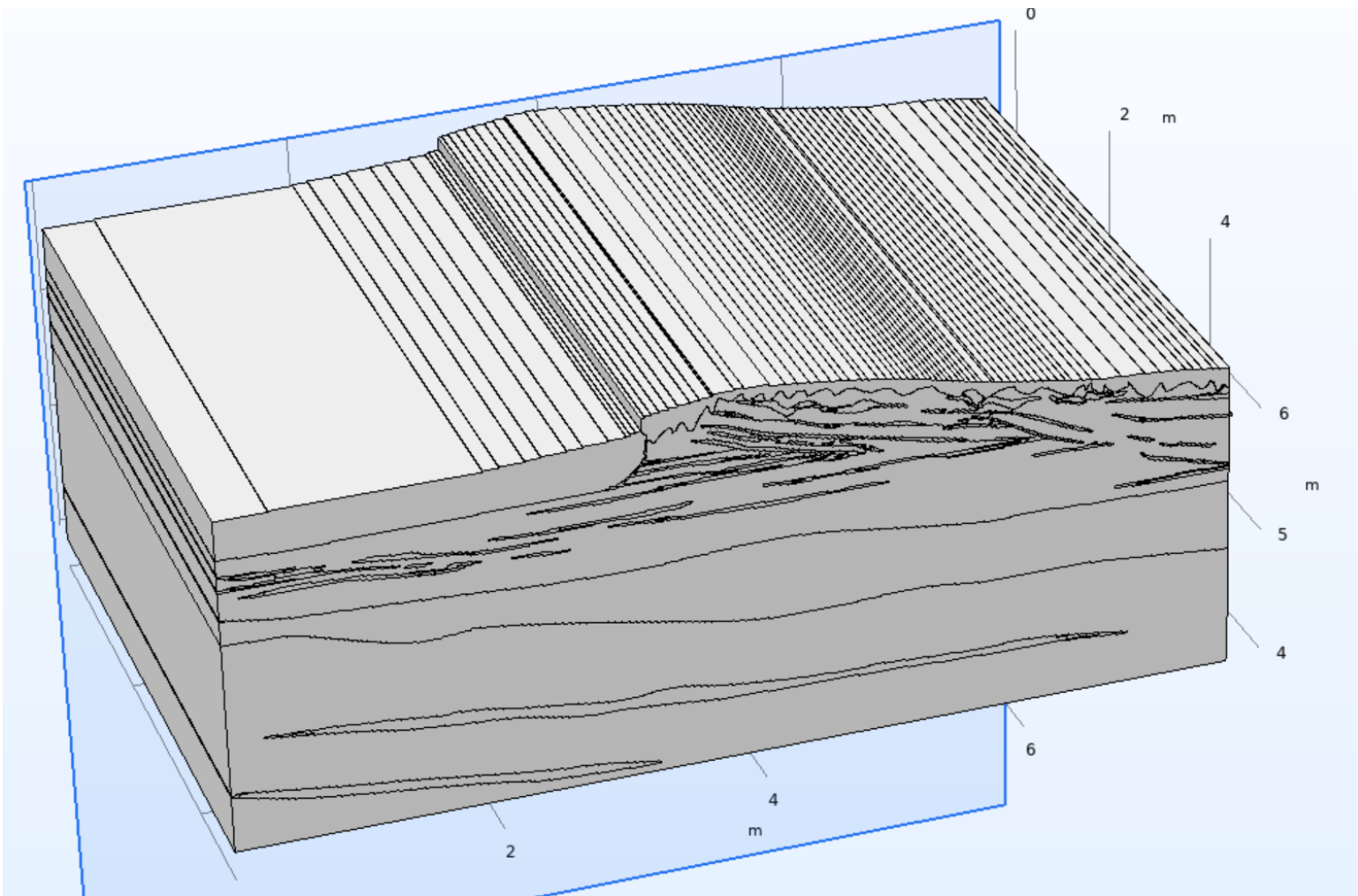
## Reconstructed –simulation domain



Using Adobe Illustrator and an algorithm in python that transforms images to CAD geometry for further exploitation

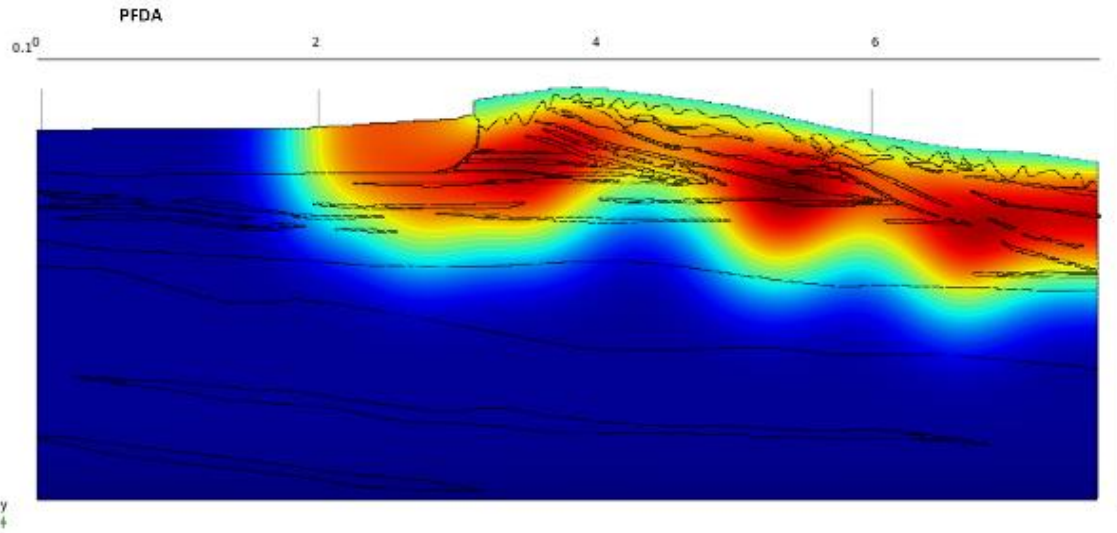
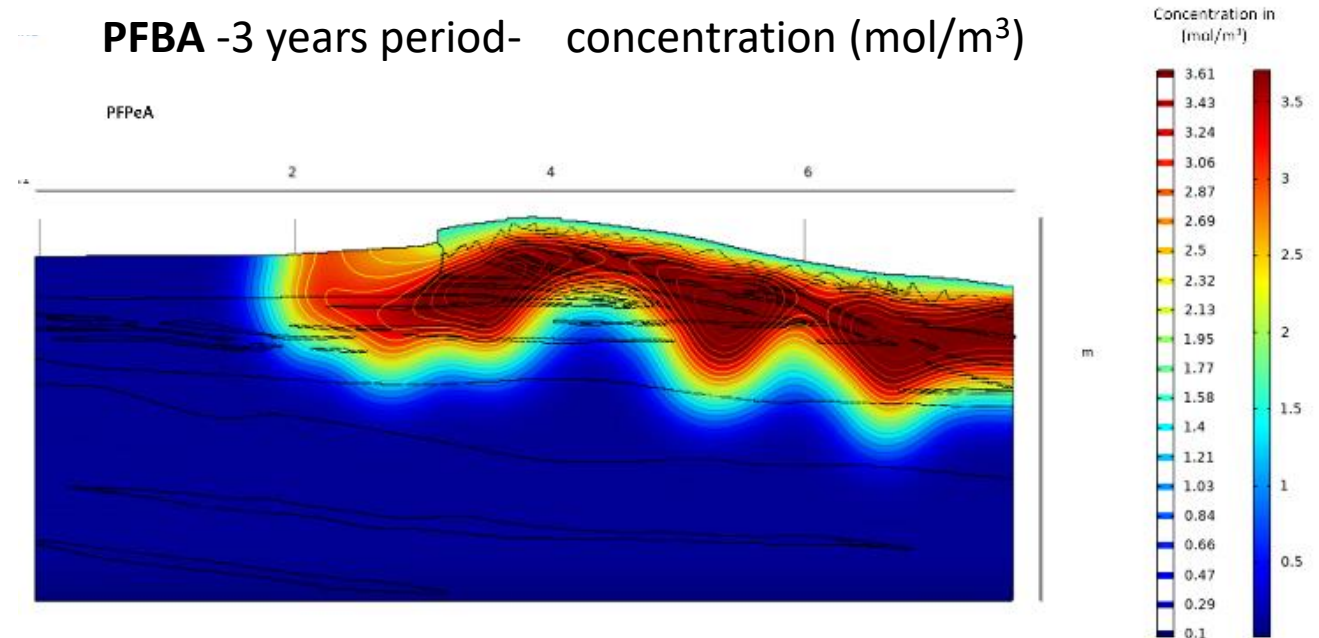
Different soil layers take into account

# Parameter estimating



Soil type	Parameter	Value	Description
Clayey sandy till	$\epsilon$	0.22	Porosity
	K	$4.8 \cdot 10^{-13} \text{ m}^2$	Absolute permeability
	$\alpha$	$0.5 \text{ m}^{-1}$	Van Genuchten parameter
	n	1.09	Van Genuchten parameter
	$\theta_s$	0.22	Water saturation = porosity
	$\theta_r$	0.015	Water residual
Apply to all layers	aL	200 $\mu\text{m}$	Dispersivity (the default)
	$D_{pfos}$	$0.5 \cdot 10^{-9} \text{ m}^2/\text{s}$	Diffusion coefficient of PFOS
	$D_{pfoa}$	$3.5 \cdot 10^{-9} \text{ m}^2/\text{s}$	Diffusion coefficient of PFOA
	$D_{pfda}$	$2 \cdot 10^{-9} \text{ m}^2/\text{s}$	Diffusion coefficient of PFDA
	$D_{pfba}$	$8 \cdot 10^{-9} \text{ m}^2/\text{s}$	Diffusion coefficient of PFBA
	$K_{dpfos}$	$302.5 \cdot 10^{-9} \text{ mol/kg}$	Freundlich constant PFOS
	$K_{dpfoa}$	$31.3 \cdot 10^{-9} \text{ mol/kg}$	Freundlich constant PFOA
	$K_{dpfda}$	$386 \cdot 10^{-9} \text{ mol/kg}$	Freundlich constant PFDA
	$K_{dpfba}$	$38.7 \cdot 10^{-9} \text{ mol/kg}$	Freundlich constant PFBA
	$n_{pfos}$	0.63	Freundlich exponent PFOS
	$n_{pfoa}$	0.63	Freundlich exponent PFOA
	$n_{pfda}$	0.42	Freundlich exponent PFDA
$n_{pfba}$	0.35	Freundlich exponent PFBA	
Melt-water clay/silt	$\epsilon$	0.28	Porosity
	K	$2.4 \cdot 10^{-13} \text{ m}^2$	Absolute permeability
	$\alpha$	$0.8 \text{ m}^{-1}$	Van Genuchten parameter
	n	1.09	Van Genuchten parameter
	$\theta_s$	0.28	Water saturation = porosity
	$\theta_r$	0.015	Water residual
Melt-water Sand	$\epsilon$	0.38	Porosity
	K	$7.2 \cdot 10^{-12} \text{ m}^2$	Absolute permeability
	$\alpha$	$7.45 \text{ m}^{-1}$	Van Genuchten parameter
	n	1.89	Van Genuchten parameter
	$\theta_s$	0.38	Water saturation = porosity
	$\theta_r$	0.025	Water residual
Melt-water gravel/sand	$\epsilon$	0.45	Porosity
	K	$3.6 \cdot 10^{-11} \text{ m}^2$	Absolute permeability
	$\alpha$	$14.5 \text{ m}^{-1}$	Van Genuchten parameter
	n	2.68	Van Genuchten parameter
	$\theta_s$	0.45	Water saturation = porosity



PFDA -3 years period- concentration (mol/m<sup>3</sup>)PFBA -3 years period- concentration (mol/m<sup>3</sup>)

- High adsorption coefficient on soil grain for PFDA and on air/water interfaces (less concentration for transport downwards in the vadose zone)
- Differences in permeabilities (in particular in the region of clay formations) led to fingering transport

## Unikt datasæt med tidsserie data fra 24 måneder indeholdende:

- PFAS indhold i uforstyrret smeltevandssand/silt/ler og morænesand og macropore med
- Høj frekvens monitorering af PFAS indhold i nedsivende vand
- On line "real time" monitorering af vandindhold i jorden i 6 forskellige dybder
- On line "real time" monitorering af nedbør

Disse data muliggør ret præcis beregning af "Mass transfer" af forskellige PFAS typer til grundvandet



- Koncentration af PFAS i nedsivende vand stiger med højere vandmætning.
- Udvaskning/mobilisering af "kortkædede PFAS" sker med vandmætning over 5% men afhænger af vandindholdet
- Udvaskning/mobilisering af "langkædede PFAS" sker kun ved markante "Wetting front" passager (>10% vandindhold)
- Indhold af PFOS, PFOA er signifikant højere i makroporre end i matrix
- Flow sker som kombination af langsom matrixflow og hurtig makropore flow
- Mass transport af PFAS i den umættede zone bør altid kalibreres med vandindholdet i jorden, men jordspecifikke parametre som lerindhold, har også stor betydning.
- Selv homogene konfigurationer af geologiske modeller bør modelleres som dobbelt porøse medier, med både matrix og makropore flow.
- Måling af tidsserier er essentiel for forståelsen af den samlede udvaskning

- Betydning af ”udtørring/opmætnings” frekvenser
- Mere præcis estimering af betydning af andre parametre som organisk indhold, Ph, lerindhold på individuelle PFAS
- Betydningen af PFAS Cocktails. Nogle komponenter konkurrere om pladsen



Thank you for  
your attention



**SCENARIOS**

Vil du vide mere så kontakt [kek@geo.dk](mailto:kek@geo.dk)

Eller besøg Scenarios hjemmeside <https://scenarios-project.eu/>