

Vertical PFAS Transport in Glacial Tills: Field Investigations and Numerical Modelling

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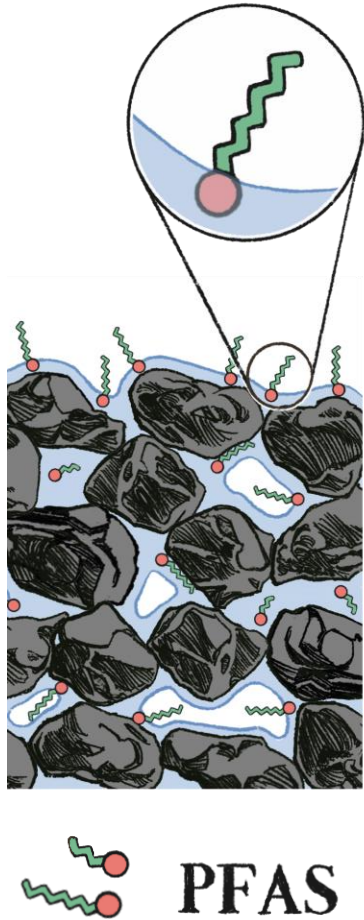
NIRAS



Funding from

- Innovation Fund Denmark
- The Capital Region of Denmark
- HOFOR
- NIRAS Fonden
- DTU

Vertical PFAS Transport – The Knowns

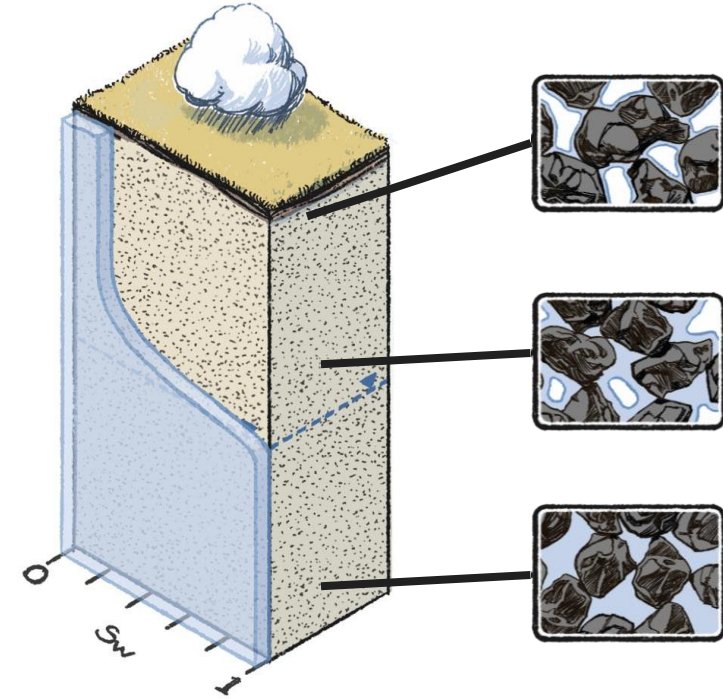


Transport Processes:

- Water Flow
- Sorption to soil
- Sorption to air-water interface (Aia)
- etc.

Impacted by:

- PFAS chain length
- PFAS functional group
- Aia
- etc.



Various estimation methods to determine **Aia based on S_w** for **sandy soils**

Vertical PFAS Transport – The **Unknowns**...

Transport Processes in

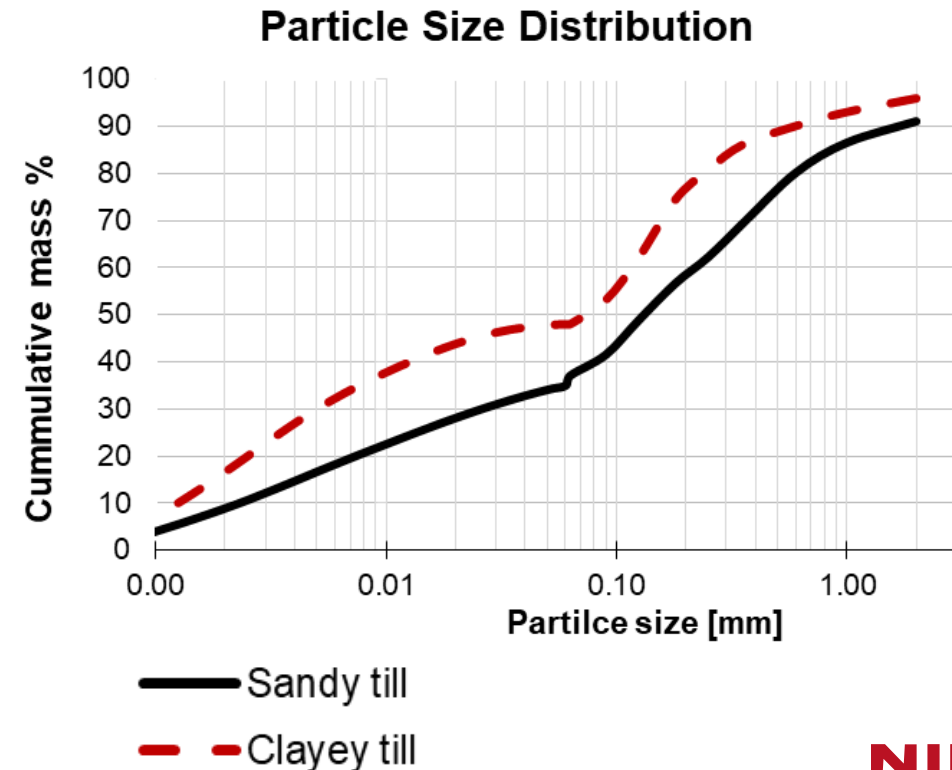
- Heterogenous soils?
- In soils different to **sandy soils**?

Example Glacial Deposits (e.g. Clayey Till and Sandy Till):

Soil	d_{50} [mm]	Uniformity coefficient, U (d_{60}/d_{10})
Sandy till, site*	0.11	81.49
Clayey till, site*	0.06	89.10
Vinton, literature**	0.23	2.4
Accusand, literature**	0.35	1.1

*Presented d_{50} and U based on <2 mm fraction

**Brusseau, M. L., El Ouni, A., Araujo, J. B., & Zhong, H. (2015). Novel methods for measuring air–water interfacial area in unsaturated porous media. *Chemosphere*, 127, 208-213.



Objective

Identify the **governing transport processes of PFAS** in unsaturated **glacial tills** to improve the **risk assessment** strategies for PFAS contaminated sites ...

Method

... by combining high resolution **laboratory** and **field data** in a **numerical model**.

Field & Laboratory Data

Field Site

- Active fire training area (FTA) since 1969
- PFAS application since ~ 1975
- ~ 14 m unsaturated zone



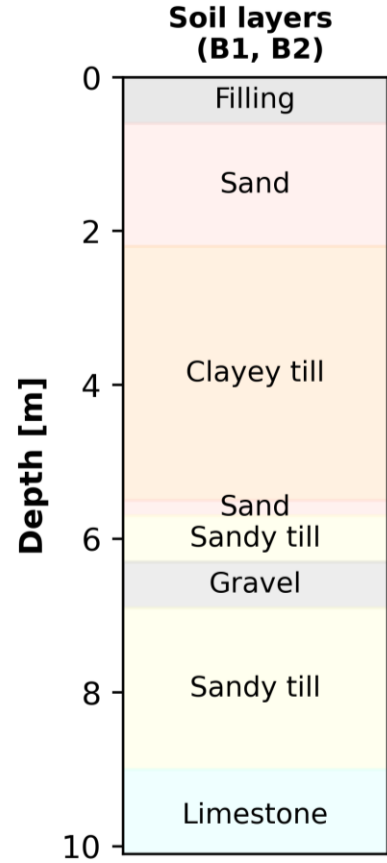
Data presented today:

3 soil cores in close vicinity

- Sampled August 2024 – B1
- Sampled October 2025 – B2 & B3
- Geoprobe samples

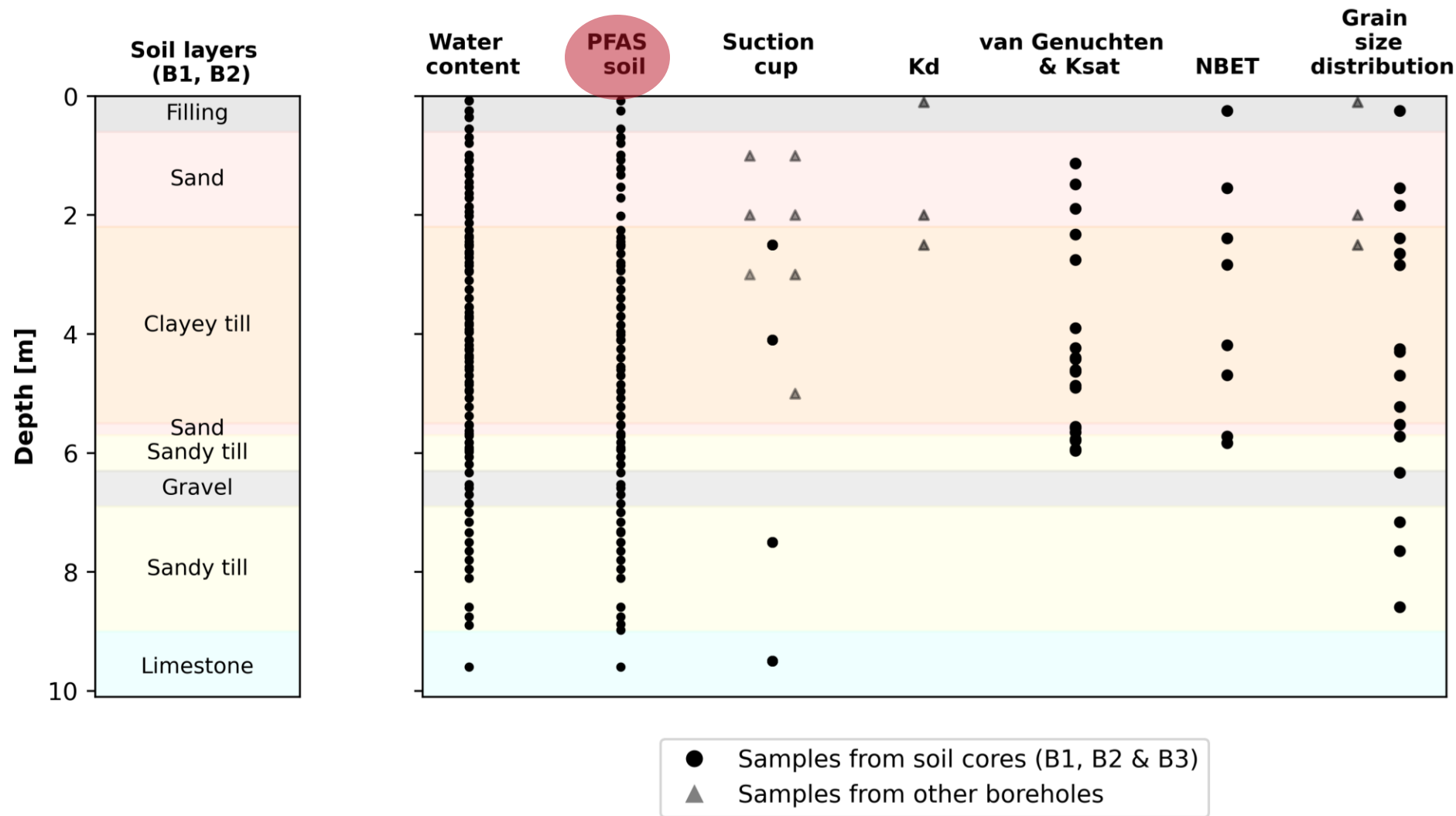


Field Site – Geology and Data



Field Site – Geology and Data

Analyzed 29 PFAS
Focus today 6 PFAS



PFAS profiles

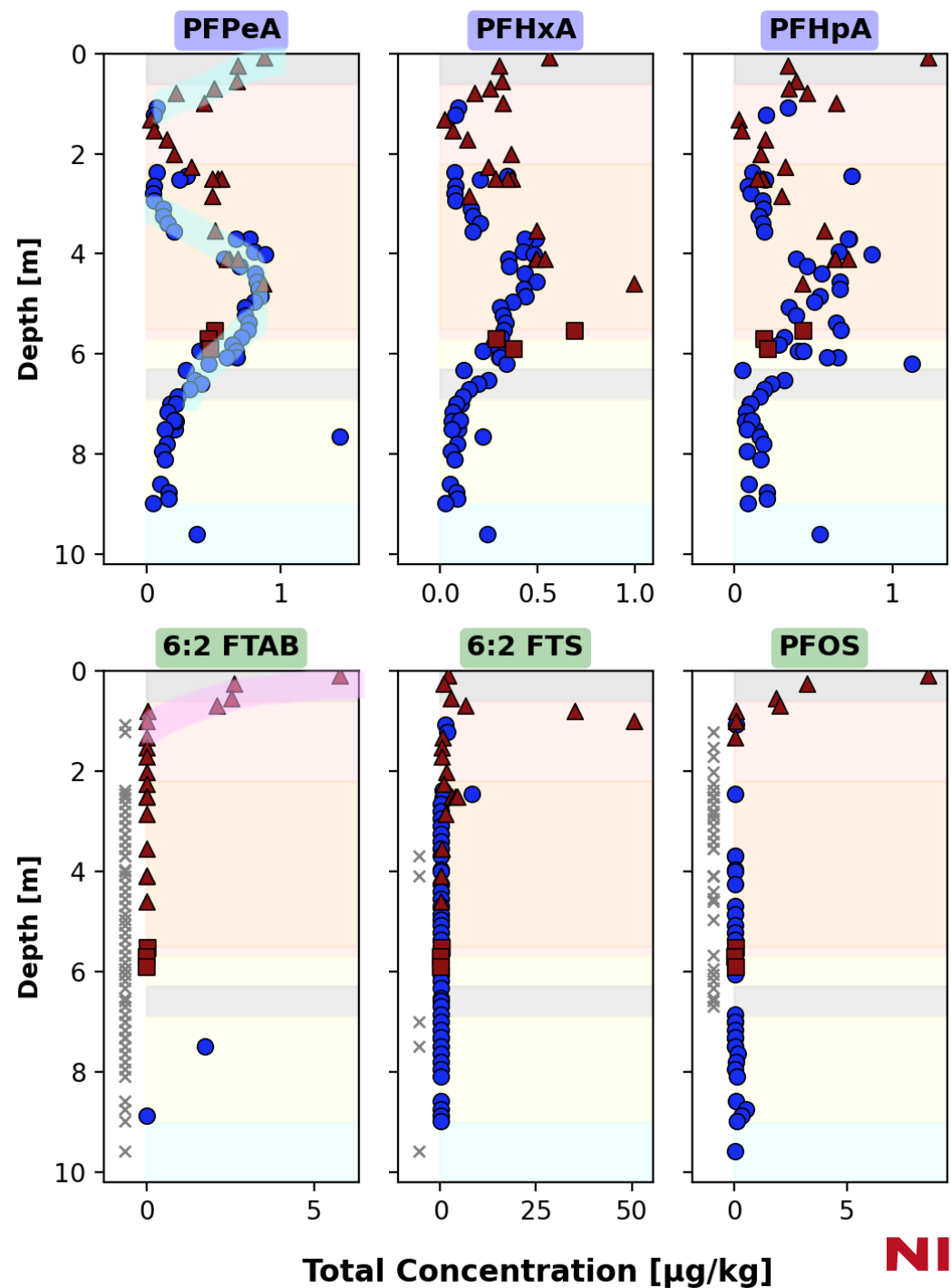


Profile type 1

- 2 peaks
- Max. conc. < 1 µg/kg dw

Profile type 2

- 1 concentration peak, close to surface
- Steep concentration decline
- Higher max. conc.



PFAS Transport Model

Model = LEACHE

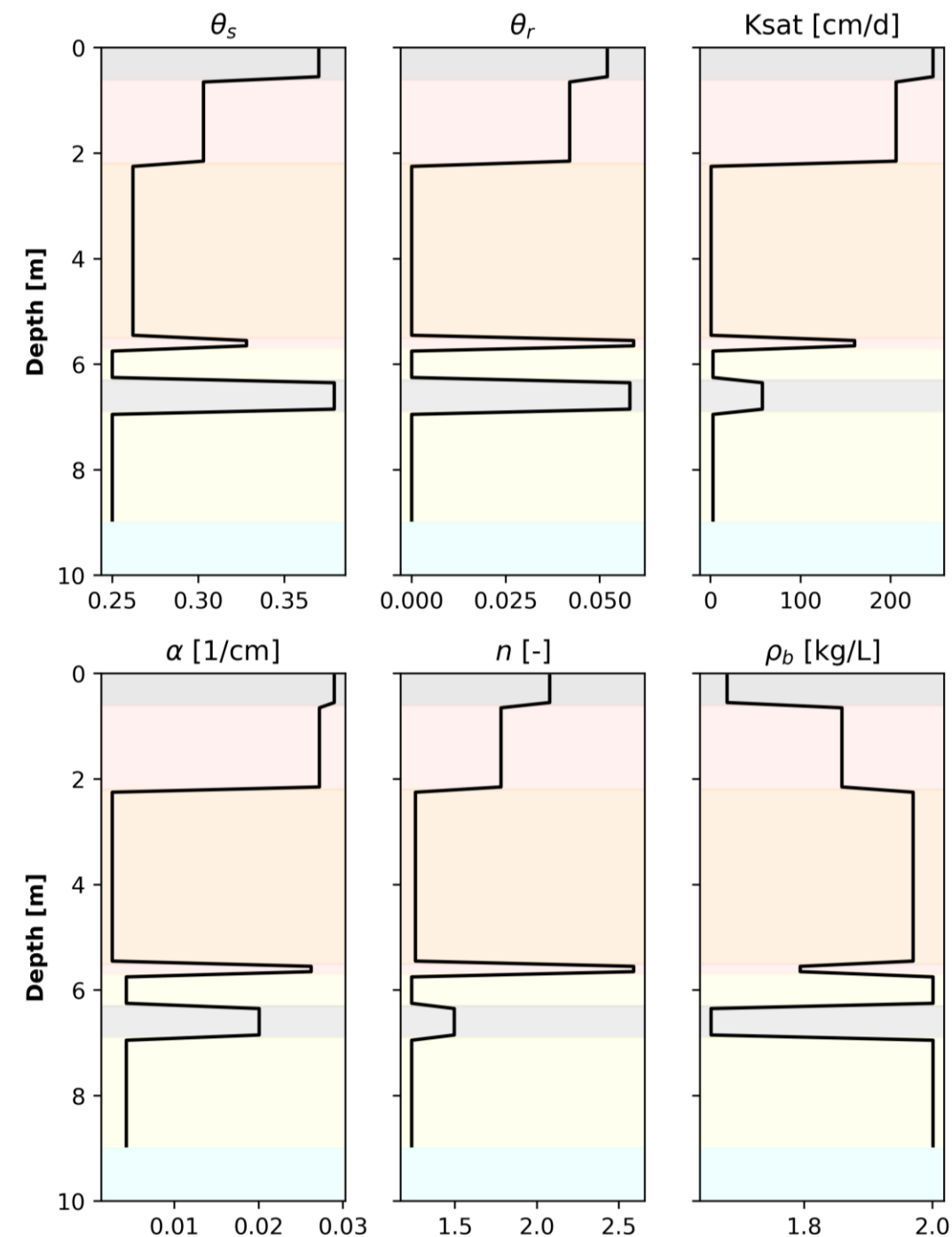
- Developed by Ilka Wallis & John Hutson (Flinders University, Australia)
- 1D numerical model (2D possible)

Flow model

- Richard's equation
- Variable infiltration, evapotranspiration, ...

Transport model

- Linear sorption to soil
- Linear sorption to air-water interface



Model calibration

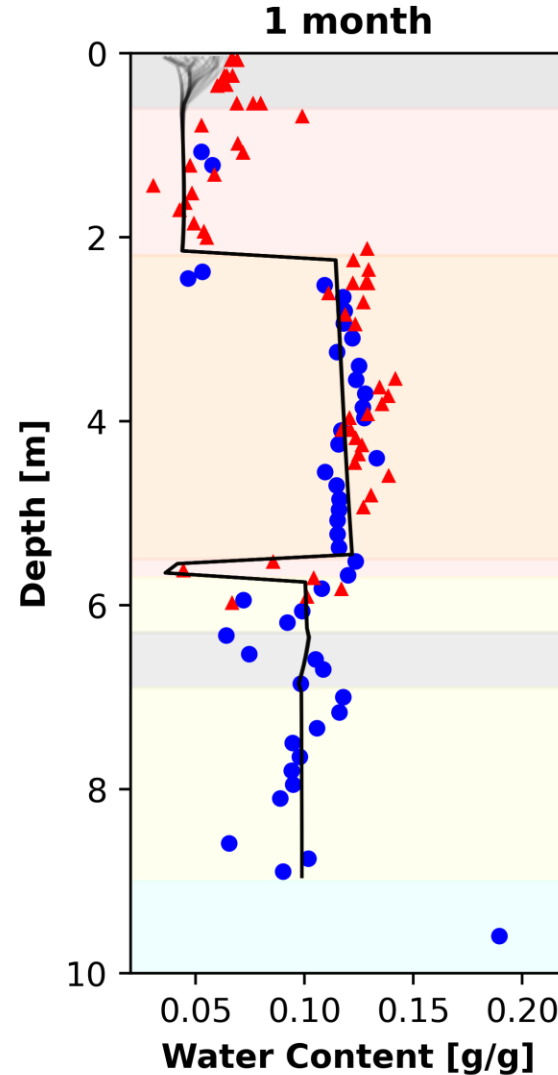
Manual calibration for **gravimetric water content [g/g]** varying:

- ρ_b (bulk density based on θ_s)
- α (van Genuchten)
- n (van Genuchten)

Results:

- Good alignment between model and measurements
- Site-specific van Genuchten parameters were valuable input
- Water content stays almost constant in clayey till and sandy till

Variation over



- | | |
|--------------------------------|--------------------------------------|
| ● measured 13.08.2024, B1 | — simulated 01.10.2025 to 31.10.2025 |
| ▲ measured 14.10.2025, B2 & B3 | — simulated 01.01.2025 to 31.12.2025 |
| | — simulated 01.01.2016 to 31.12.2025 |

Conceptual PFAS Models

Goal

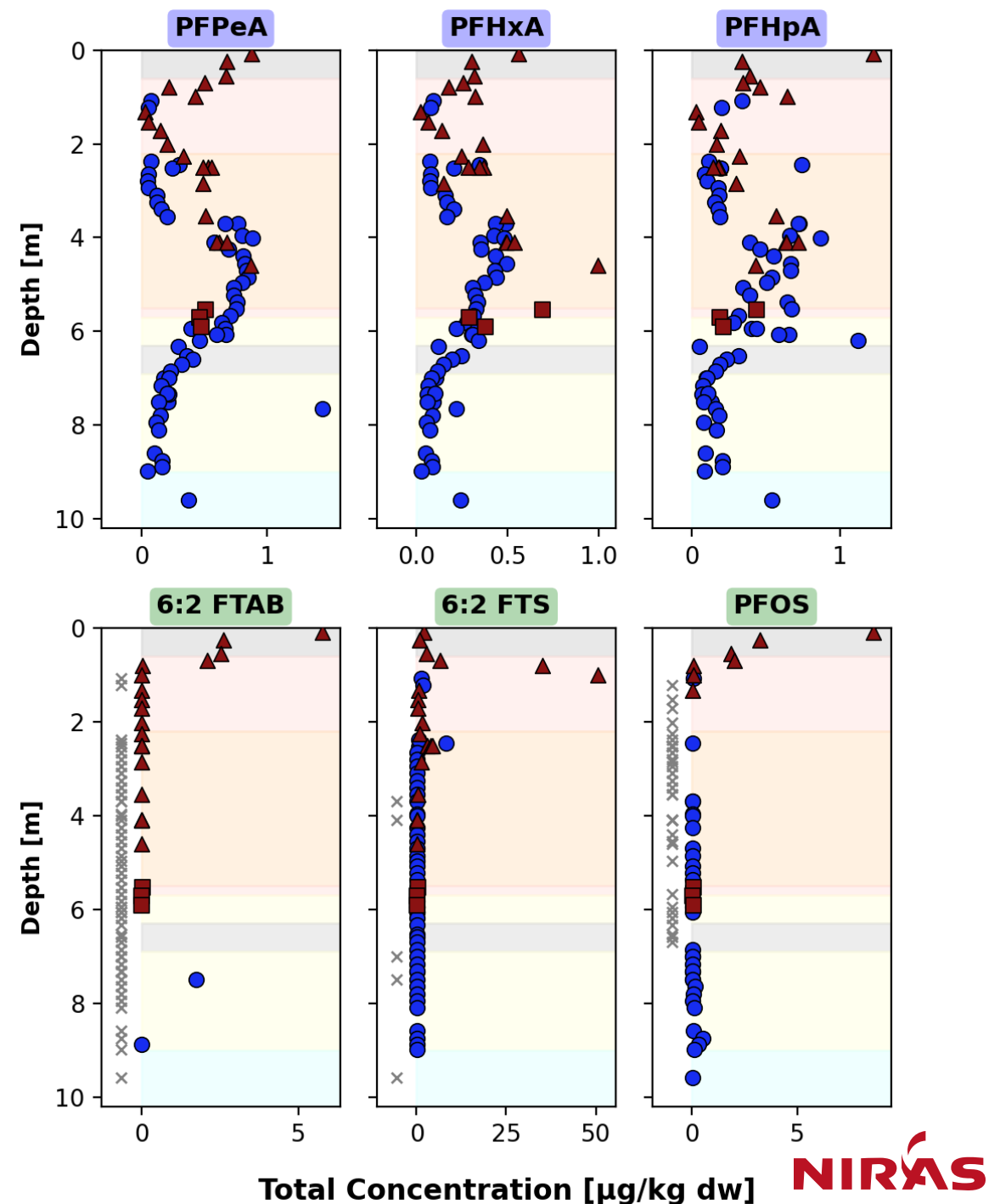
- Reproduce the profiles of PFPeA, PFHxA, PFHpA, 6:2 FTAB, 6:2 FTS and PFOS

Method

- Change input parameters within realistic ranges (K_d , A_{ia} , net infiltration, PFAS application rate)

Results

- Three conceptual numerical models



Model #1 – Base model

Model

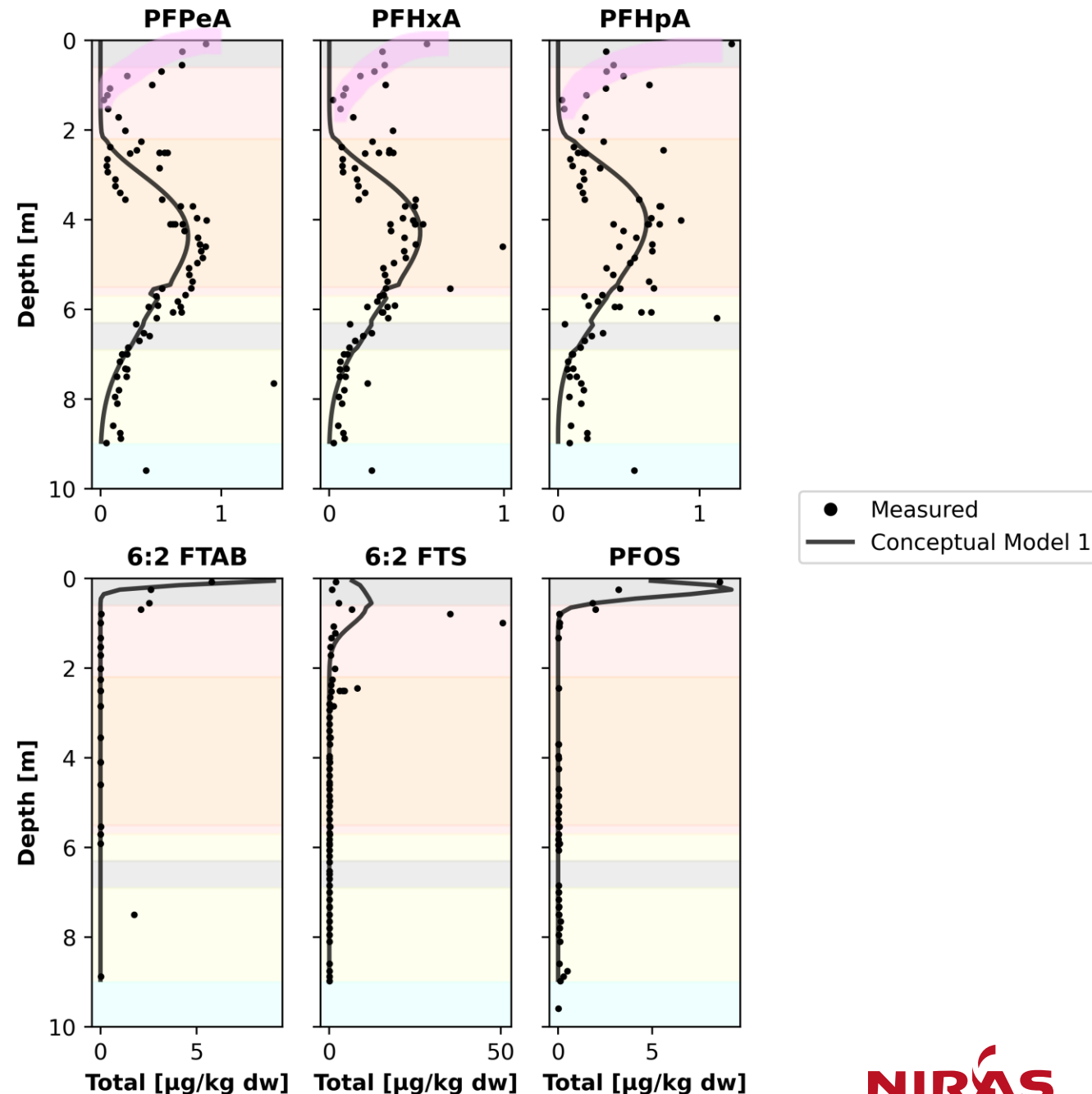
- Based on calibrated flow model
- Includes PFAS transport
 - Sorption to soil
 - Sorption to air-water interface

Results

- Good representation of bulk mass
- Impact of Aia-estimation method (*not shown*)
- Impact of groundwater recharge rate (*not shown*)

Limitations

- Surface-near peak of PFPeA, PFHxA, PFHpA



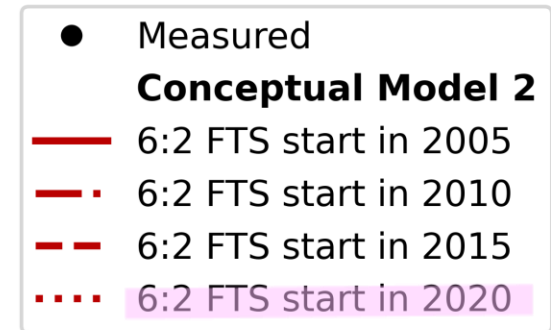
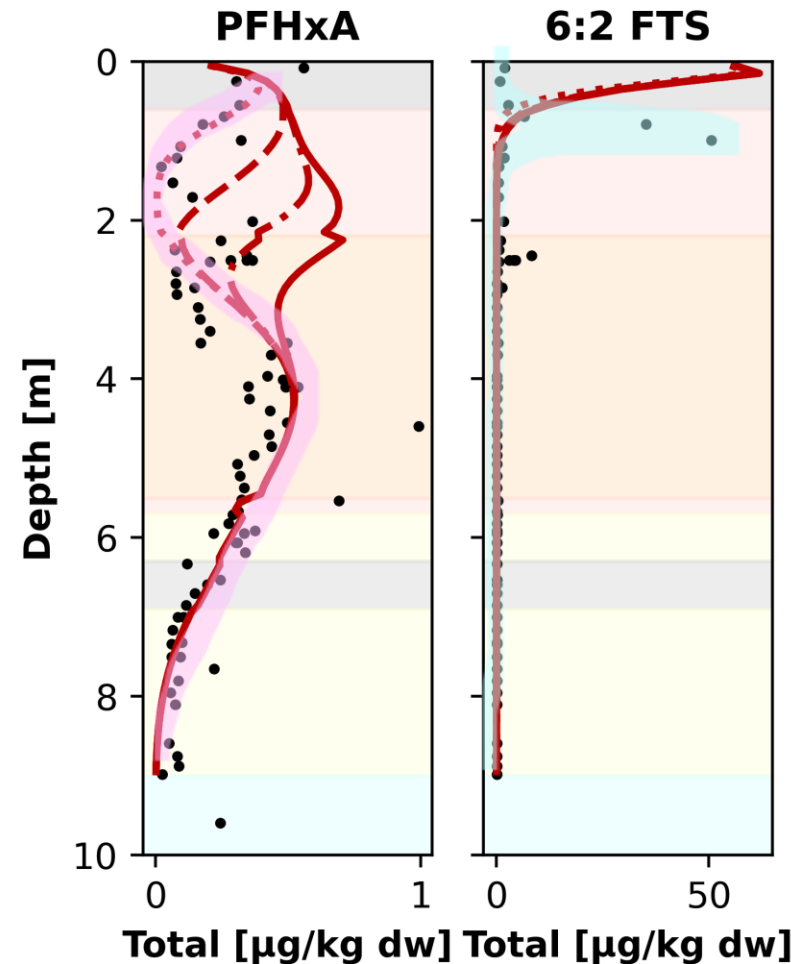
Model #2 - Transformation

Implementation of Transformation

- 6:2 FTS $\xrightarrow{\text{transformation}}$ PFHxA
- “degradation”
represents other transformations $\rightarrow \dots$
- Varying
 - application patterns for 6:2 FTS
 - transformation & degradation rates

Results & Limitations

- Can only reproduce the correct shape if 6:2 FTS is applied after 2020
- Cannot reproduce the 6:2 FTS profile



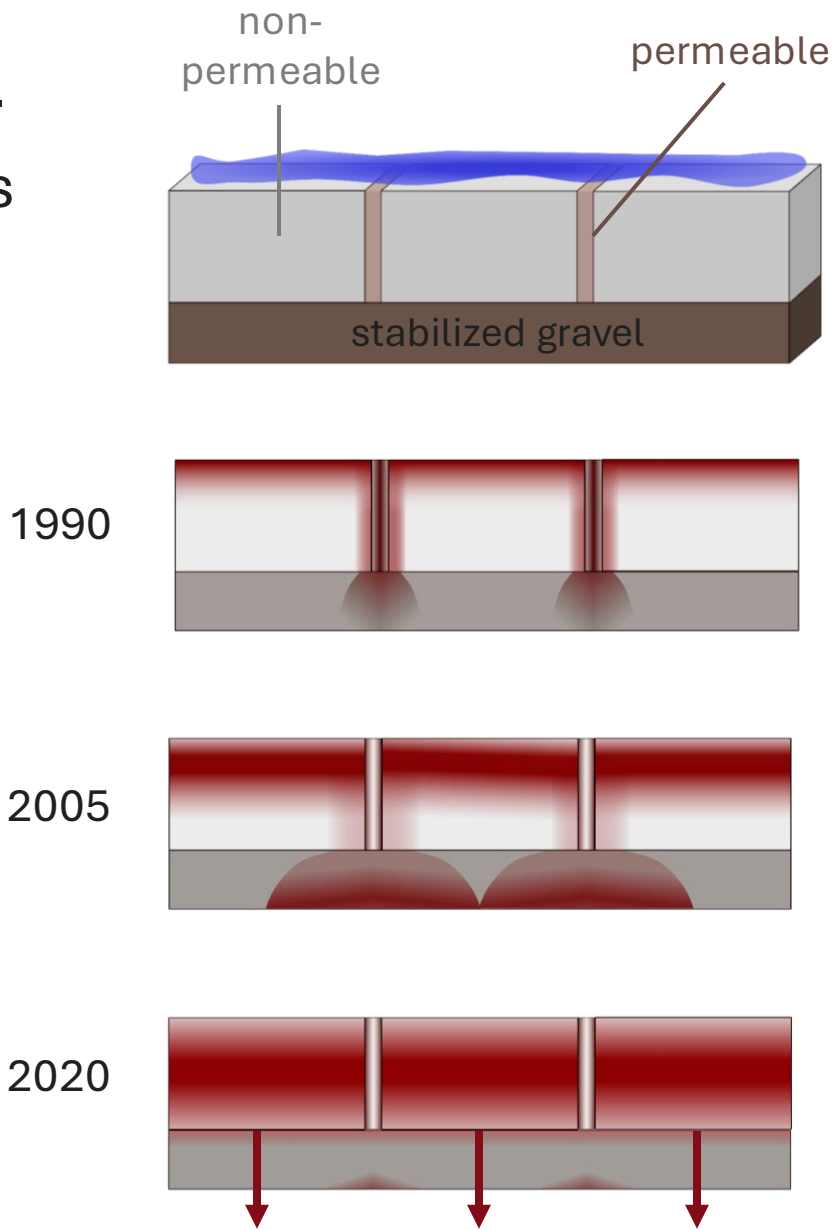
Model #3 – Secondary source

Adaptation:

- Change of application rate of PFHpA, PFHxA & PFHpA
- Theory - slow leaching/diffusion process through the top non-permeable stone layer (“SF-stones”)

PFAS	application old	Application new
PFPeA	1975-2004	1975-2004 + 2020-2025
PFHxA	1975-2004	1975-2004 + 2020-2025
PFHpA	1975-2004	1975-2004 + 2020-2025
PFOS	1975-2004	1975-2004
6:2 FTS	2005 - 2024	2005 - 2024
6:2 FTAB	2005 - 2024	2005 - 2024

Top Layer SF-Stones



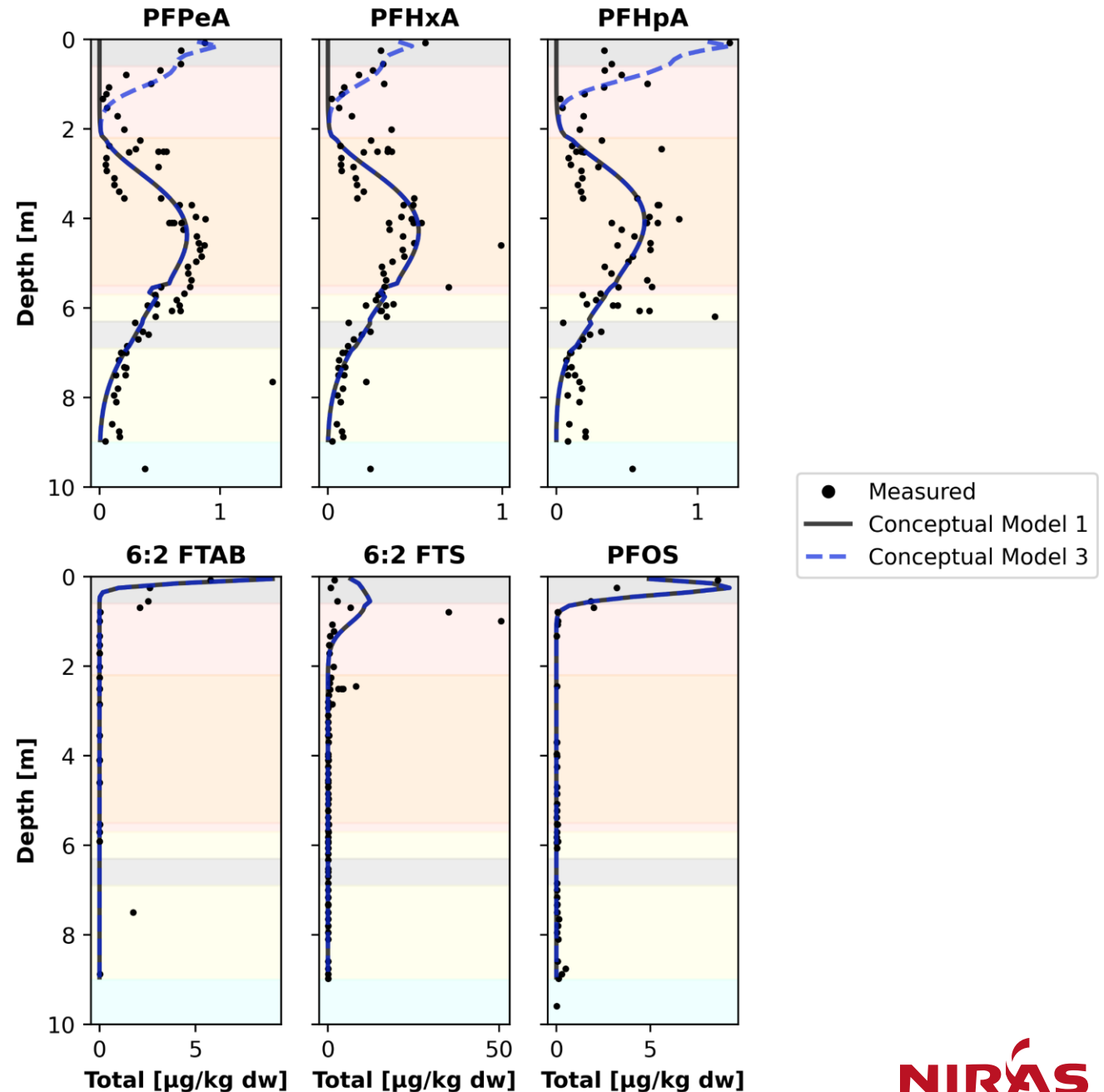
Model #3 – Secondary source

Adaptation:

- Change of application rate of PFHpA, PFHxA & PFPeA
- Theory - slow leaching/diffusion process through the top non-permeable stone layer (“SF-stones”)

Results and limitations:

- Profiles of PFPeA, PFHxA, PFHpA, 6:2 FTAB, PFOS are very well reproduced
- Requires further research in the “SF-stones”



Governing transport processes

Retardation coefficient

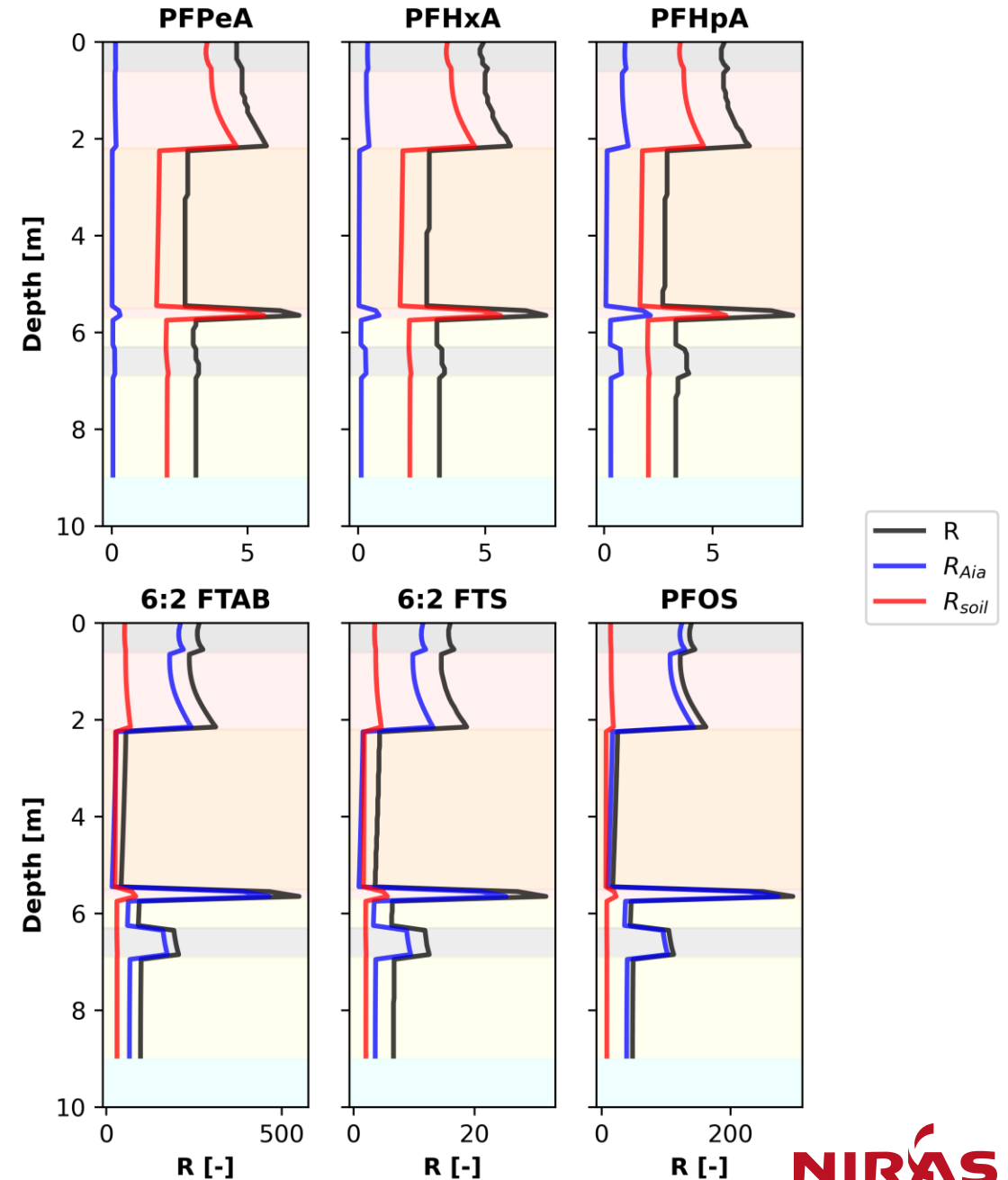
“how much is the compound slowed down”

$$R = 1 + \underbrace{\frac{K_d \cdot \rho_b}{\theta_w}}_{R_{Soil}} + \underbrace{\frac{K_{ia} \cdot A_{ia}}{\theta_w}}_{R_{Aia}}$$

The **sorption to the soil** plays major part for the total retention for PFPeA, PFHxA, PFHpA.

The **sorption to the air-water interface** plays the major role for the retention of 6:2 FTAB, 6:2 FTS and PFOS.

The retention in **glacial tills**, is typically lower than sandy soils.



Take Home Messages

1. Combination of **high-resolution vertical profiles** and **numerical modelling** is a powerful tool to **investigate the governing transport processes** of contaminants in the subsurface and thus **improve risk assessments**
2. **Site-specific van Genuchten parameter & water content measurements & net infiltration rates** were highly valuable for the model calibration
3. Field work – **detailed screening at the top** is important to catch the main mass of long-chain PFAS (e.g. PFOS, 6:2 FTAB)
4. Retardation in clayey till & sandy till is expected to be lower than in sandy soils
5. Profiles of PFPeA, PFHxA, PFHpA could be reproduced if there if including a **second delayed input** . Possibly due to slow release from the **SF-stones**.

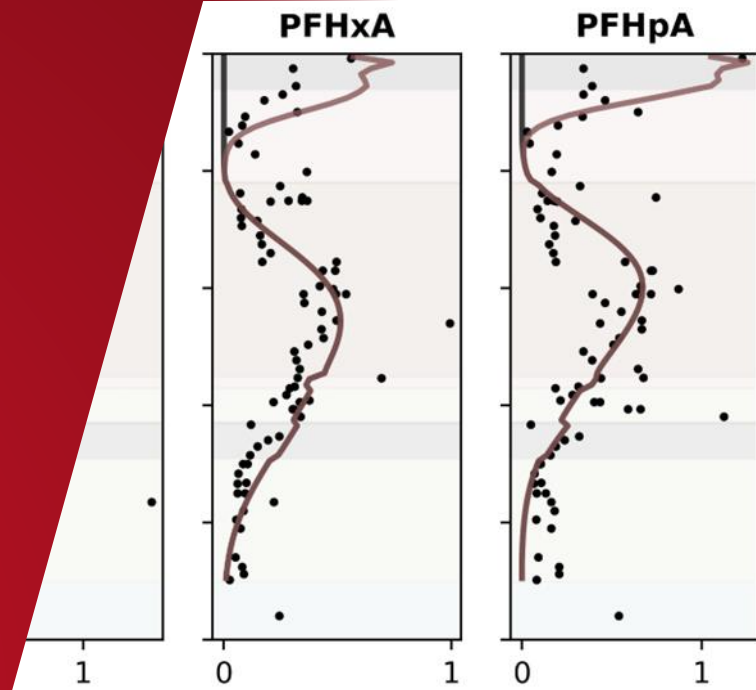


Thanks for the attention!

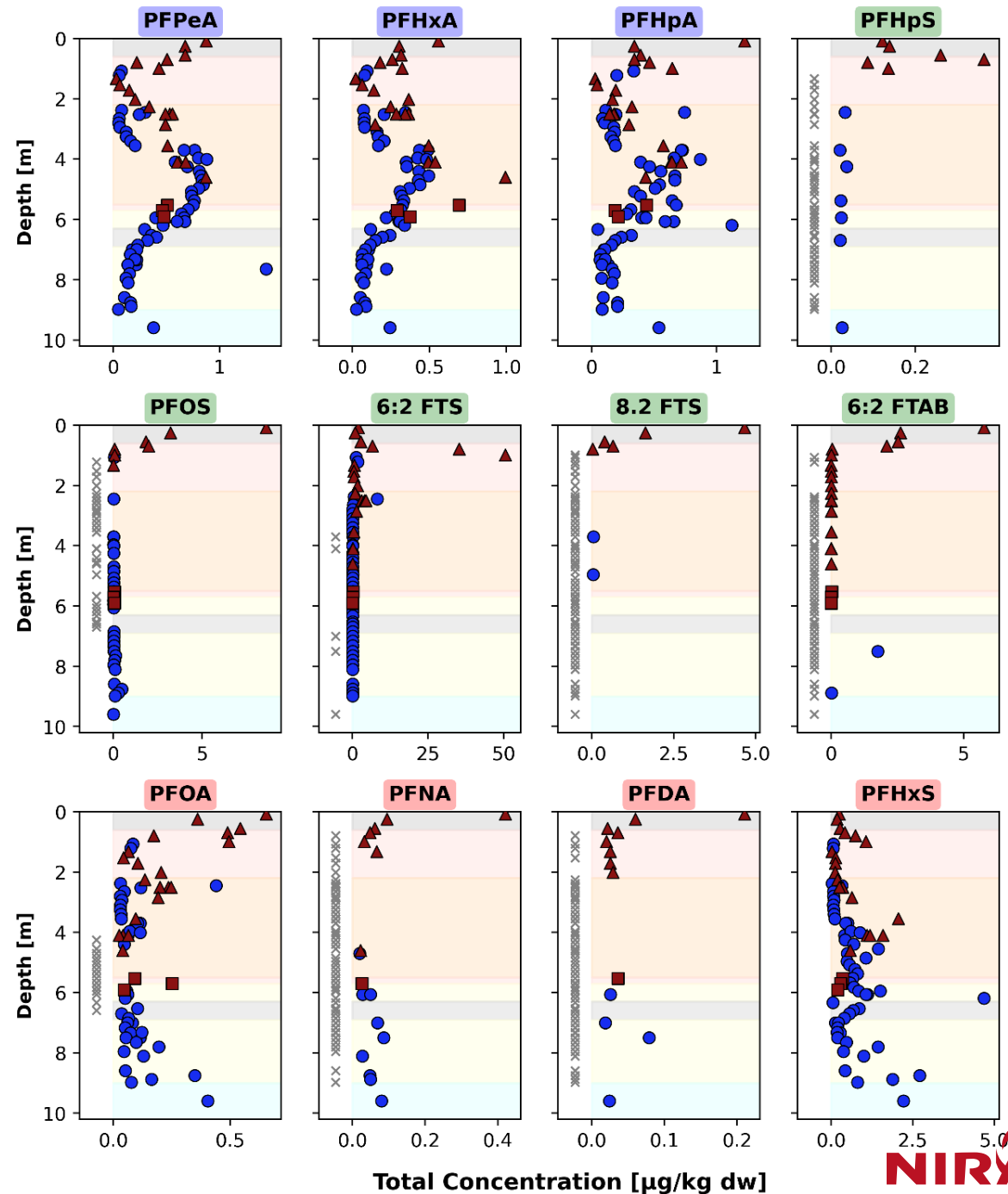
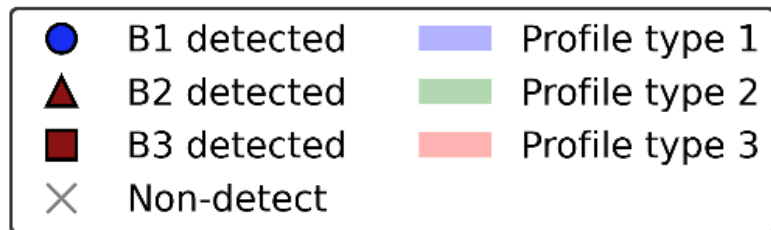


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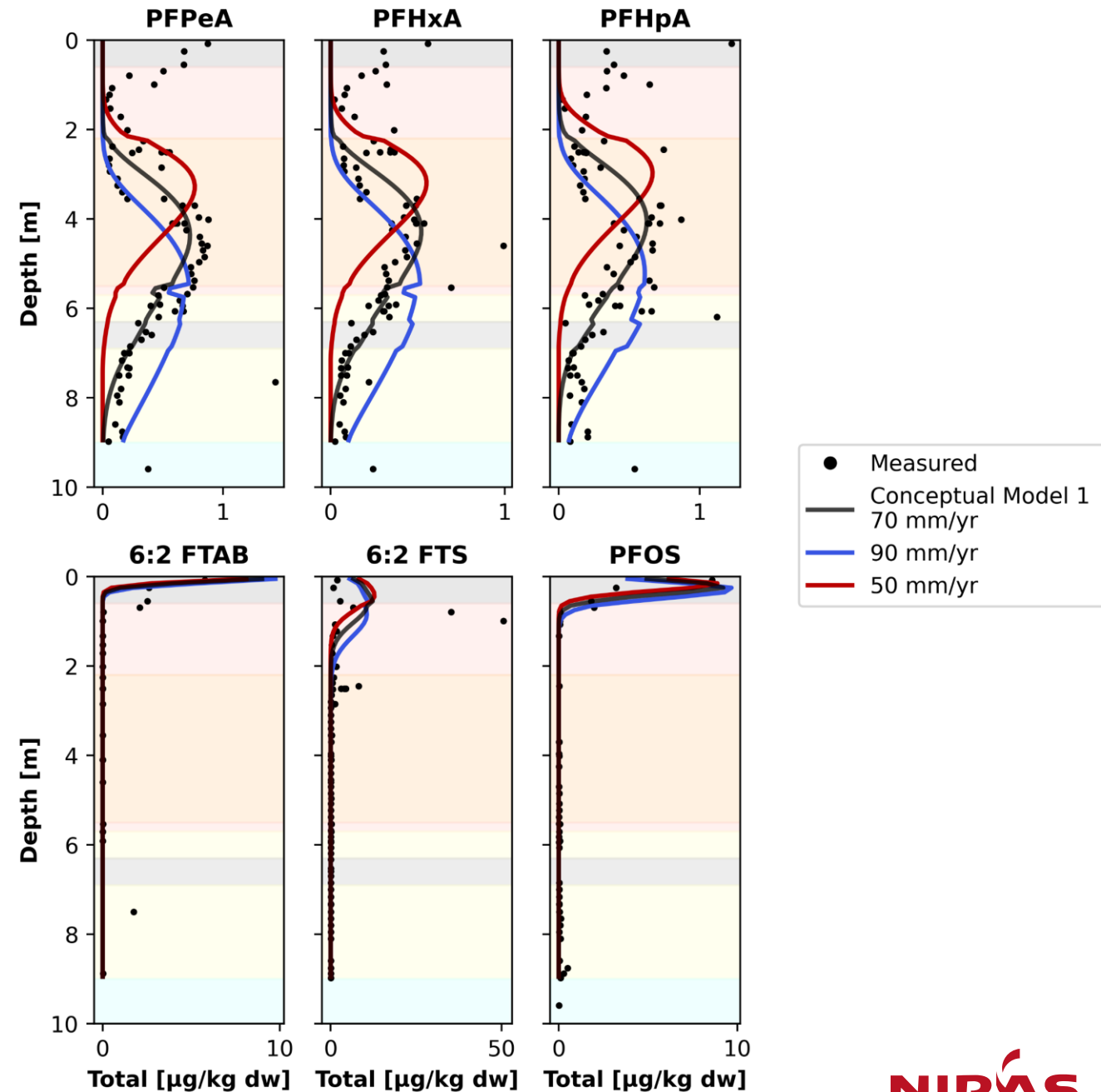
essc@niras.dk
PhD student



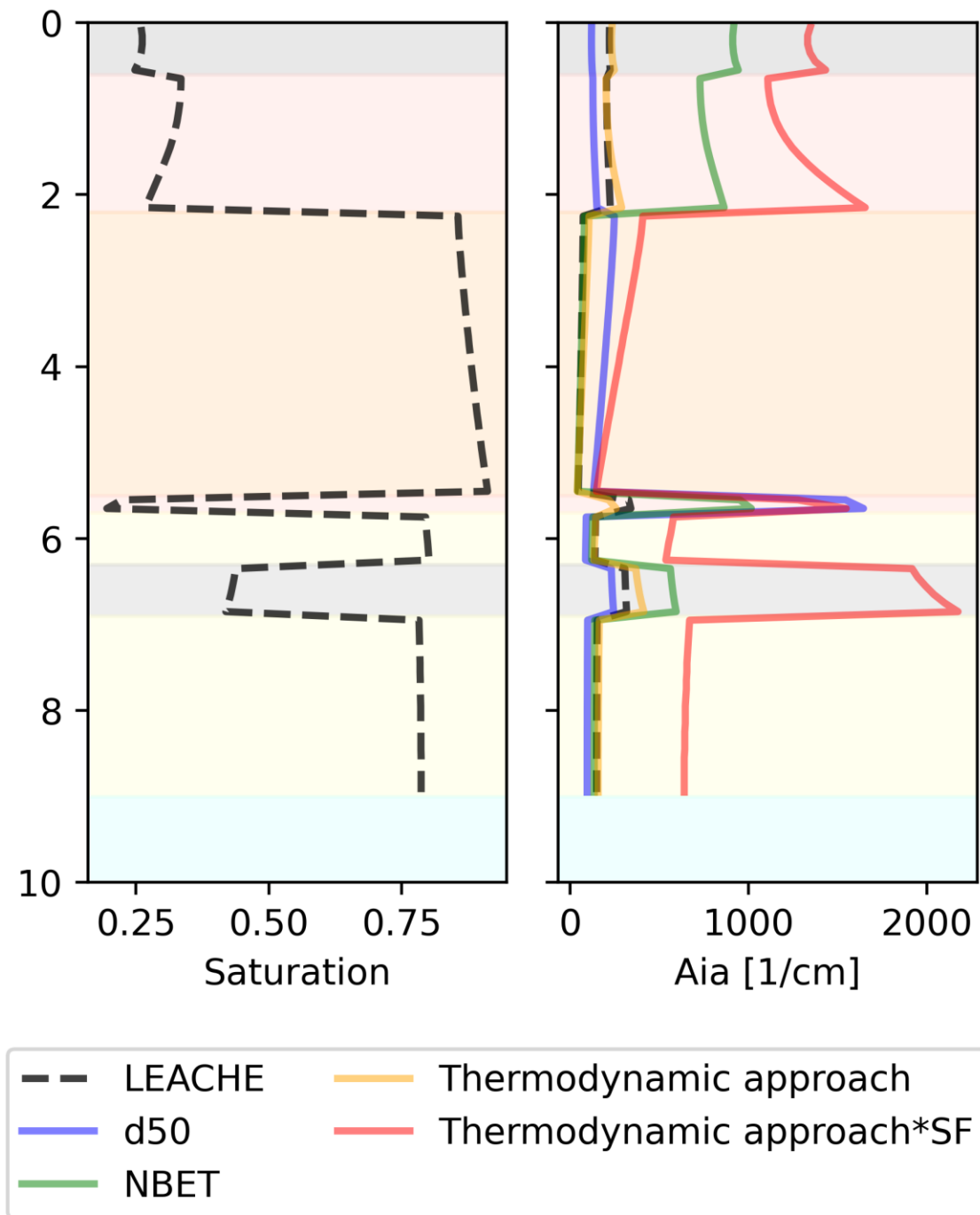
PFAS Depth Profiles



Model #1 – varying net groundwater recharge rate



Aia vs. Depth

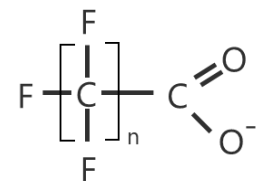


Field Site –

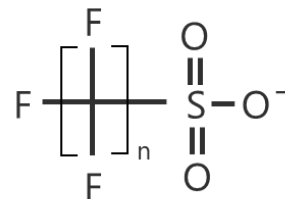
PFAS analysis (in soil)

Analyzed for 29 PFAS - Focus today 6 PFAS

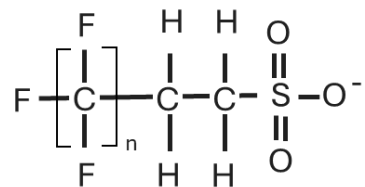
PFCAs



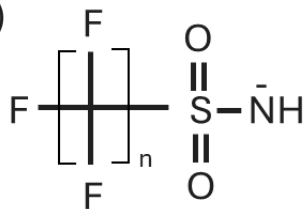
PFSAs



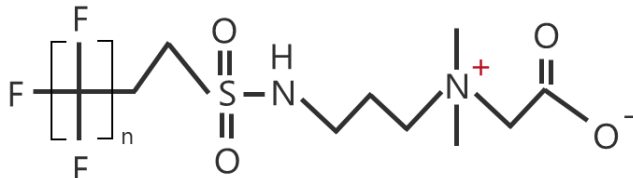
n:2 FTS



FASA (e.g. FBSA, FHxSA, PFOSA)



6:2 FTAB



PFCAs + precursors			PFSA's + precursors		
PFAS	# C in chain	Ion	PFAS	# C in chain	Ion
PFTeDA*	13		PFTrDS	13	
PFTrDA	12	-	PFDoDS	12	
PFDoA	11	-	PFUnDS	11	
PFUdA	10		PFDS	10	
PFDA	9	-	PFNS	9	-
PFNA	8	-	PFOS	8	-
PFOA	7	-	PFHpS	7	-
PFHpA	6	-	PFHxS	6	-
PFHxA	5	-	PFPeS	5	-
PFPeA	4	-	PFBS	4	-
PFBA	3	-			
6:2 FTS	6	-	FBSA*	4	-
6:2 FTAB*	6	+ / +/-	FHxSA*	6	-
8:2 FTS *	8	-	AmPr-FHxSA*	6	+/-
			TAmPr-FHxSA*	6	+/-
			PFOSA	8	-

Precursors

*Not included in Danish soil & GW quality criteria