

The filter function of agricultural soils, exemplified by PFAS transport and retention

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PHISHES : PHysically-based Integrated Soil HHealth Simulation



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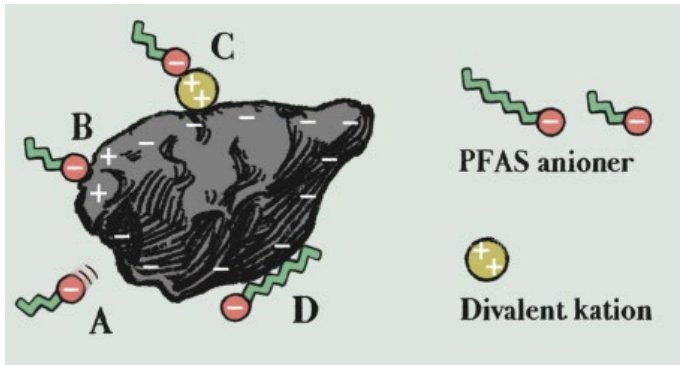
PFAS – fate in agricultural soils

- 1 **Soil organic carbon:** high OC → higher sorption
- 2 **Soil texture:** higher retention in loam & clay soils
- 3 **PFAS chain length:** long-chain bind stronger
- 4 **Soil water content:** air-water-interphase area change over seasons



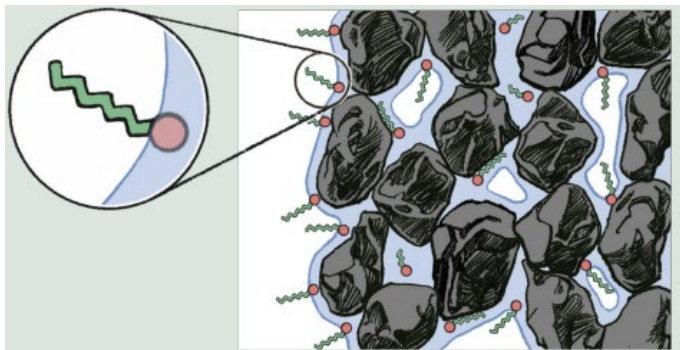
Retention mechanism in soil

PFAS contain a **hydrophobic tail** and a **hydrophilic head**



Solid phase adsorption (K_d)

- Hydrophobic interactions with organic carbon (OC)
- Electrostatic interactions with mineral fraction



Air-water-interface adsorption (K_{AWI})

- Due to the amphiphilic structure, PFAS accumulates at interfaces between air and water in the soil pores
- Important in the unsaturated zone

[1]



Calculating PFAS in the soil with Daisy

PFAS concentration in the matrix:

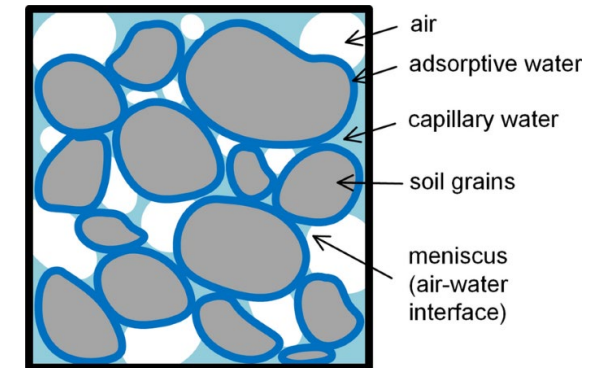
An equilibrium between water, solid phase, and air-water-interface area

$$M = \underbrace{C \cdot \theta}_{\text{water}} + \underbrace{Kd \cdot C}_{\text{soil}} + \underbrace{A_{AWI} \cdot K_{AWI} \cdot C}_{\text{air-water interface}}$$

Air-water interfacial area [2]

a function of water saturation and particle size distribution

$$A_{AWI} = \left(-2.85 \cdot \frac{\theta}{\theta_{sat}} + 3.6 \right) \left(\left(1 - \frac{\theta}{\theta_{sat}} \right) \cdot 3.9 \cdot d_{50}^{-1.2} \right)$$



Air-water interface distribution coefficient [3]

$$K_{AWI} = \frac{\sigma_0 b}{RT(c+a)}$$

At low PFAS concentration, K_{AWI} is constant

M: PFAS conc in soil+water+air (g/cm³)

C: PFAS conc in water (g/cm³)

θ : water content (-)

d_{50} : median grain size (cm)

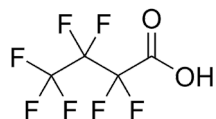
A_{AWI} : Air-water interfacial area (cm²/cm³)



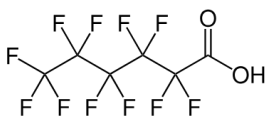
Simulating PFAS fate in agricultural soils

- Two soils types: Loamy and Sand
- Conventional Agricultural practices
- 2 PFAS
- PFAS entry as wet deposition
1 ng/L in precipitation

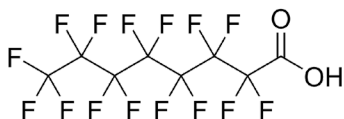
PFBA



PFHxA



PFOA



PFOS



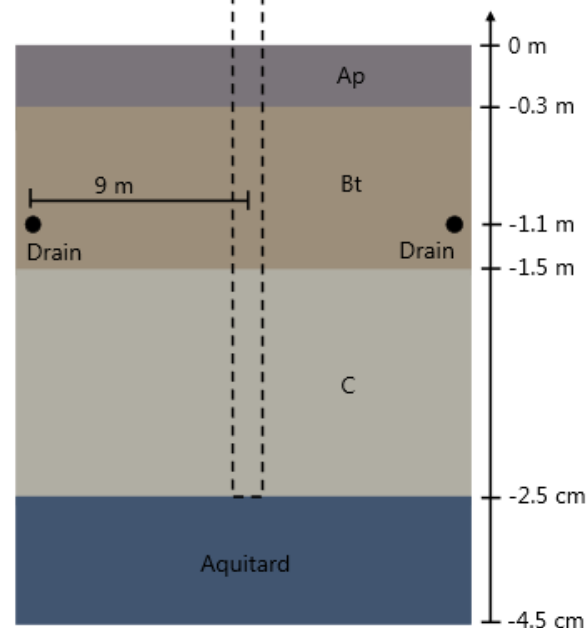
Wet
deposition



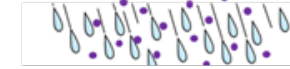
Wet
deposition



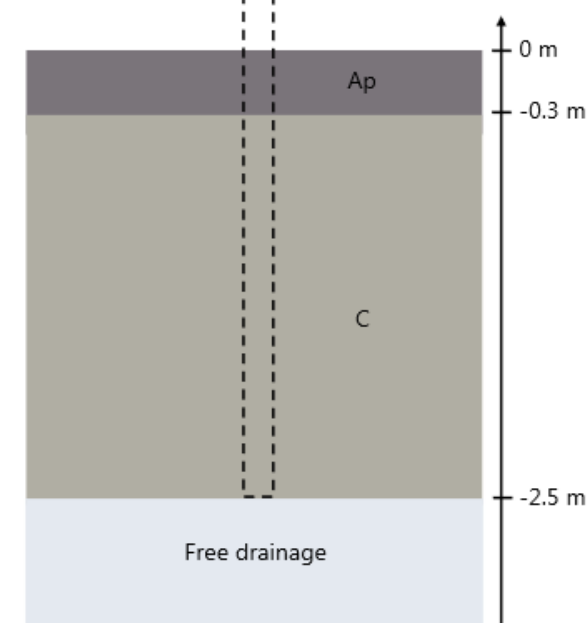
Daisy 1D column



Sandy loam



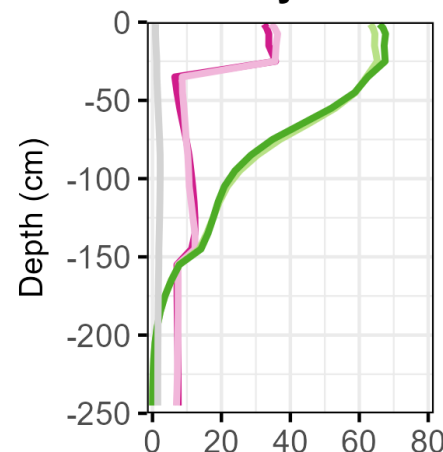
Daisy 1D column



Sand

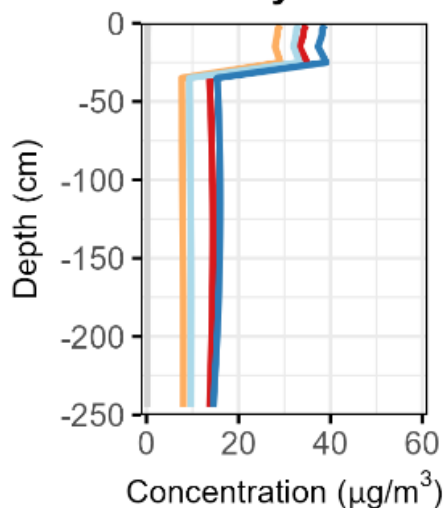
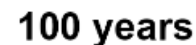
Fc1ccc(cc1)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)S(=O)(=O)O

1 year



- All scenarios include OC adsorption
- Including clay, results in enhanced PFOS retention in the top 25 cm
- AWI adsorption has no impact in this soil

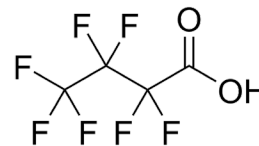
1 year



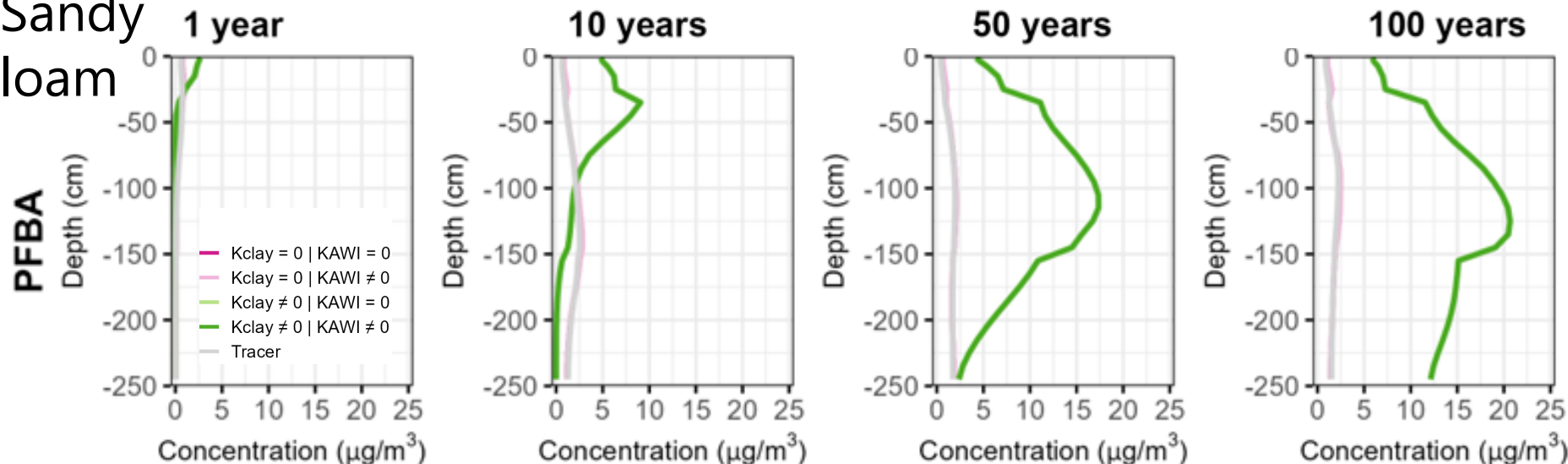
- All scenarios include OC adsorption
- Including clay, results in a slightly more PFOS retention in the top 25 cm
- AWI adsorption result in increased retention, more so than clay over long term



Results – PFBA

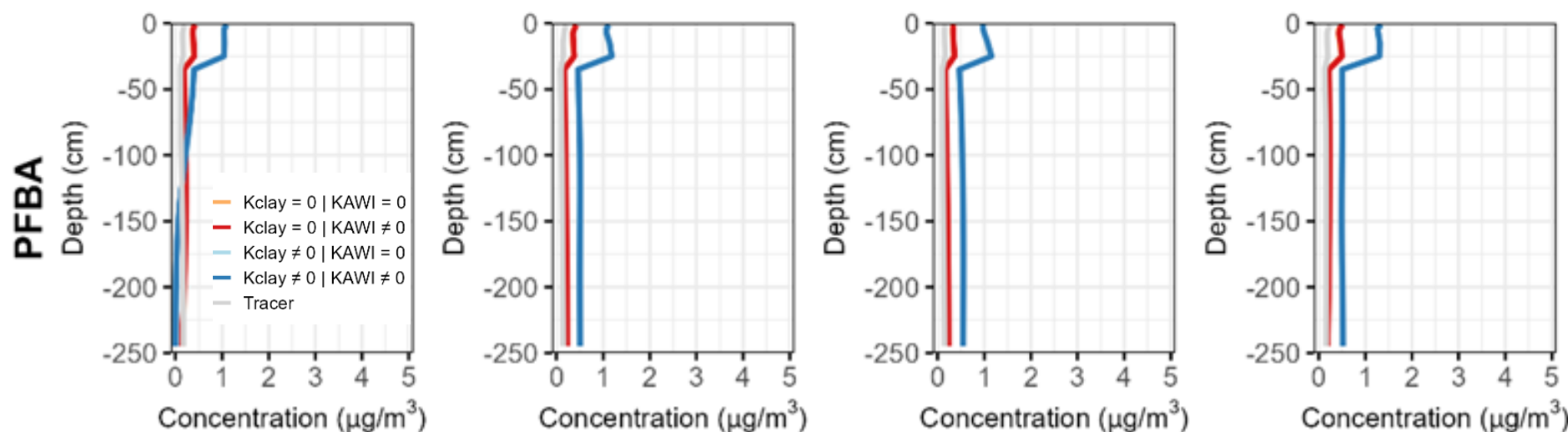


Sandy
loam



- All scenarios include OC adsorption
- Including clay, results in enhanced PFBA retention
- Without clay adsorption, PFBA is as mobile as a non-reactive tracer (low OC content)
- PFBA is more mobile than PFOS
- AWI adsorption has no effect for this compound

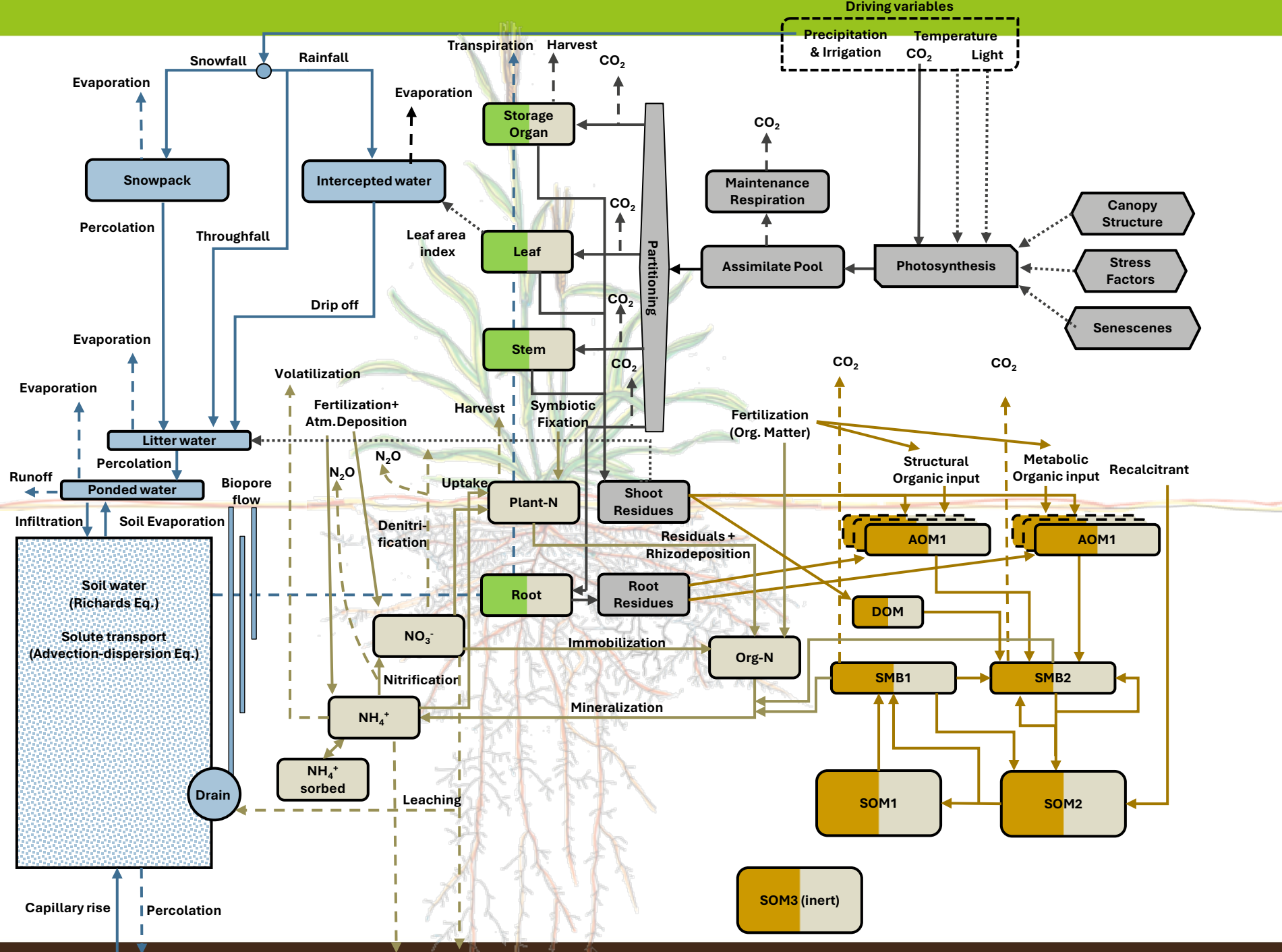
Sand



- All scenarios include OC adsorption
- Including clay, results in a slight bigger PFBA retention in the top 25 cm
- AWI adsorption has no effect for this compound



Daisy model [4]





Take home messages

- The fate of PFAS in agricultural soils can be estimated using mechanistic soil models (Daisy)
- AWI is important for long-chain PFAS in **sandy soils**, but no effect for short-chain PFAS.
- AWI was negligible in **sandy loam soils** for all PFAS.
- Inclusion of clay adsorption resulted in enhanced PFAS retention in both sandy loam and sand soil.

References

- [1]: Jakobsen, C, Holbak, M., Svane, S.F., Abrahamsen, P., & Strobel, B.W. 2026. Modelling PFAS Fate in Agricultural Soils: Clay and Air-Water Interface Adsorption. *Vadose Zone J.*, 2026;25:e70114. <http://doi.org/10.1002/vzj2.70114>, 18 pp.
- [2]: Brusseau, M. L. (2023). Determining air-water interfacial areas for the retention and transport of PFAS and other interfacially active solutes in unsaturated porous media. *Science of The Total Environment*, 884, 163730. <https://doi.org/10.1016/j.scitotenv.2023.163730>
- [3]: Guo, B., Zeng, J., & Brusseau, M. L. (2020). A Mathematical Model for the Release, Transport, and Retention of Per- and Polyfluoroalkyl Substances (PFAS) in the Vadose Zone. *Water Resources Research*, 56(2), e2019WR026667. <https://doi.org/10.1029/2019WR026667>
- [4]: Holbak, M., Abrahamsen, P., Grønning, C.R. , Klöffel, T., Schwartzkopff, M.V., Styczen, M.E., Svane, S.E.& Diamantopoulos, E. . 2026. The Daisy model: A tool for simulating agricultural systems - Recent (2012-2025) developments, calibrations and validations. *Agricultural Systems*, 238, 104846. <http://doi.org/10.1016/j.agry.2026.104846>

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