

”Simpel” bestemmelse af vertikal flux – hvad kan man gøre i praksis på de ”almindelige” sager

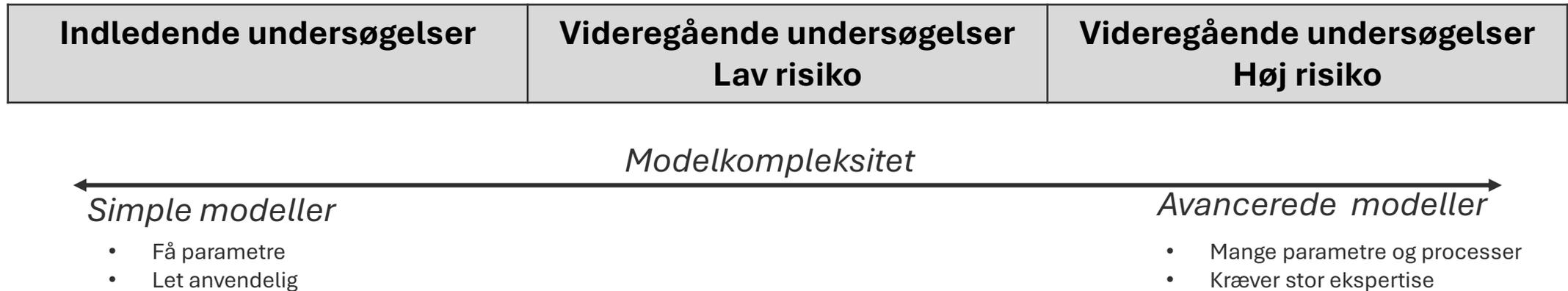
Therese L. Petersen, Gro Lilbæk, Søren Dyreborg, NIRAS A/S
Henning Wienkenjohann, Klaus Mosthaf, Poul L. Bjerg, DTU
Louise Rosenberg og Nina Tuxen, Region Hovedstaden

ATV vintermøde, Temadag 2. marts 2026



Formål

- Hvordan kan ”simplere” modeller bruges til risikovurdering af PFAS?
- Hvilke PFAS risikovurderingsværktøjer har vi og hvornår kan de bruges?
- Hvornår kan de bruges uden at ”begå” store fejl?



- Vi bruger flux i risikovurderingen.

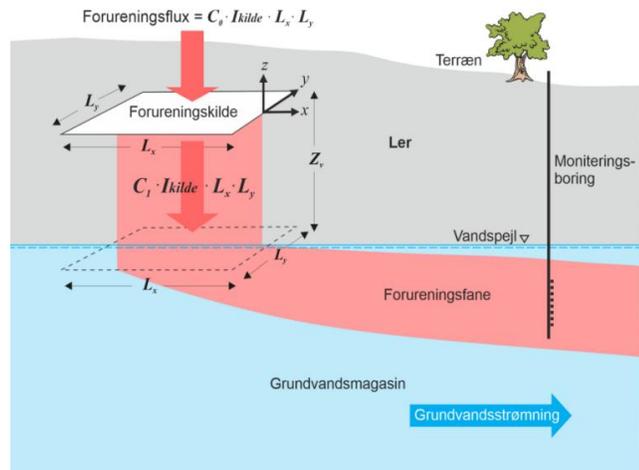
Husk PFAS ≠ PFAS

Modeller/risikovurderingsværktøjer

Simpel model

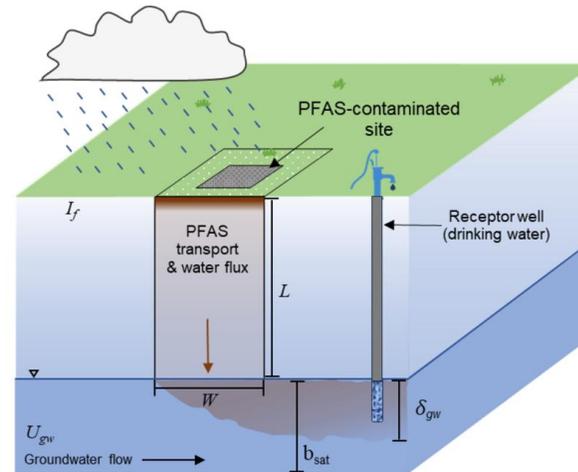
$$J = \sum_{i=1}^n C_i \cdot A_i \cdot I_i$$

GrundRisk



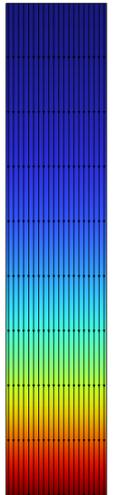
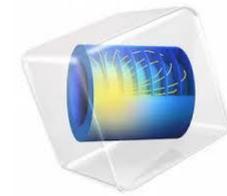
(VMR, 2022)

PFAS-LEACH



(Smith et al., 2025)

COMSOL



Module0 Input Screen - Basic Analysis

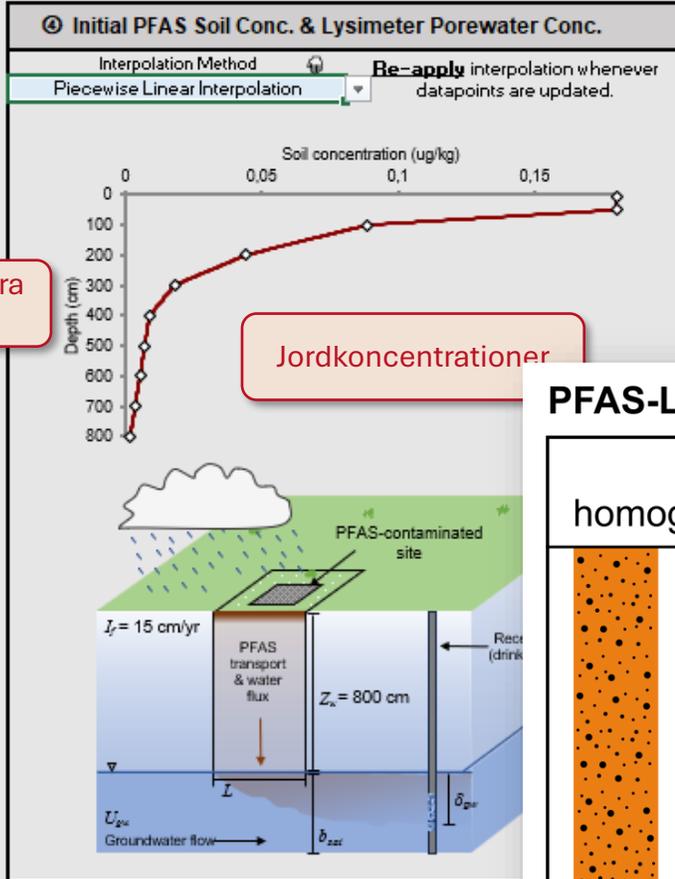
READ BEFORE START:

Read Section 2 of the User Guide for parameter descriptions and work through Boxes ① to ⑤ sequentially.
 Blue cells can be filled with reference values using the **blue cells** icon.
 White cells can be either estimated using the **functional** icon.
 Default values for all cells can be set by clicking the **green** icon.
 Parameters with asterisks (*) are the bare minimum to run the simulation.
 When copying and pasting, please paste **values only** to avoid changing the sheet's formatting.

Mange felter behøver ikke at blive udfyldt

Soil Properties and Site Conditions		Parameter Values	Set Default Values
Depth to groundwater*	Z_w	cm	800
Contaminated site area (or unit area)	A	m^2	100
Temperature	T	$^{\circ}C$	User defined
Net infiltration*	I_f	cm/yr	15.00
Soil bulk density*	ρ_s	g/cm^3	1.78
Saturated hydraulic conductivity	K_s	cm/day	
Residual water content	θ_r	cm^3/cm^3	
Saturated water content*	θ_s	cm^3/cm^3	0.330
Median grain size	d_{50}	cm	
Organic carbon fraction	f_{oc}	%	
van Genuchten parameter	α	cm^{-1}	
van Genuchten parameter	n	(-)	
Longitudinal dispersivity*	α_L	cm	10.00
Water content*	θ	cm^3/cm^3	0.200
Air-water interfacial area scaling factor	SF	(-)	
Air-water interfacial area*	A_{aw}	cm^2/cm^3	250.0

Parameterværdier fra PFASen



PFAS-LEACH

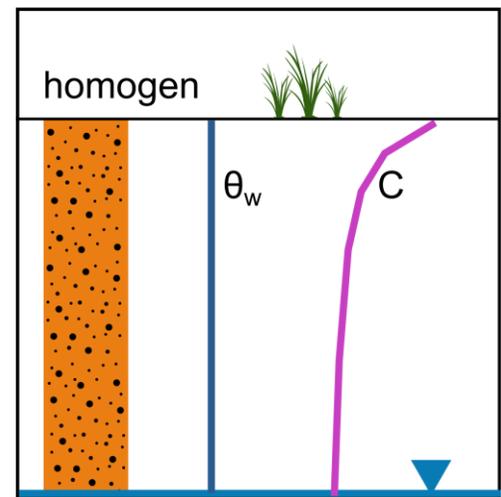


Illustration of Henning Wienkenjohann

PFAS Properties		Parameter Values	PFAS Type
Surface tension parameter	a	mg/L	
Surface tension parameter	b	(-)	User defined
Surface tension parameter	σ_p	dyn/cm	
Molar mass*	M	g/mol	214.04
Molecular diffusion coefficient*	D_p	cm^2/s	5.62E-06
Molar volume	V	cm^3/mol	
Organic carbon-water partition coefficient	K_{oc}	cm^3/g	
Solid-phase adsorption coefficient*	K_d	cm^3/g	0.06
Air-water interfacial adsorption coefficient*	K_{aw}	cm^3/cm^2	2.06E-05

NOTE: F_s and α_s are only needed for using the advanced solver.

Groundwater Dilution		Parameter Values	Estimate $\alpha_s, \delta_{gw}, DF$
Groundwater darcy flux	U_{gw}	m/yr	
Lateral site width	L	m	
Saturated zone thickness	b_{sat}	m	
Vertical dispersivity	α_v	m	
Mixing zone thickness	δ_{mix}	m	
Dilution Factor*	DF	(-)	150.0

Simulation Information		Parameter Values	Advanced Solver
Simulation time (time series)*	t	yr	100
Output time interval (time series)*	Δt	yr	1
Output time points (profiles)*	t_p	yr	5,10,30,50
Acceptable groundwater concentration*	$C_{gw,c}$	ug/L	0.002

(Equilibrium solid-phase sorption)

(Kinetic solid-phase sorption)

Outputs fra PFAS-LEACH

Computed Results from PFAS-LEACH-Analytical

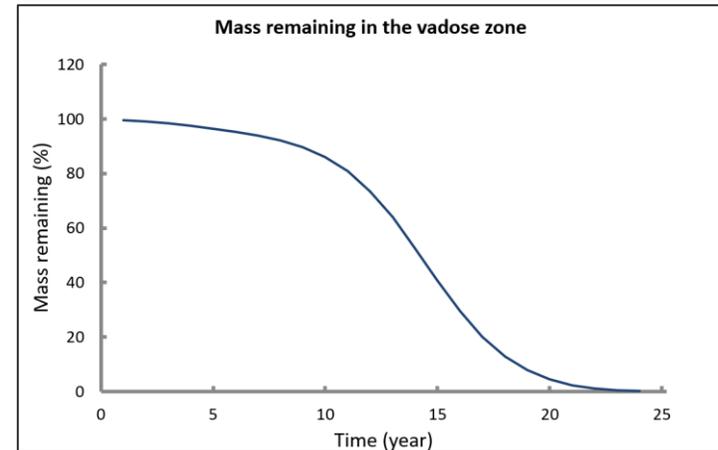
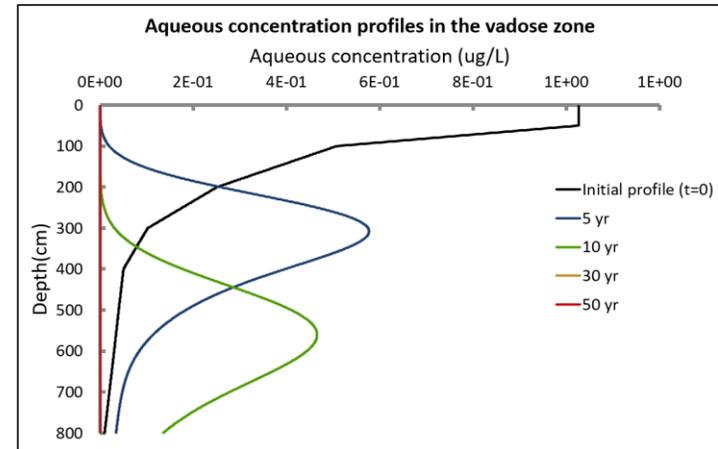
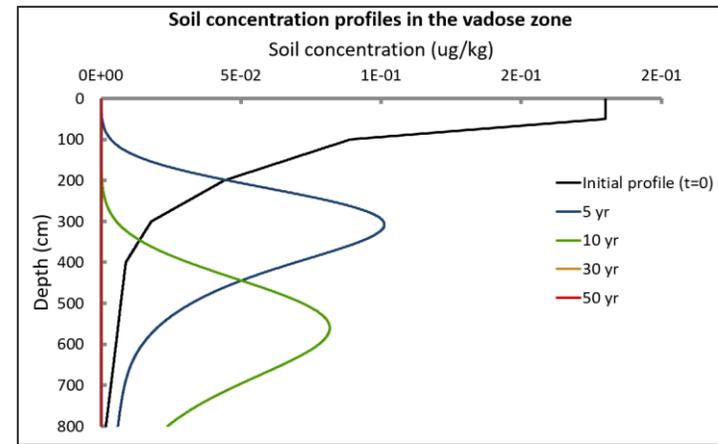
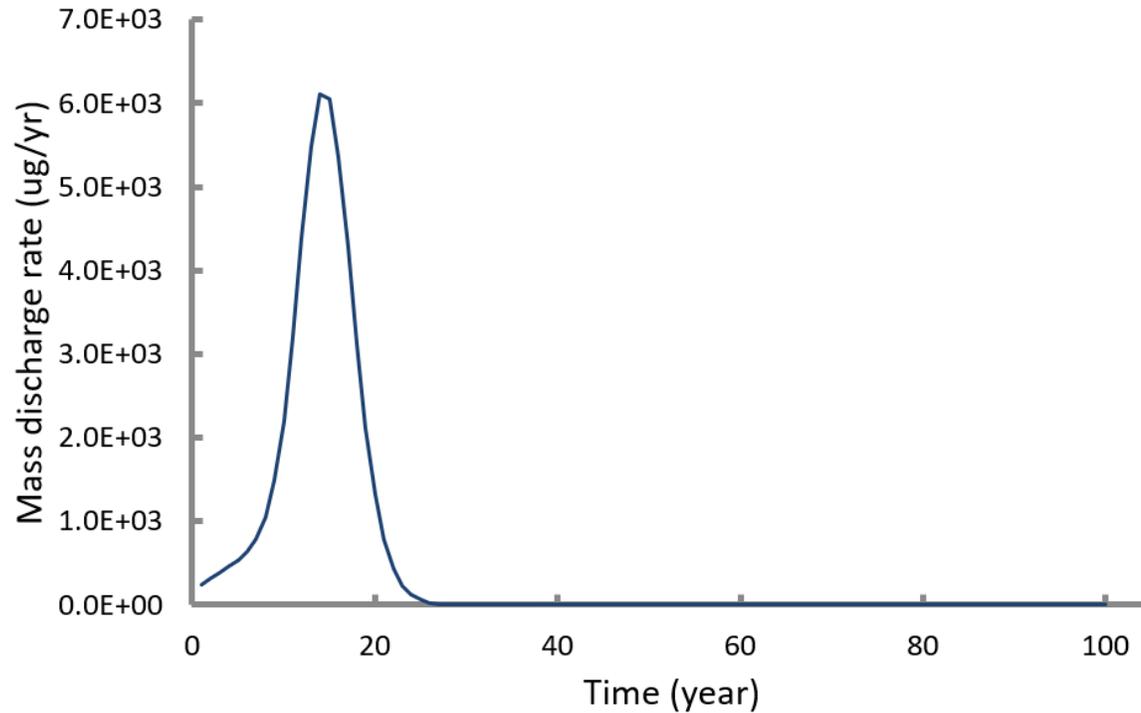
Select what to plot



Vadose-zone mass discharge rate

Download data

Vadose-zone mass discharge rate



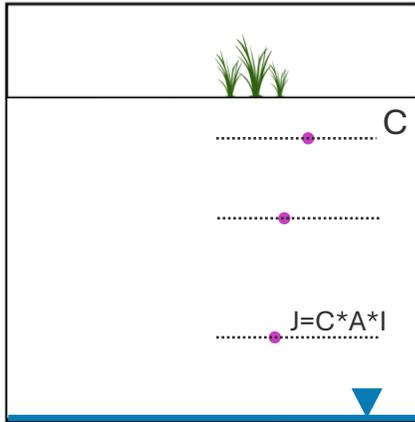
Konceptuelle forskelle

Simple modeller

Avancerede modeller



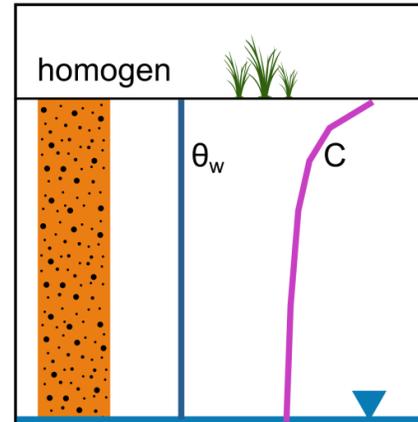
Simpel model



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

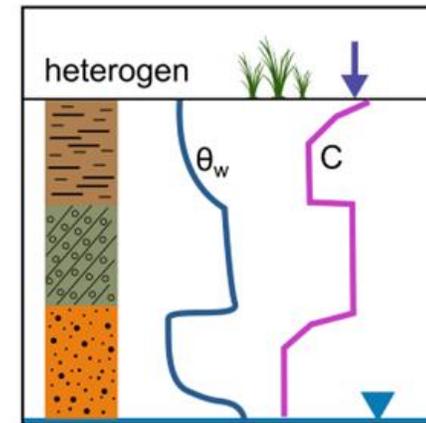
- Steady state
- Én koncentration

PFAS-LEACH



- Tidsafhængig
- Homogen geologi
- Konstant vandmætning
- Kun jordkoncentration med mulighed for at definere et koncentrationsprofil
- Ingen kilde

COMSOL



Illustrationer af Henning Wienkenjohann

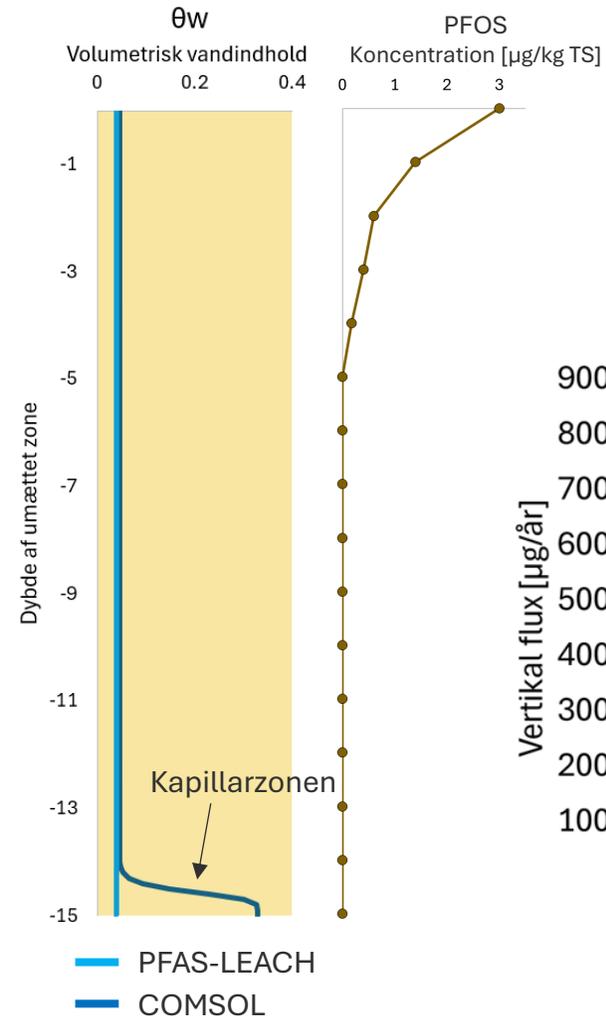
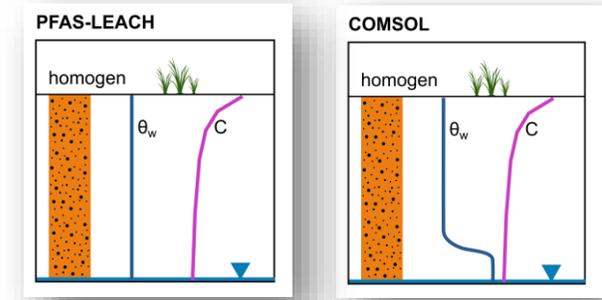
- Tidsafhængig
- Mulighed for variabel geologi og vandmætning
- Mulighed for at definere et koncentrationsprofil
- Mulighed for at tilføje en kilde
- Mulighed for at tilføje heterogenitet (lenser, sprækker)
- Mulighed for at variere infiltration

Region Hovedstadens typologier

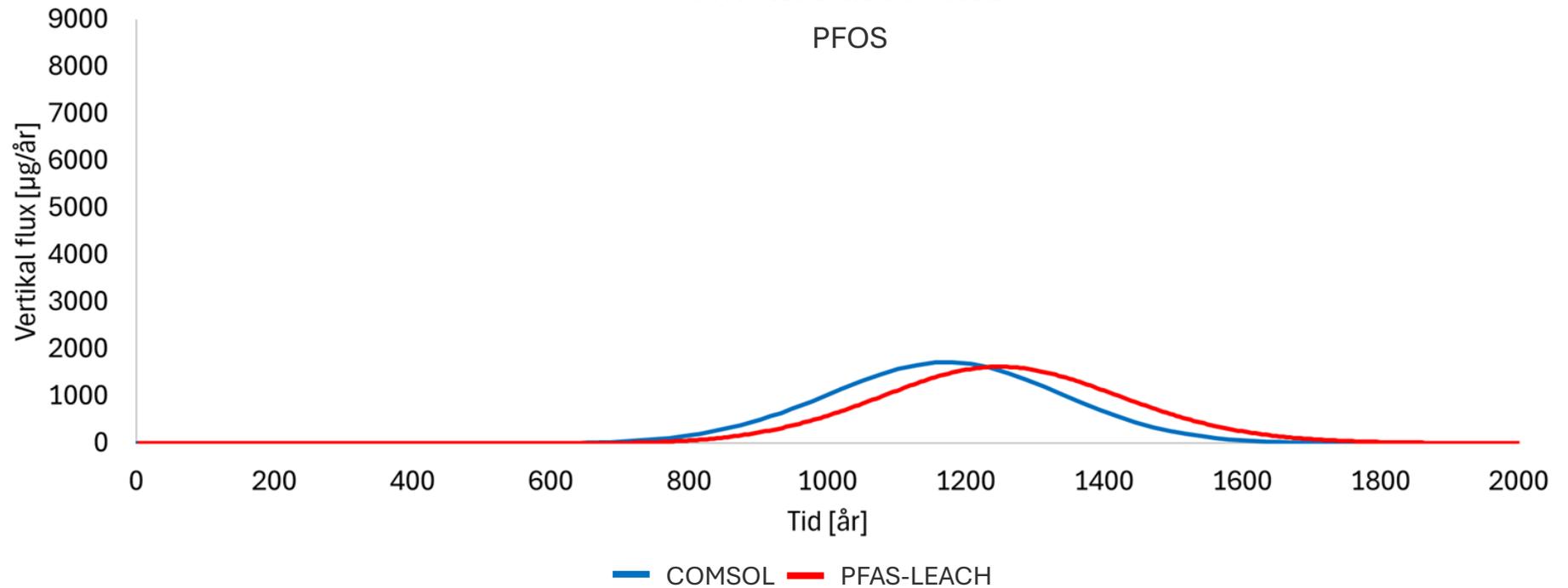
- Hvilke modeller kan bruges?
- Hvilke opmærksomhedspunkter er der ved de individuelle typologier?
- Tre jordtyper dominerer den umættede zone
 - Smeltevandssand
 - Oxideret moræneler
 - Reduceret moræneler



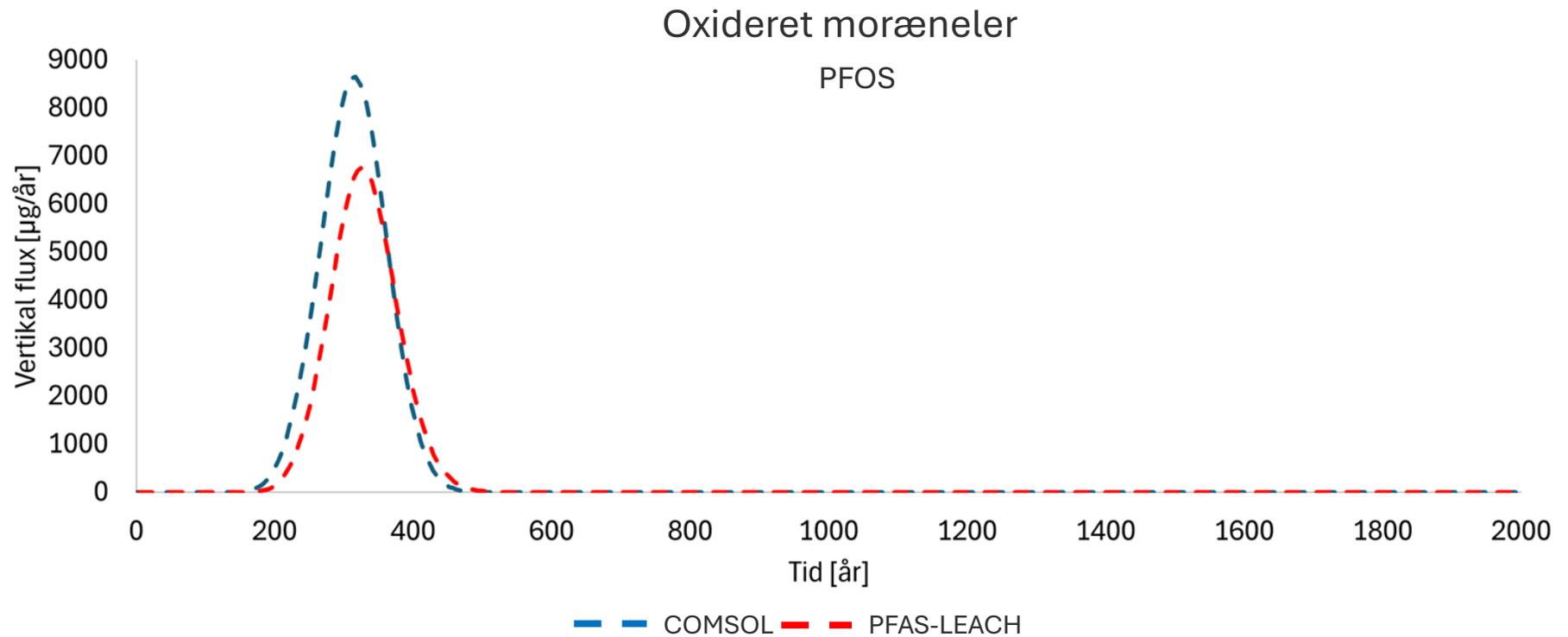
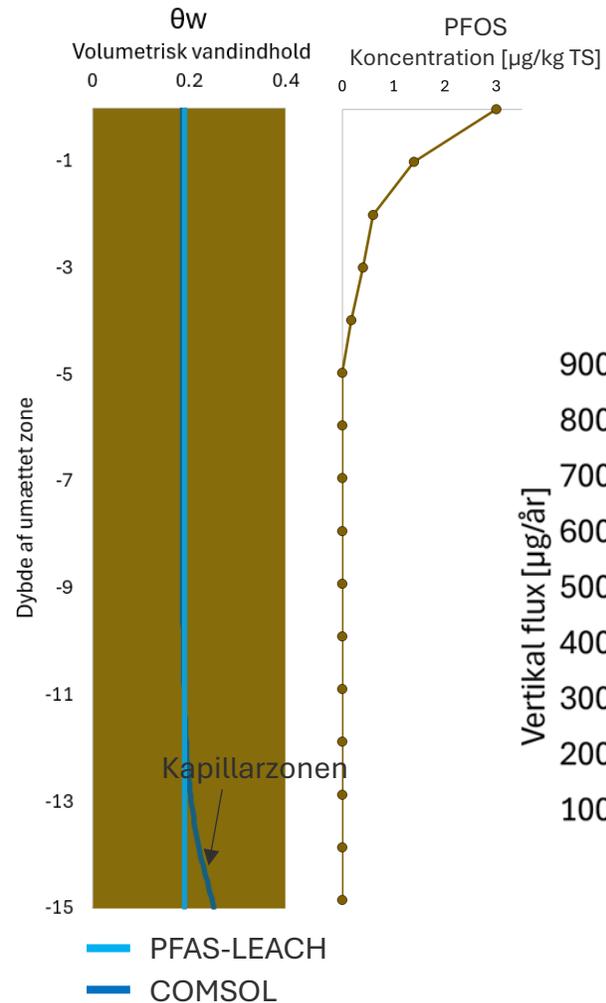
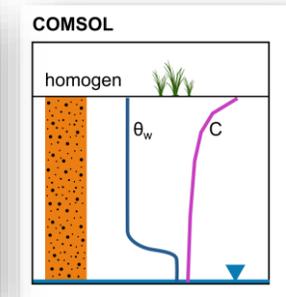
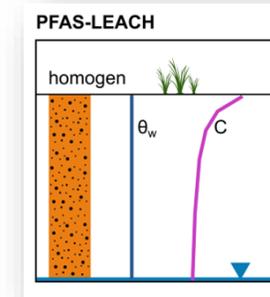
Sammenligning af PFAS-LEACH med COMSOL



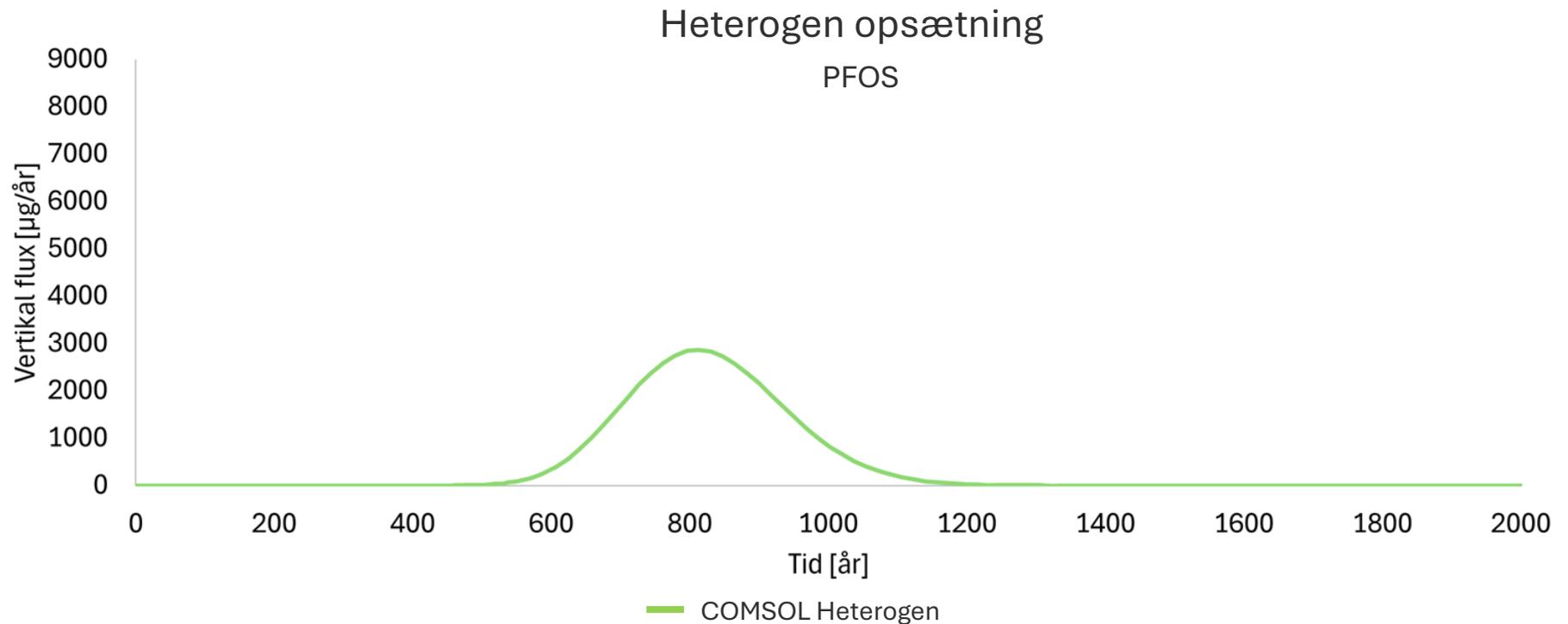
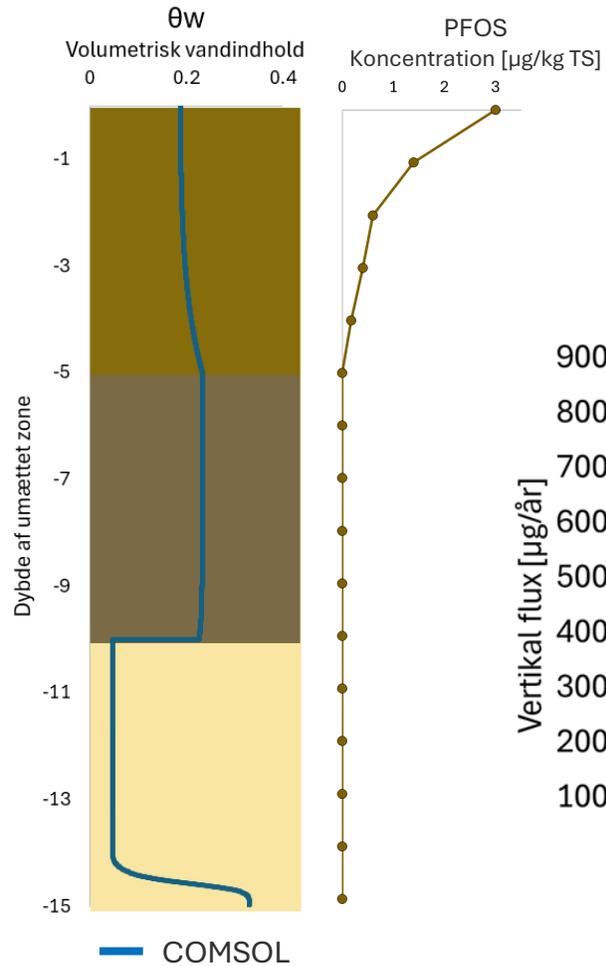
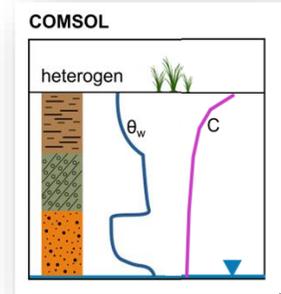
Smeltevandssand
PFOS



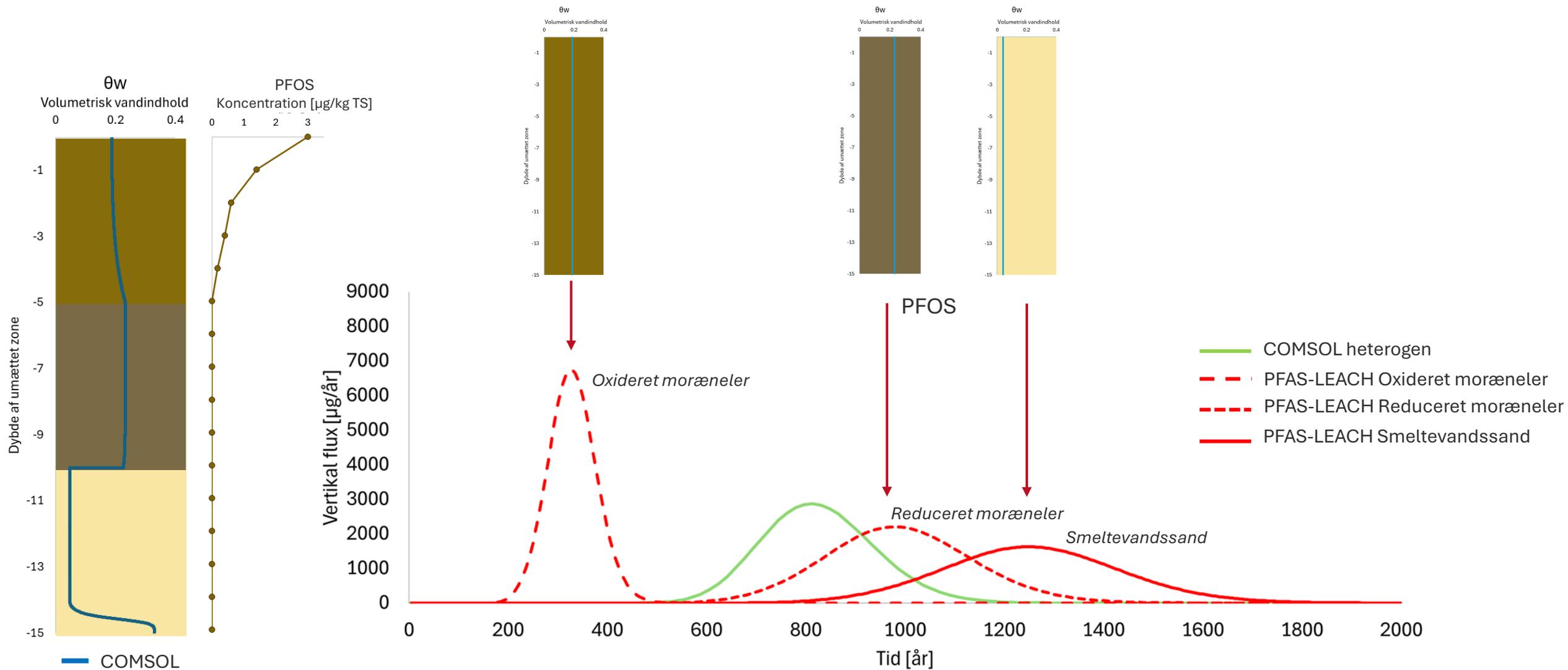
Sammenligning af PFAS-LEACH med COMSOL



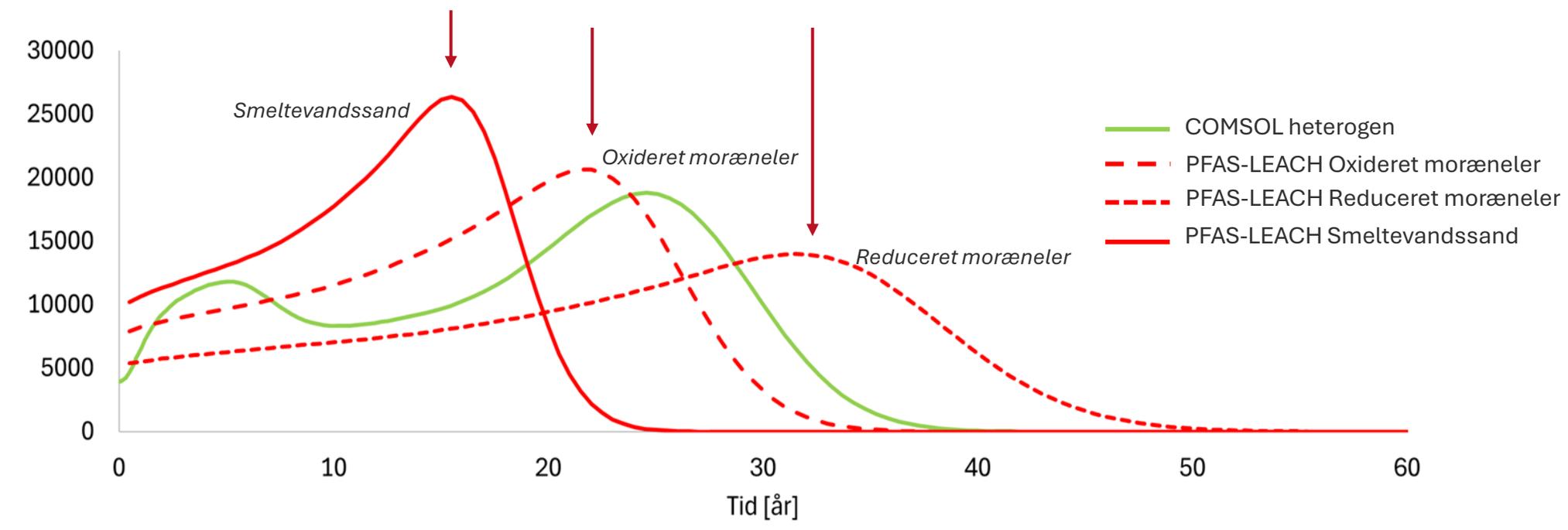
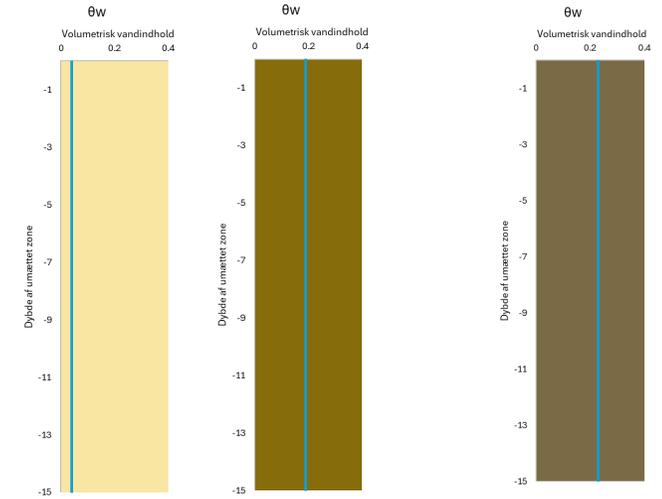
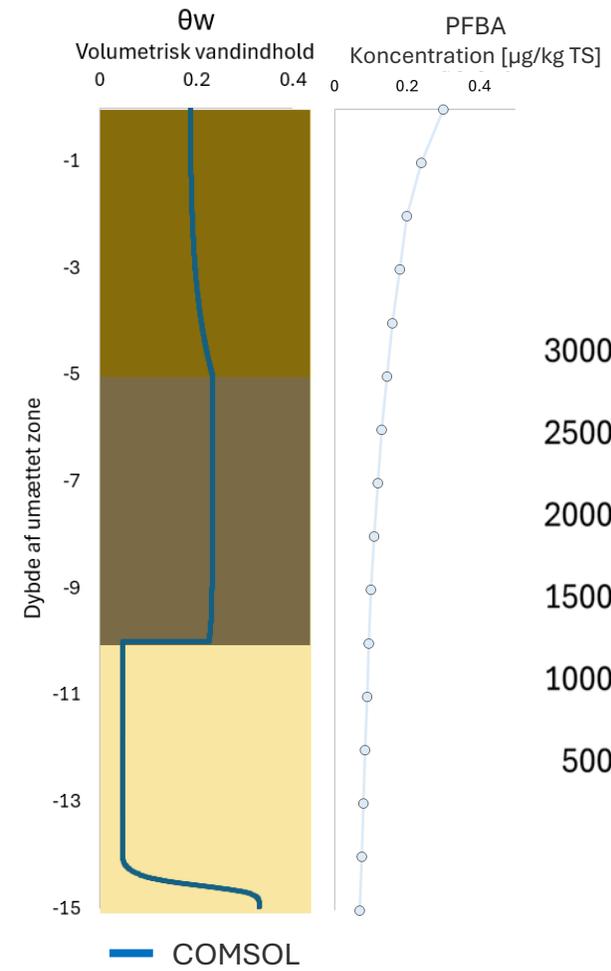
Sammenligning af PFAS-LEACH med COMSOL



Sammenligning af PFAS-LEACH med COMSOL

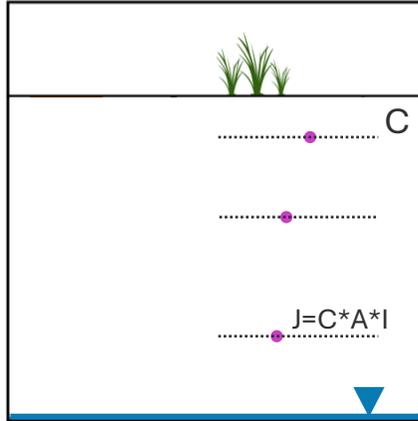


PFBA

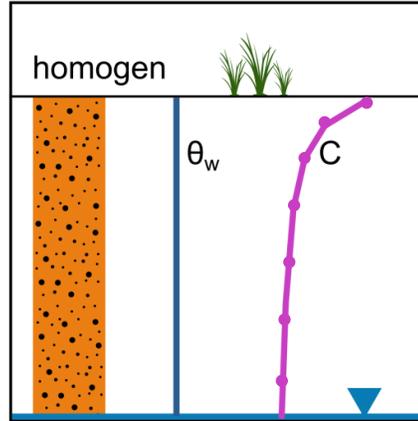


Hvordan defineres kilden?

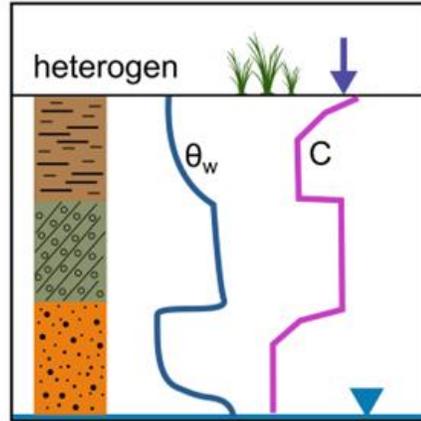
Simpel model



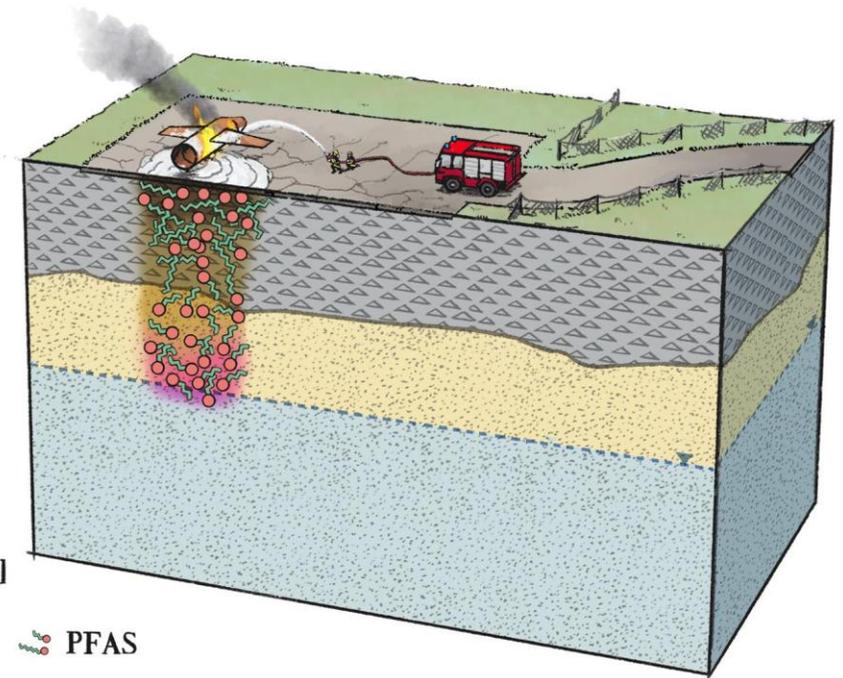
PFAS-LEACH



COMSOL



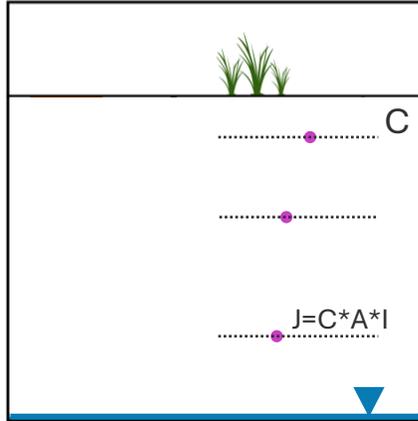
Illustrationer af Henning Wienkenjohann



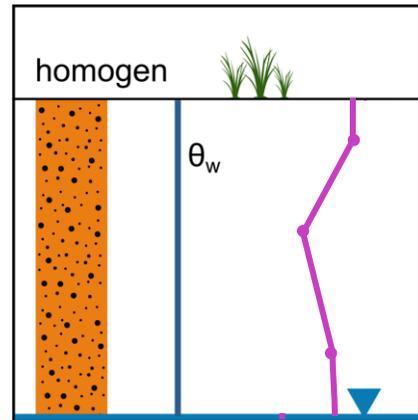
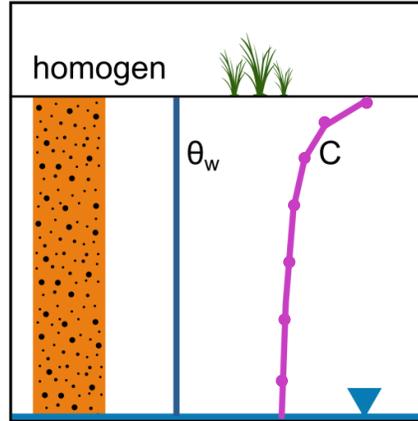
Morsing et al. (2025)

Hvordan defineres kilden?

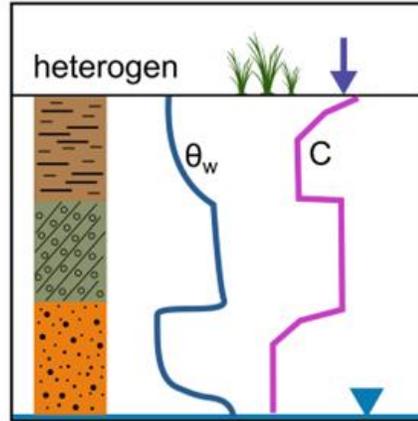
Simpel model



PFAS-LEACH

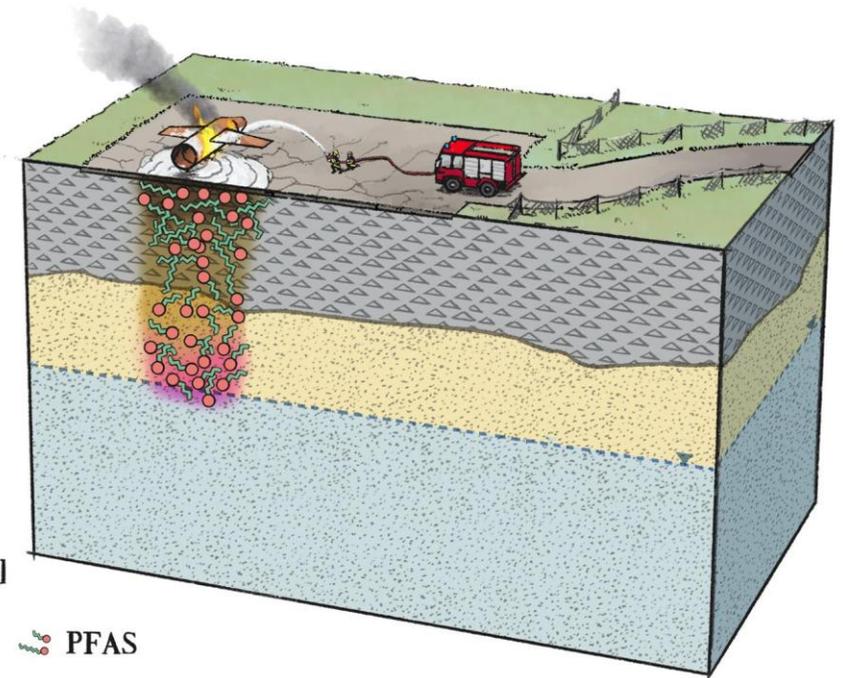


COMSOL



Illustrationer af Henning Wienkenjohann

- Grundvandsspejl
- Sand
- Moræner
- PFAS

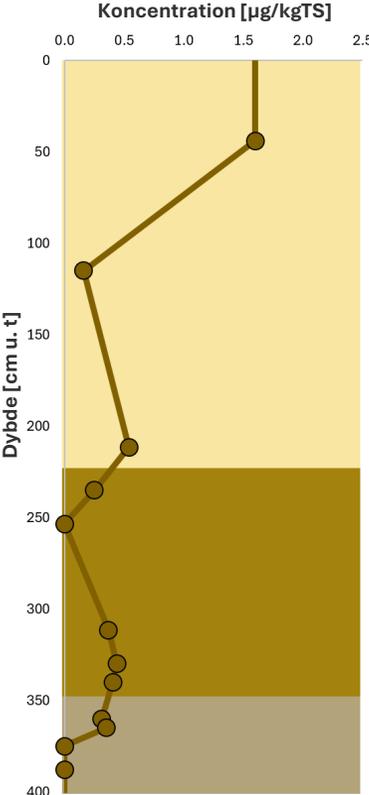


Morsing et al. (2025)

PFOS flux

Konkrete data

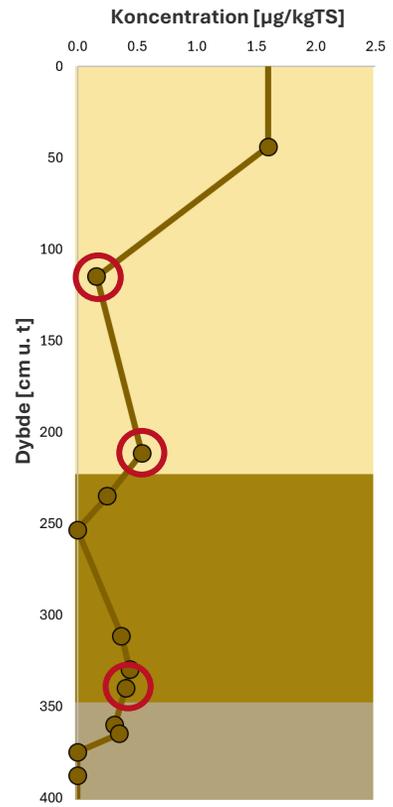
Diskretiseret
koncentrationsprofil



PFOS flux

Konkrete data

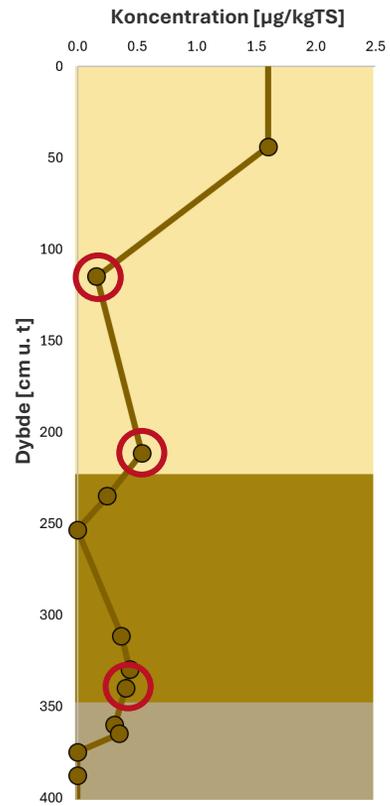
*Diskretiseret
koncentrationsprofil*



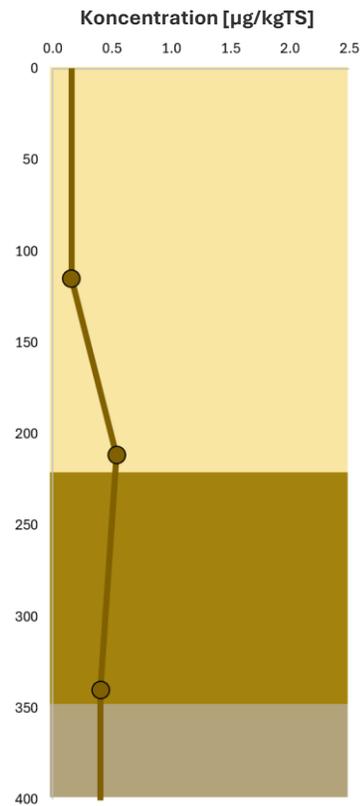
PFOS flux

Konkrete data

Diskretiseret
koncentrationsprofil



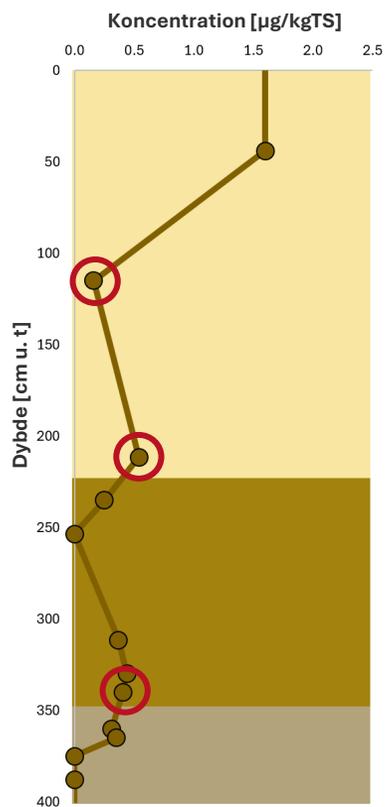
Reduceret datasæt



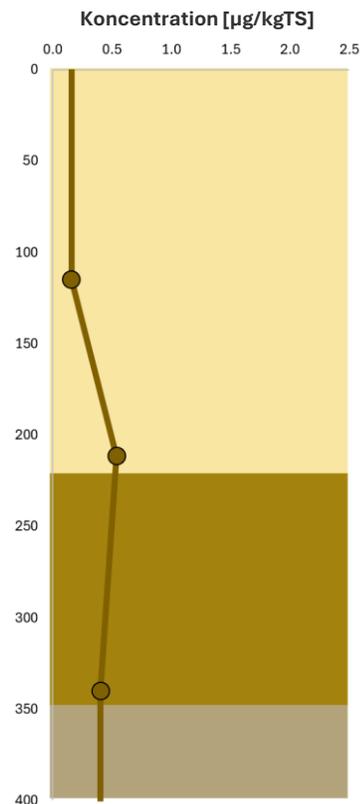
PFOS flux

Konkrete data

Diskretiseret
koncentrationsprofil



Reduceret datasæt

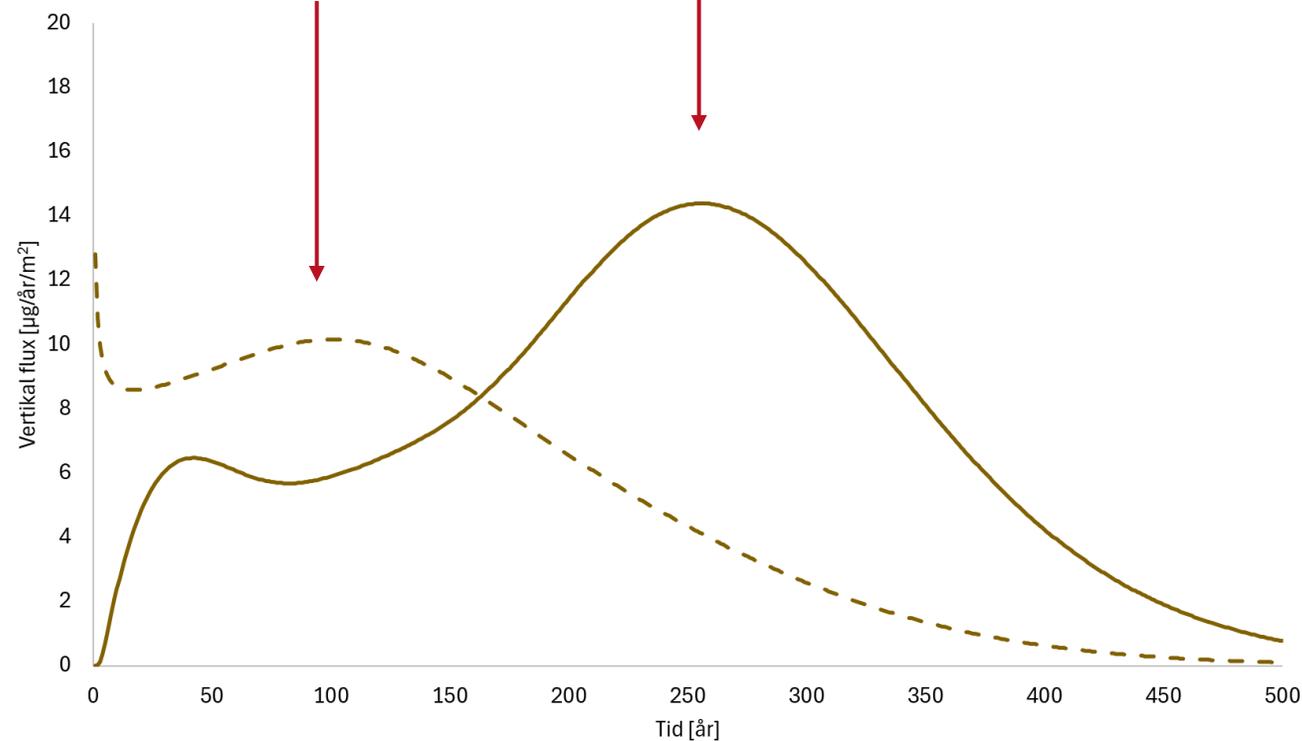


Fluxresultat PFAS-LEACH

Smeltevandssand

Reduceret datasæt

Diskretiseret
koncentrationsprofil



— PFAS-LEACH, diskretiseret profil — PFAS-LEACH, reduceret datasæt

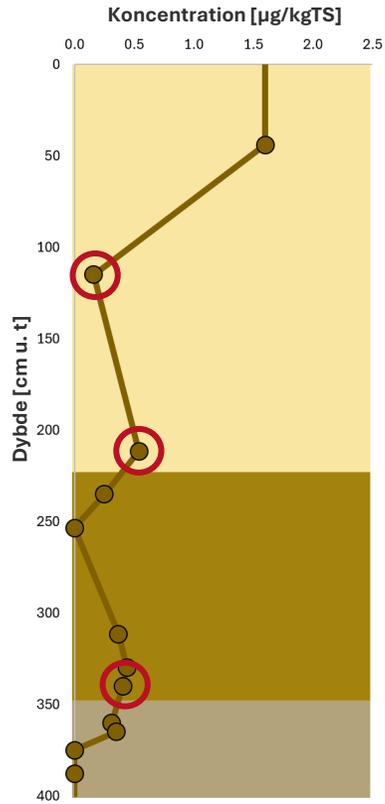
PFOS flux

Konkrete data

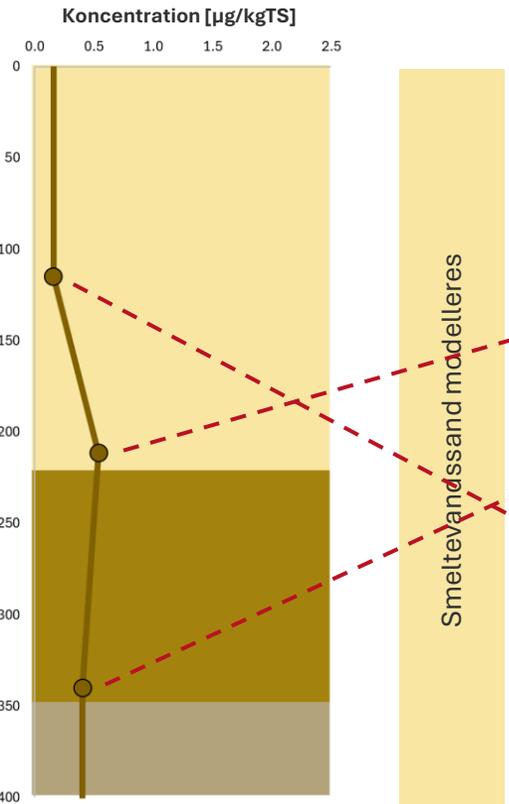
Jordkoncentrationer omregnet til vandkoncentrationer med *PFASen*

Analyseresultater	Fra jordprøve		Fra vandprøve		Estimerede resultater (afrundede)	
	# fluorerede C-atomer	Forkortelse	Koncentration (C) [µg/kg TS]	Koncentration (C _v) [ng/L]	C _v [ng/L]	C _v [ng/L]
4 Trifluorbenzen	3	PFBA				
5 Perfluorbutansulfon	4	PFBS				
6 Perfluorbutansulfon	4	PFBS				
7 Perfluorpentansulfon	5	PFPeA				
8 Perfluorhexansulfon	6	PFHxA				
9 Perfluorheptansulfon	7	PFHpA				
10 Perfluoroktansulfon	8	PFOSA				
11 Perfluoroktansulfon	8	PFOSA				
12 6,2 Fluortelomersulfon	6	6,2 FTSt				
13 Perfluordecansulfon	10	PFDS				
14 Perfluordecansulfon	10	PFDS				
15 Perfluordecansulfonamid	10	PFDSa				
16 Perfluorundecansulfon	11	PFUnA				
17 Perfluorundecansulfon	11	PFUnA				
18 Perfluorundecansulfon	11	PFUnA				
19 Perfluorundecansulfon	11	PFUnA				
20 Perfluordecansulfon	10	PFDS				
21 Perfluordecansulfon	10	PFDS				
22 Perfluordecansulfon	10	PFDS				
23 Perfluordecansulfon	10	PFDS				
24 Perfluordecansulfon	10	PFDS				
25 Perfluordecansulfon	10	PFDS				
26 Perfluordecansulfon	10	PFDS				
27 Sum af alle (PFBA, PFBA, PFDA, PFDS)		PFAS				
28 Sum af påviste PFAS, 22 stoffer		PFAS22				

Diskretiseret koncentrationsprofil



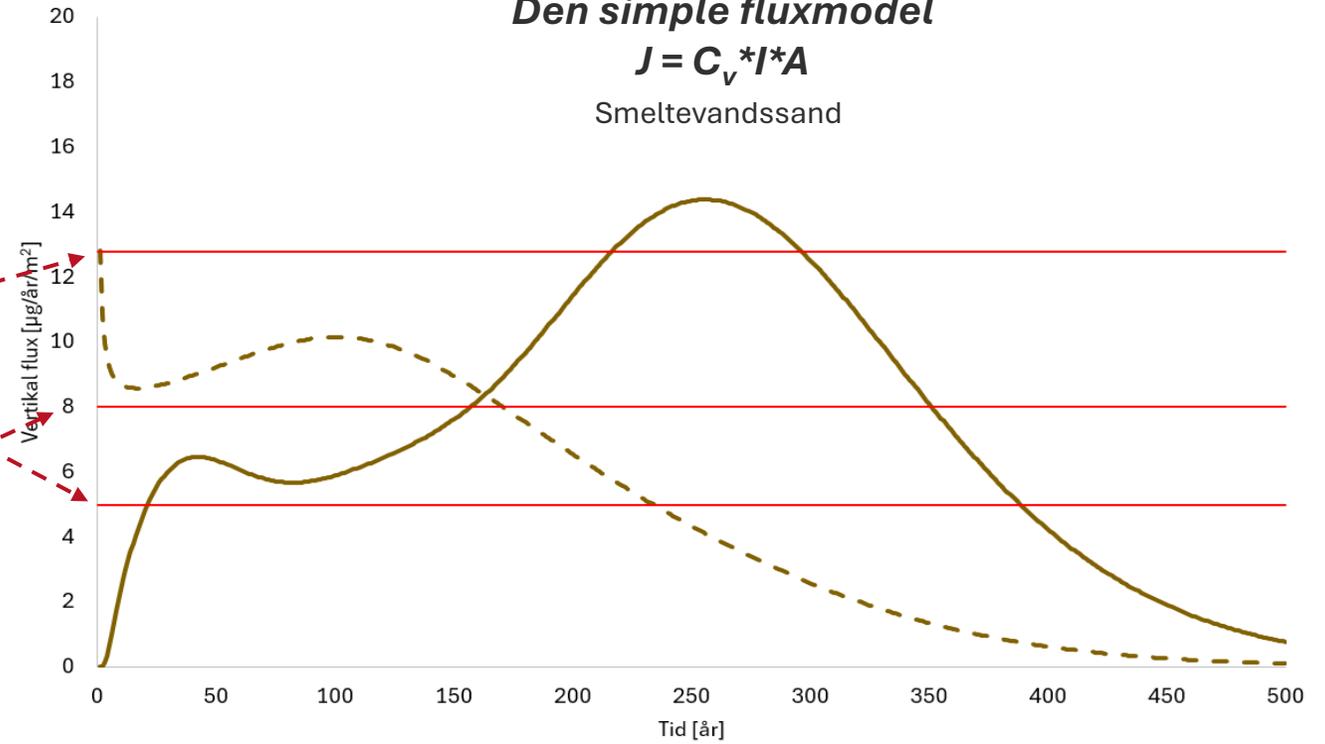
Reduceret datasæt



Den simple fluxmodel

$$J = C_v * I * A$$

Smeltevandssand

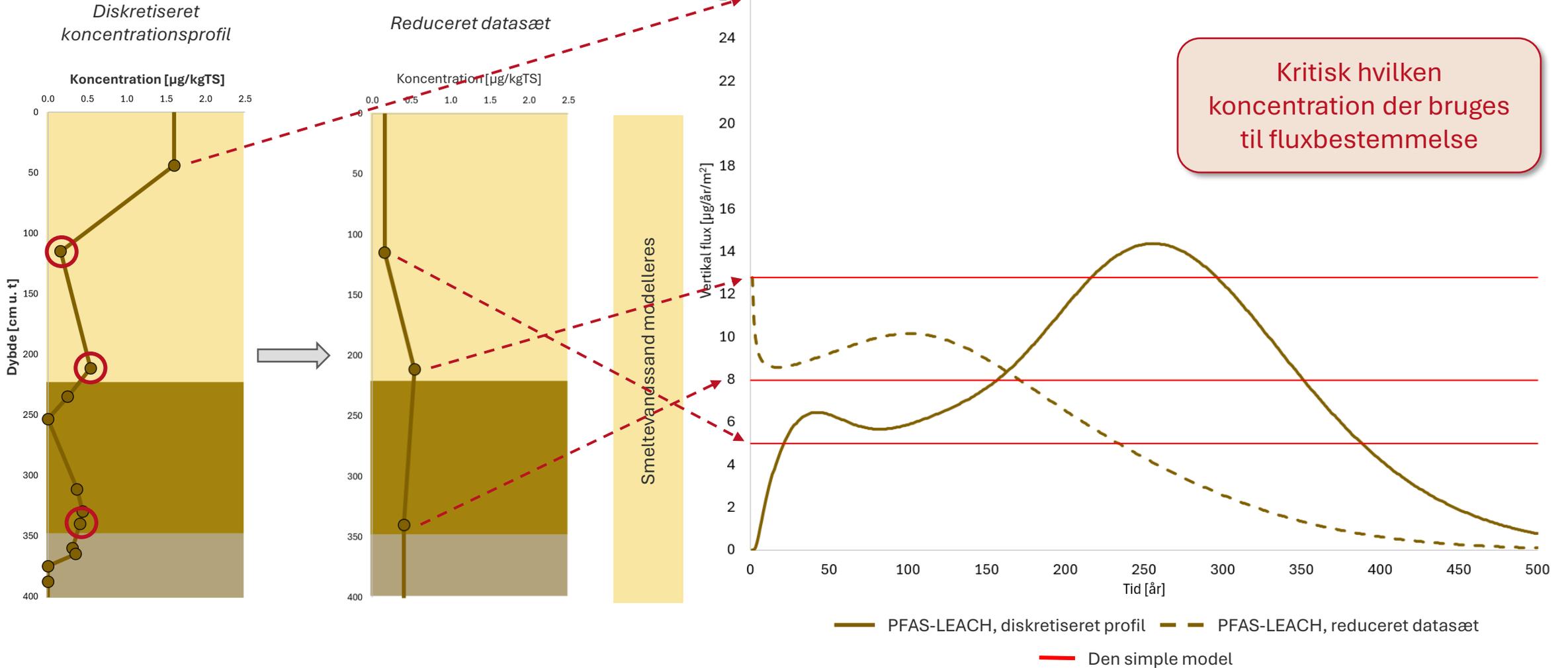


— PFAS-LEACH, diskretiseret profil - - - PFAS-LEACH, reduceret datasæt

— Den simple model

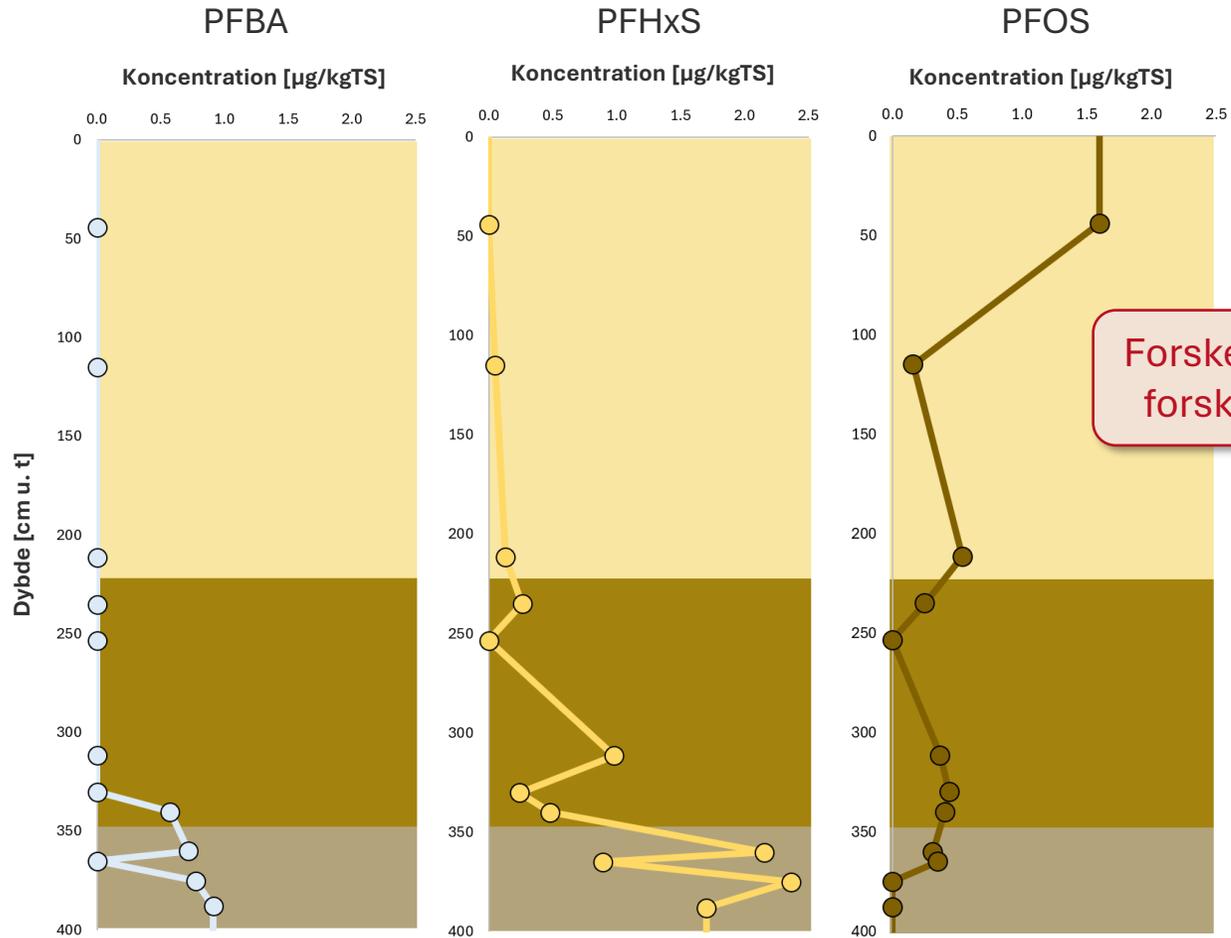
PFOS flux

Konkrete data

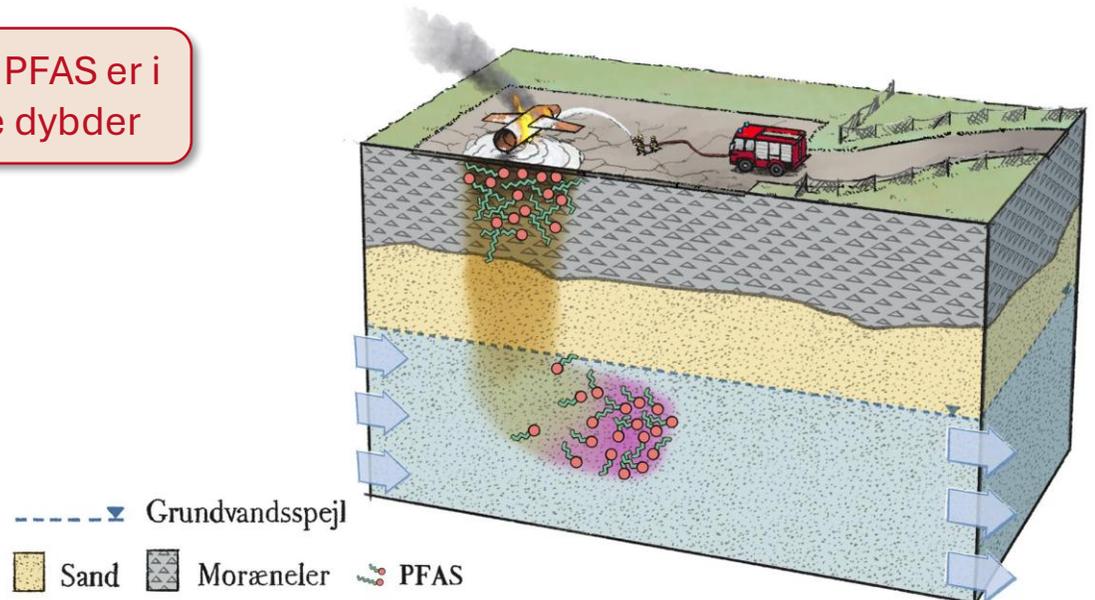


Koncentrationsprofiler

Konkrete data



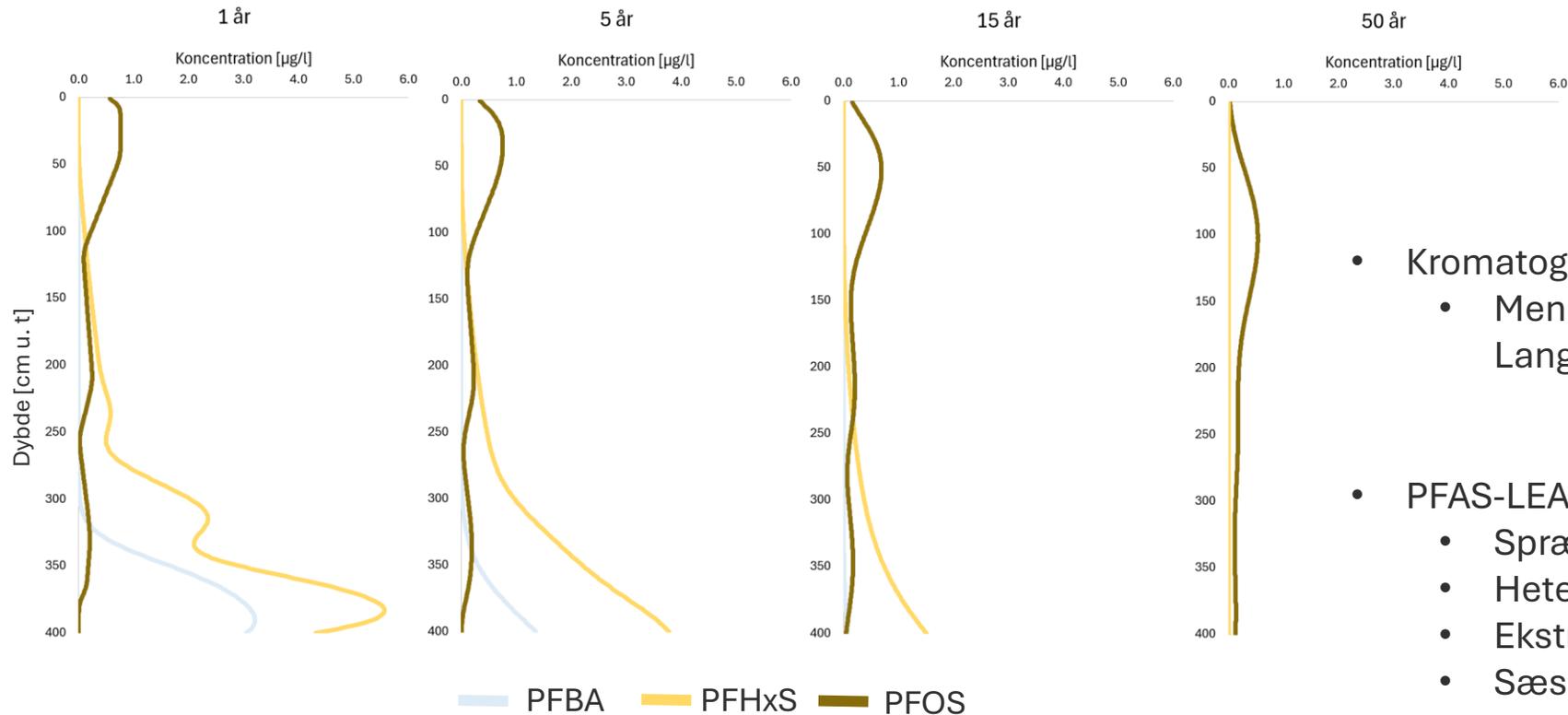
Forskellige PFAS er i forskellige dybder



Morsing et al. (2025)

Udvaskning af PFAS

Konkrete data



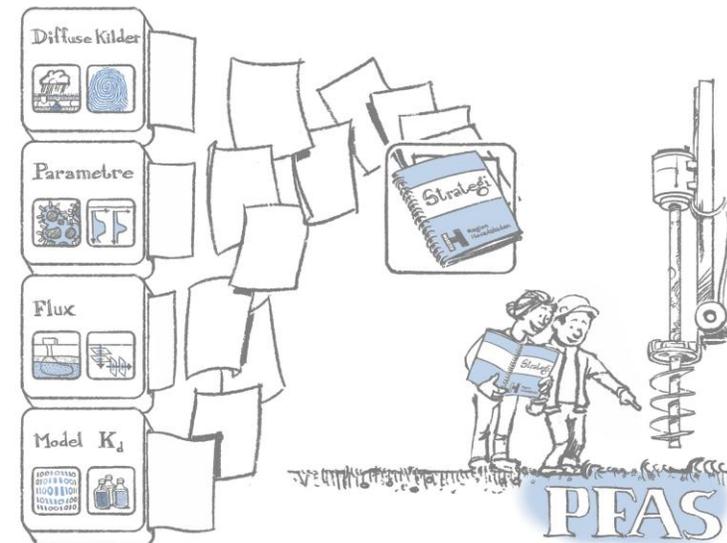
- Kromatografering ses tydeligt i PFAS-LEACH
 - Men....
Langkædede PFAS findes også i grundvandet
- PFAS-LEACH kan ikke tage højde for alle processer
 - Sprækker
 - Heterogenitet
 - Ekstreme regnhændelser
 - Sæsonvariationer

Opsummering

- Den simple model
 - **Hurtig** at anvende
 - Meget sensitiv overfor hvilken koncentration der bruges
 - Fortæller ikke noget om *hvornår* forureningsfluxen forventes at ramme grundvandet
- PFAS-LEACH
 - **Anvendelig for de fleste**
→ i kombination med PFASen
 - Mange sager har flere jordprøver
 - Tager højde for vigtige tilbageholdelsesprocesser
 - Medtager tidsaspekt
 - Øger den konceptuelle forståelse af PFAS transport i umættet zone

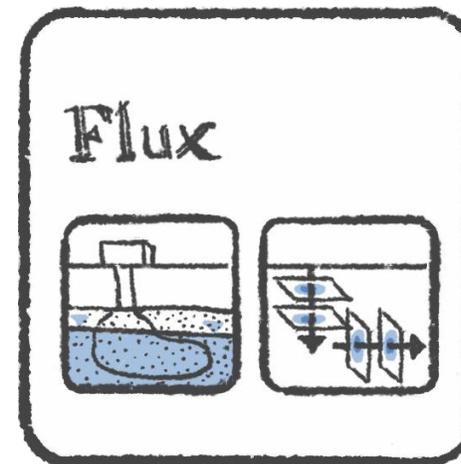
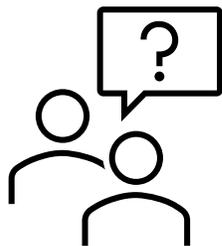
Næste skridt

- Hvordan kan vi bedst tage højde for:
 - *Sprækker*
 - *Heterogenitet*
 - *Ekstreme regnhændelser*
 - *Sæsonvariationer*
- Hvordan kan en typisk rådgiver/myndighedsperson bruge ”simplere” modeller i risikovurderinger og hvilke faldgruber er der?



Tak for opmærksomheden!

Spørgsmål?



Projekt for  **Region Hovedstaden**

Samarbejde mellem



REGION
ZEALAND



For yderligere spørgsmål

Kontakt:
Therese Lyng Petersen
tepe@niras.dk

NIRAS