University of Stuttgart
Institute for Modelling Hydraulic and Environmental Systems (IWS)
Research Facility for Subsurface Remediation (VEGAS)

EGU General Assembly 2022

Testing PFAS Immobilisation

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EGU General Assembly 2022 (SSS7.5)

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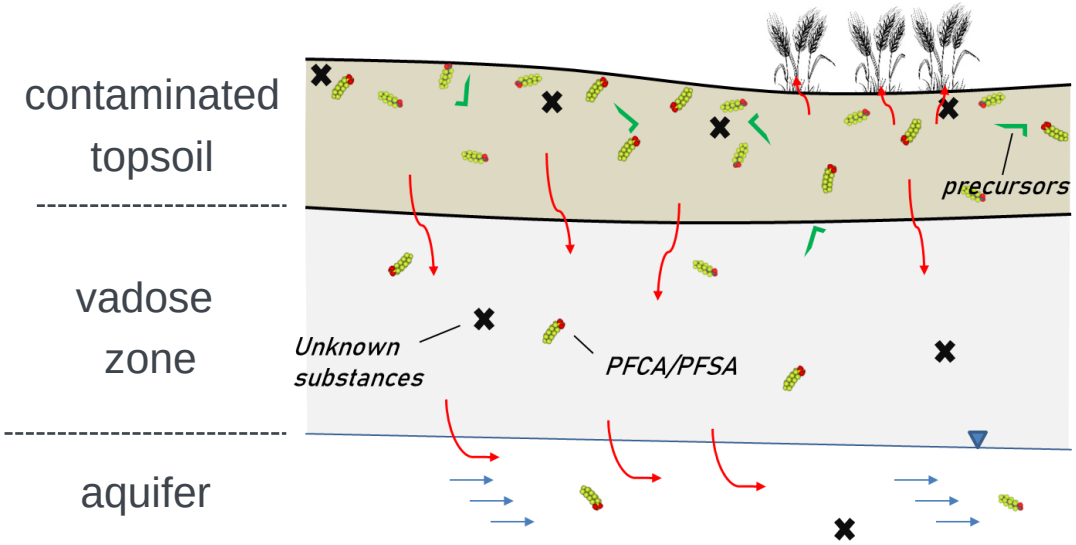
VEGAS Research Facility for Subsurface Remediation

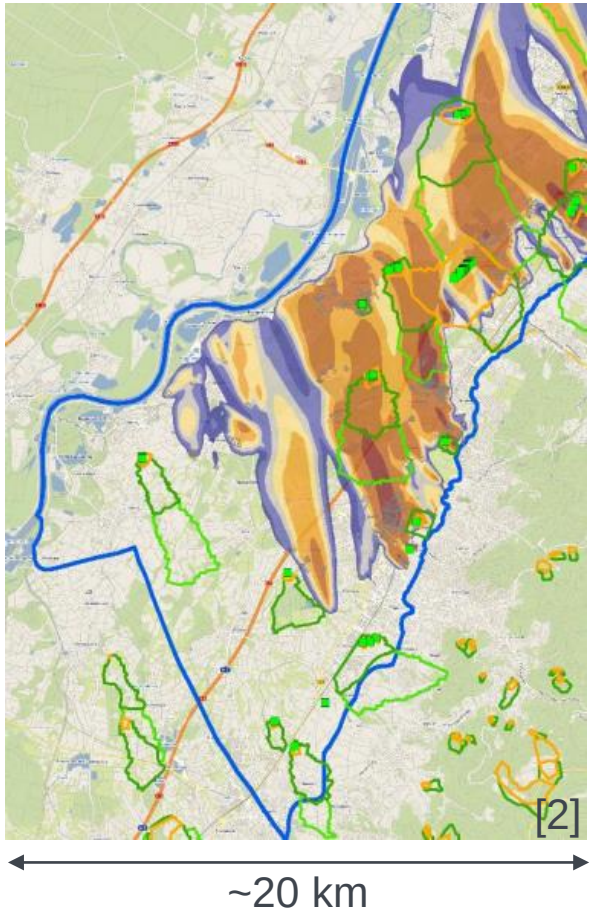
DVGW

TZW Technologiezentrum Wasser

PFAS Large-scale Non-point Source
Upper Rhine Valley

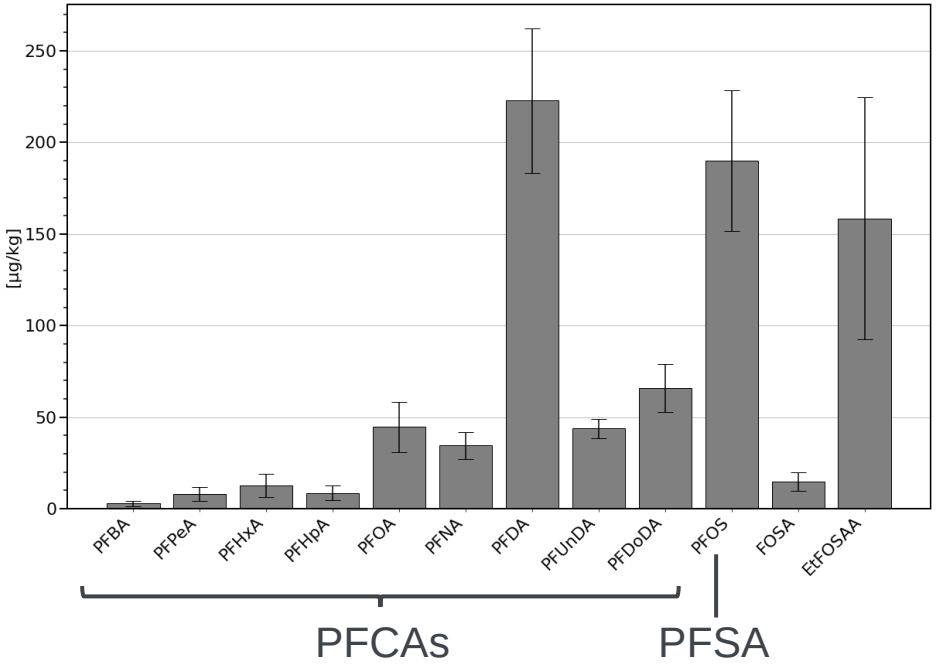
- Contamination of agricultural soil (>1000 ha) due to application of polluted paper-fibre biosolids



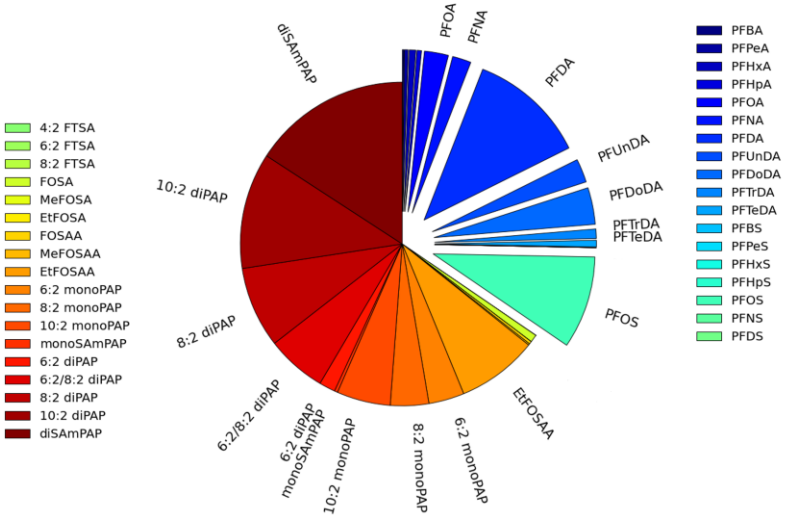


Contaminated Soil

PFAS concentrations in the studied soil (**N-1**)

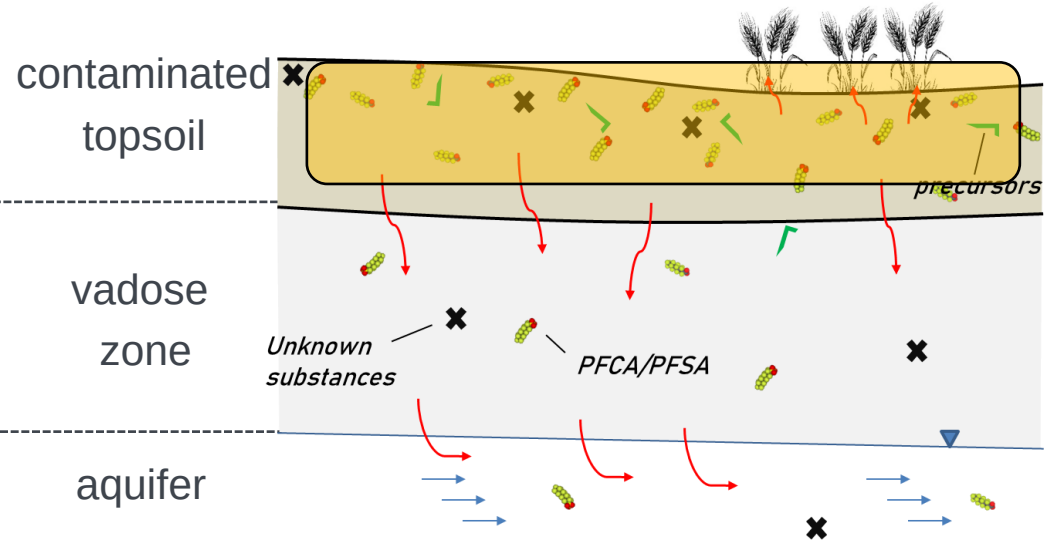


Target analysis with some precursors



organic fluorine fractions

Immobilisation of PFAS
Managing Contaminated Sites



Immobilisation

- goal: stop/reduce PFAS leaching from hot spots
- treatment of contaminated soil with additives
  - to increase sorption capacity
  - to solidify soil material
- in-situ and ex-situ applications

Soil Treatments
Immobilisation

Sorptive treatment:

- **R-1**: N-1 + 2.5 wt% powdered activated carbon
- **R-2**: N-1 + 2.5 wt% active-carbon based product (+ clay minerals, $AL(OH)_3$, …)

Soil solidification:

- **R-3**: N-1 + 7 wt% cement, bentonite, activated carbon

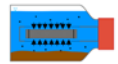
Application in concrete production:

- **R-4**: N-1 + 94 wt% concrete constituents

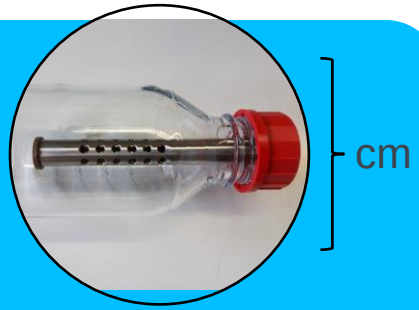
N-1 R-1 R-2 R-3 R-4

Original soil

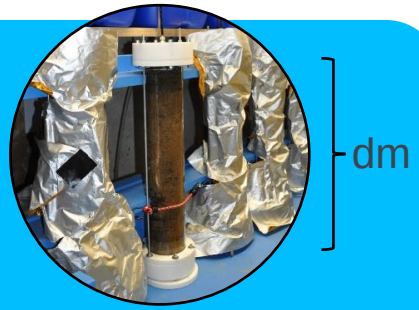
Laboratory Experiments
Investigation of PFAS Immobilisation



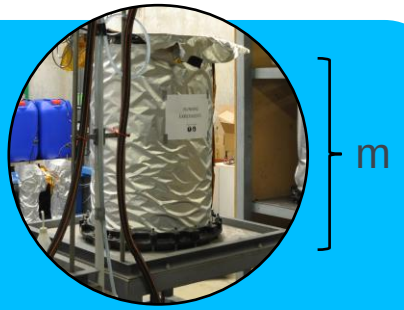
Evaluation of PFAS immobilisation in experiments and models



Infinite Sink (IS) Experiment



Column Experiment
(saturated)

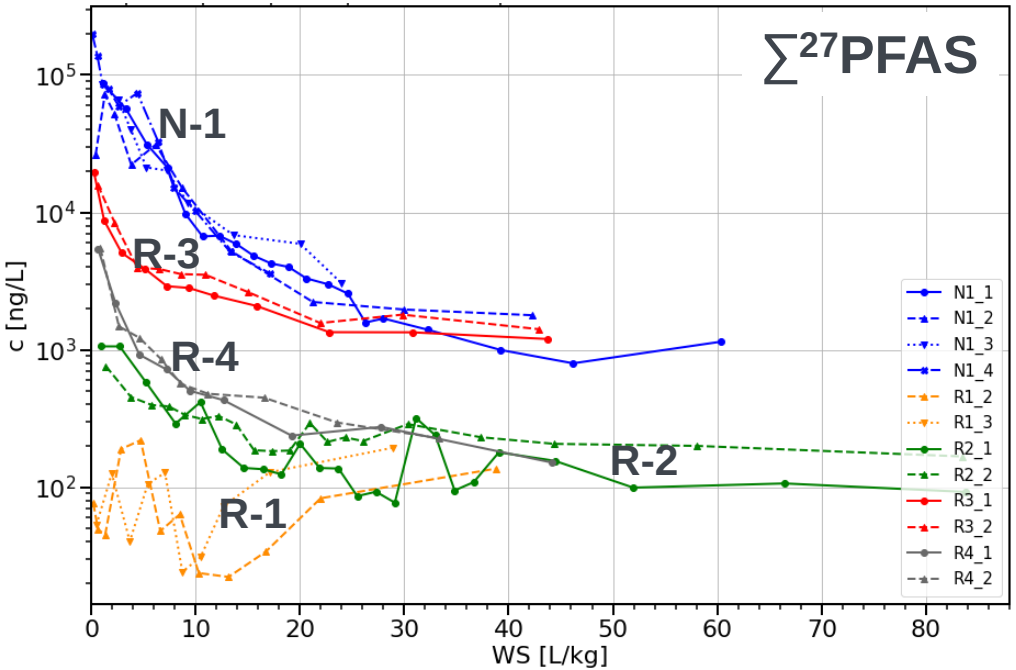


Lysimeter
(variably saturated)

Analytical tools: target analysis, EOF, AOF, TOP-Assay

Laboratory Experiments
Column Experiment

Eluate concentrations

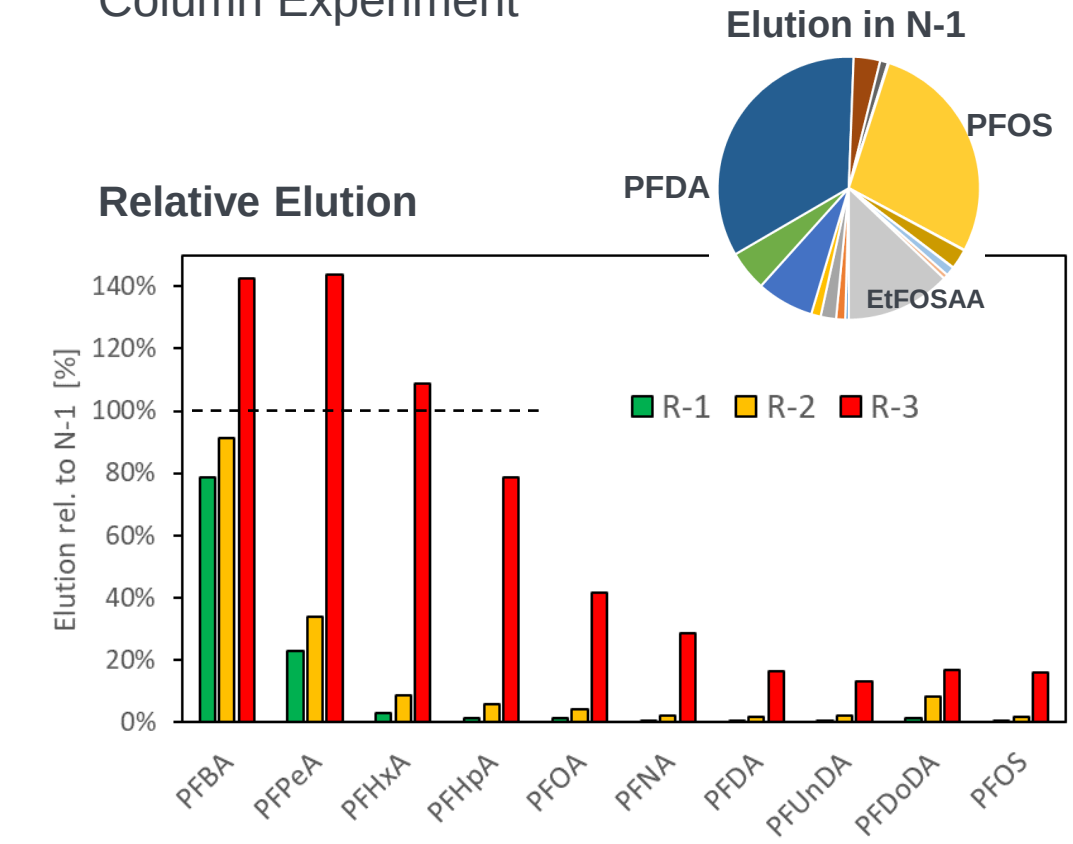


- Long elution process
- Similar immobilisation efficiencies in IS and columns:

	R-1	R-2	R-3	R-4
Infinite Sink	97 %	95 %	82 %	-6 %
Column Experiment	99 %	97 %	73 %	17 %

- ∑27PFAS: effective reduction of PFAS desorption possible
  - ➢ Fate of single substances?

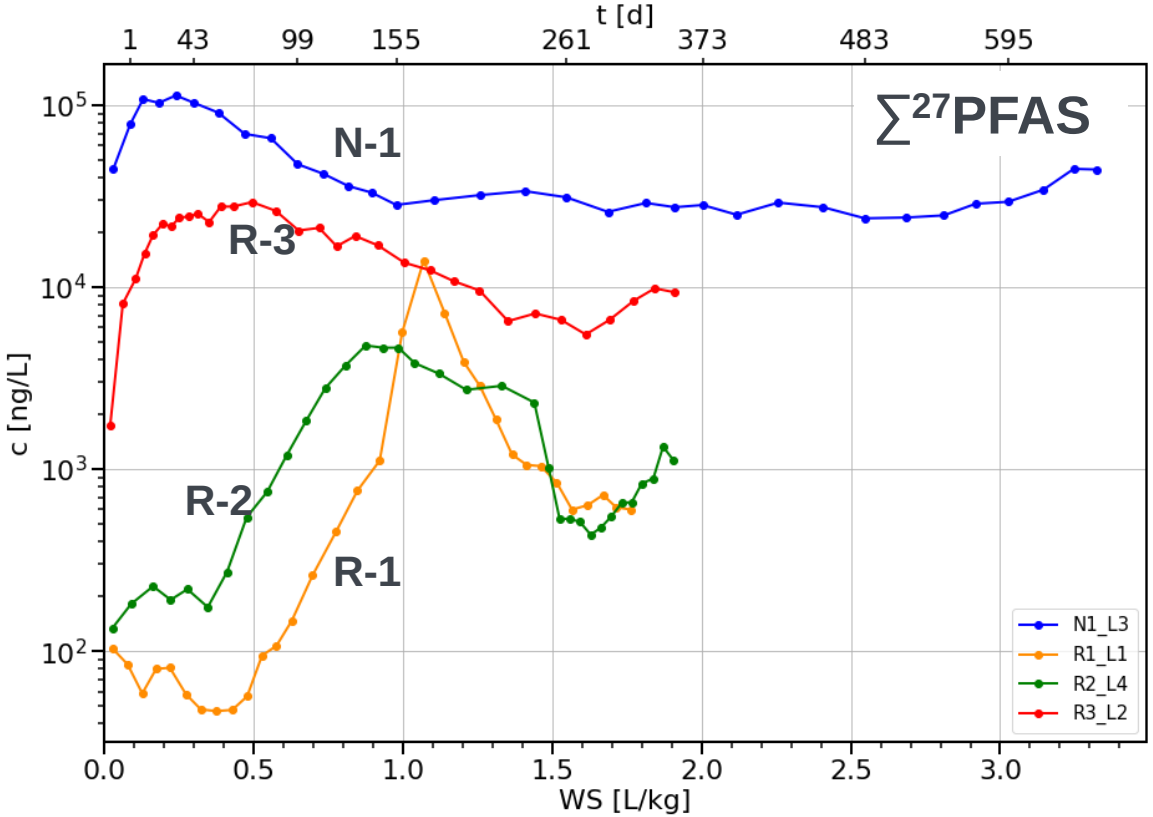
Laboratory Experiments
Column Experiment



- Similar leached PFBA mass in treated soils (water-to-solid ratio: 40 L/kg)
  - ➢ lower immobilisation efficiency for short-chain PFCAs
- exceeding elution in R-3 (and R-4)
  - ➢ enhanced desorption
    + transformations (abiotic)

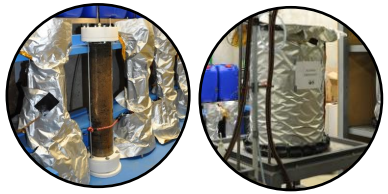
Laboratory Experiments
Lysimeter

Eluate concentrations

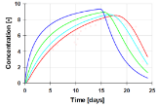


- Delayed leaching of short-chain PFCAs in R-1 and R-2
- Indication of biotransformations
  - Competitive Sorption? (Gellrich et al., 2012 [3]; McCleaf et al., 2017 [4])
- Affects evaluation of long-term stability

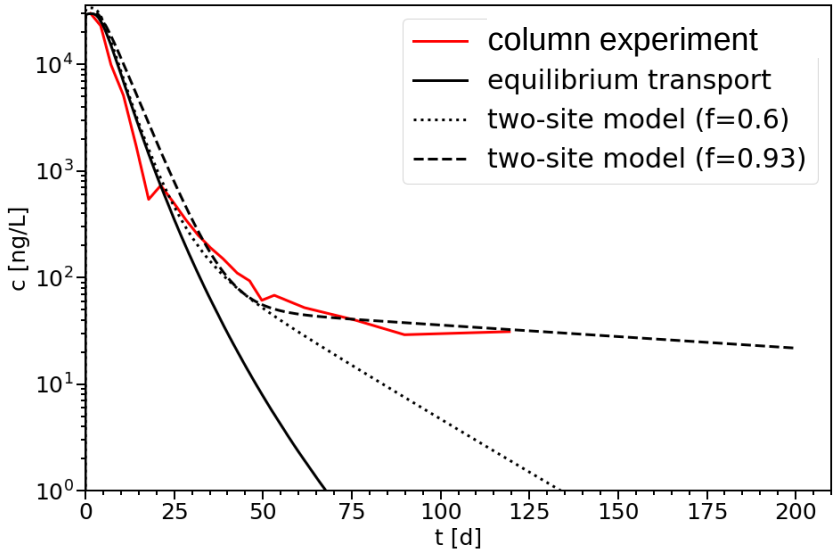
Numerical Modelling
Sorption models



column lysimeter



Eluate concentrations (PFOS in N-1)



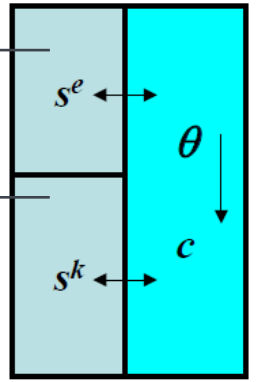
$$s = k_d c^{\beta}$$

instantaneous

$$\frac{\partial s_e}{\partial t} = f \frac{\partial s}{\partial t}$$

kinetic

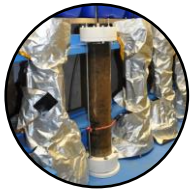
$$\frac{\partial s_k}{\partial t} = \omega \left[(1-f) \quad k_d c^{\beta} \quad - s_k \right]$$

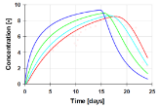


[5]

- Sorption model with Freundlich and kinetic sorption can reproduce observed concentration time-series (long tailing)

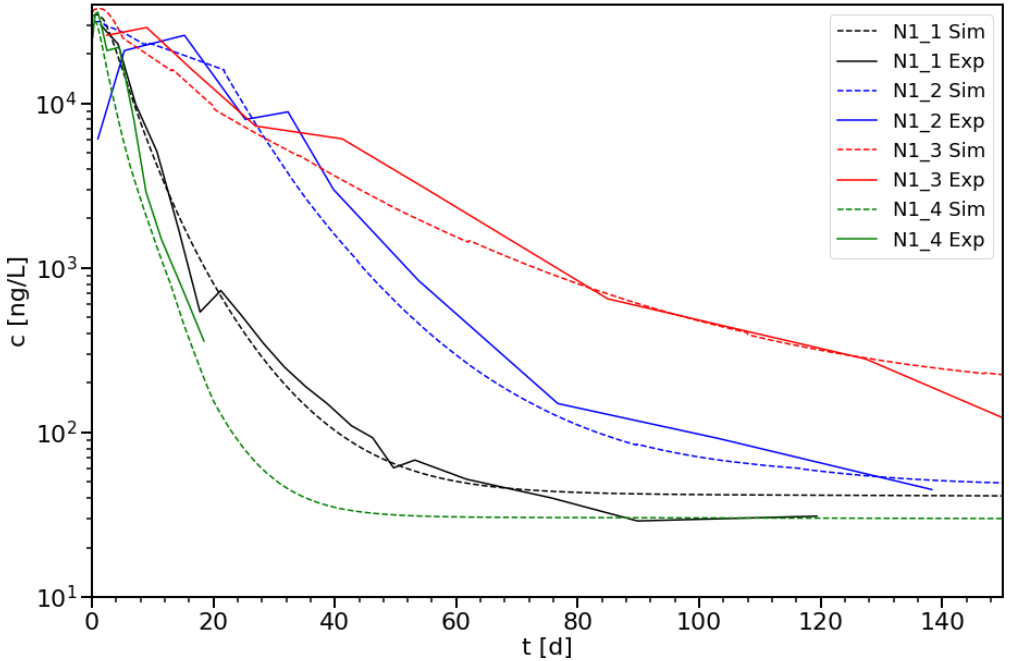
Numerical Modelling
Column Experiments





Eluate concentrations in simulations and experiments

(PFOS in N-1 with various flow rates)



- Parameter estimation for various PFAS

➢ **Parameter sets for N-1-experiments**

substance	k_d [L/kg]	β [-]	ω [d^{-1}]	f [-]
PFBA	0.7	0.9	0.01	0.6
PFOA	1.0	1.0	0.01	0.93
PFOS	4.5	0.98	0.005	0.93

- Further work:
  reactive transport models

Conclusion

- Typical **PFAS leaching behavior** observed
  (retardation, transformations, long leaching process)
- **Significant reduction of mass loading** with active-carbon based products
- **Delayed elution** of short-chain PFCAs in soils treated with active-carbon based products
- **Transformation of precursors** may affect immobilisation efficiency and/or long-term stability
- **Several experiments** with various saturation conditions **necessary** for investigation of PFAS immobilisation
- Data-based **comparison of experimental methods** helpful for identifying dominant **processes**
- **Long-term effects** in soils treated with immobilisation agents challenging to assess in lab
- Long-tailed elution (without biotransformation) possible to simulate in **model with Freundlich and kinetic sorption**

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Thank you!

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