Soil macropore-matrix mass exchange tracer experiments that account for sorption at macropore walls

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Hypotheses & Objectives

Hypotheses

➢ Macropore – matrix interface is a key for understanding local non-equilibrium processes and preferential flow

Objective

➢ Simulation of percolation experiments

- Sorption heterogeneity along macropore walls

➢ Extension of dual-permeability modeling towards chemical sorption for reactive solute transport modeling

Dual-Permeability model

1D vertical

"macroscopic scale"

SPM

Water flow: 2 Richards-equations

$$C_f \frac{\partial h_f}{\partial t} = \frac{\partial}{\partial z}\left(K_f \frac{\partial h_f}{\partial z} - K_f\right) - \frac{\Gamma_w}{w_f} - S_f$$

$$\boxed{C_m \frac{\partial h_m}{\partial t} = \frac{\partial}{\partial z}\left(K_m \frac{\partial h_m}{\partial z} - K_m\right)} + \frac{\Gamma_w}{1-w_f} - S_m$$

Water transfer, Γ_w:

$$\Gamma_w = \alpha_w (h_f - h_m) \qquad \boxed{\alpha_w = \frac{\beta}{a^2} \gamma_w K_a(h)}$$

Solute transport: 2 CDE

$$\frac{\partial}{\partial t}(\theta_f R_f c_f) = \frac{\partial}{\partial z}\left(\theta_f D_f \frac{\partial c_f}{\partial z} - q_f c_f\right) - \theta_f \mu_f c_f - \frac{\Gamma_s}{w_f}$$

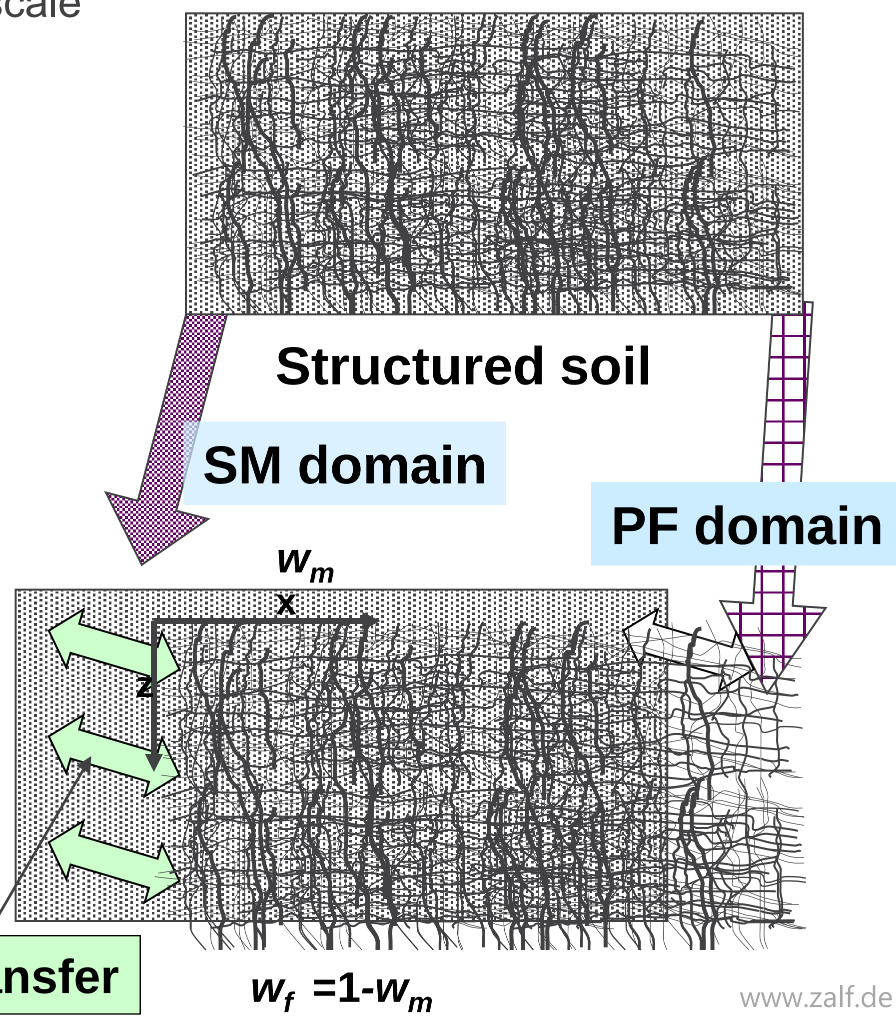
$$\boxed{\frac{\partial}{\partial t}(\theta_m R_m c_m) = \frac{\partial}{\partial z}\left(\theta_m D_m \frac{\partial c_m}{\partial z} - q_m c_m\right)} - \theta_m \mu_m c_m + \frac{\Gamma_s}{(1-w_f)}$$

Solute transfer, Γ_s:

$$\Gamma_s = (1-d)\,\Gamma_w c_f + d\,\Gamma_w c_m + \alpha_s (1-w_f)\,\theta_m (c_f - c_m)$$

$$\boxed{\alpha_s = \frac{\beta}{a^2} D_a(\theta)}$$

Two-domain concept



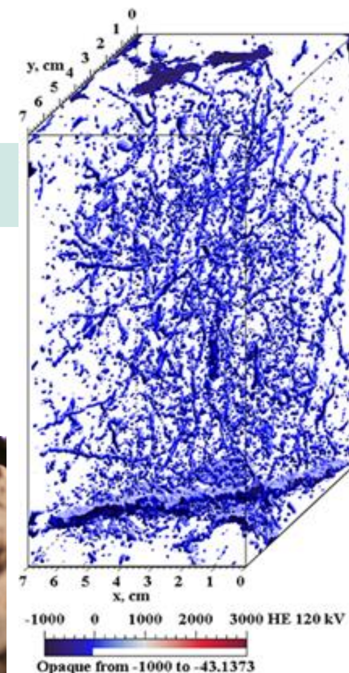
Gerke & van Genuchten WRR 1993a, 1993b; AWR 1996

Problems & Objectives

- High sensitivity of the solute mass transfer coefficient, α_s,
- Effective solute diffusion coefficient, D_a, not evaluated, yet

$$\boxed{\alpha_s = \frac{\beta}{a^2} D_a(\theta)}$$

Extension towards chemical sorption for reactive solutes



➢ Upscaling local properties to "effective" macroscopic scale parameters of the pore network

➢ Heterogeneity of sorption properties along macropore walls

Coating Analyses

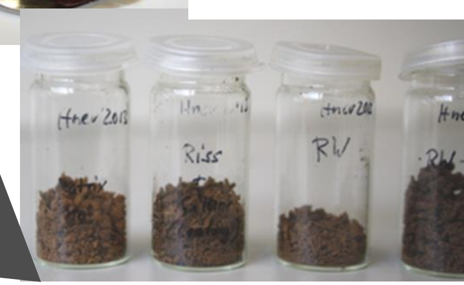
→Focus on Luvisol Bt-horizons

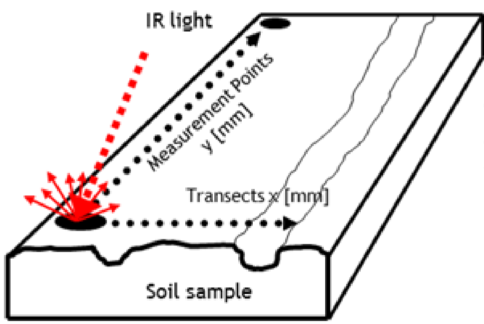
Separation

Destructive

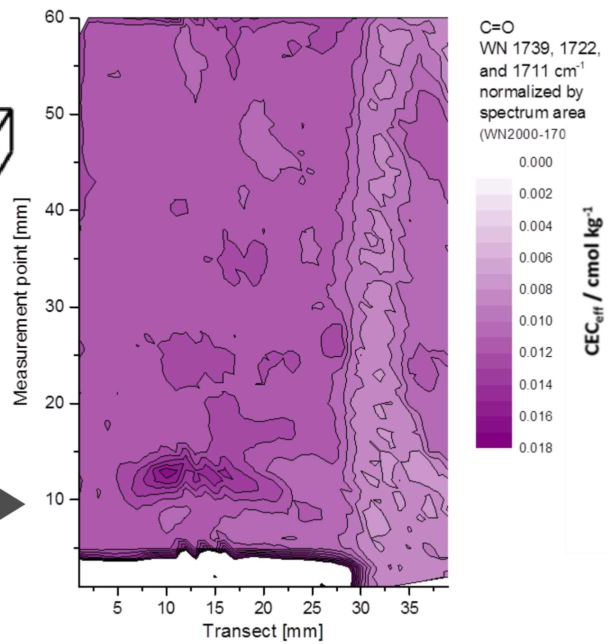
Intact, DRIFT

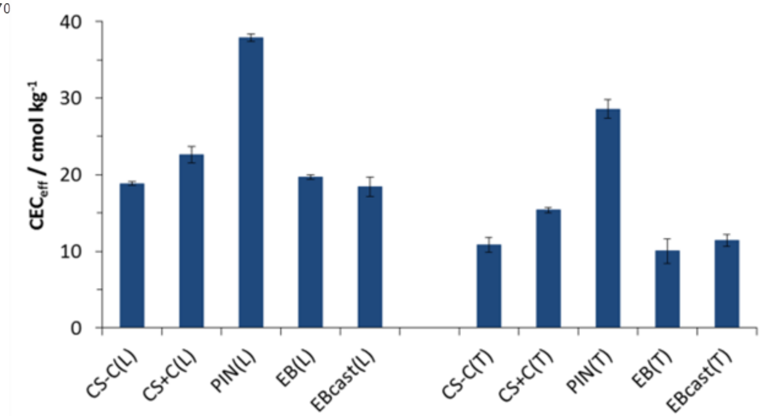
Mixed Prop.





Mapping

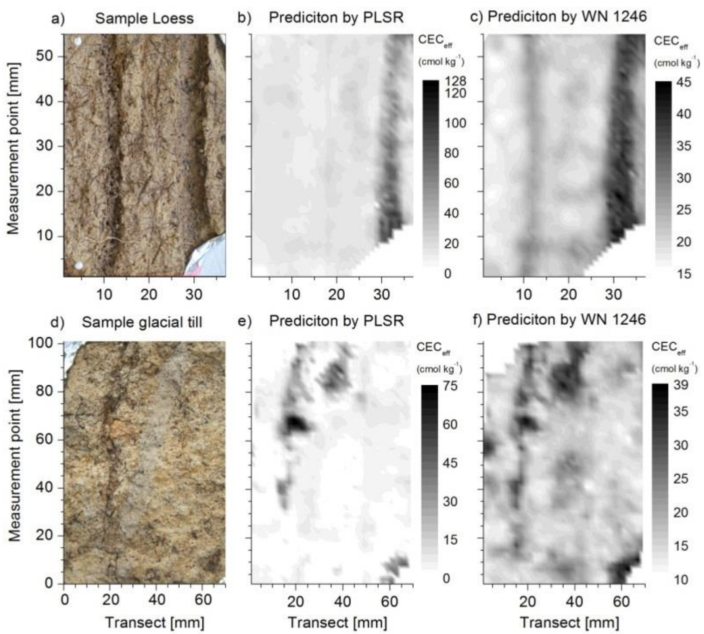




Loess Bt

Till Bt

CEC & OM maps from DRIFT

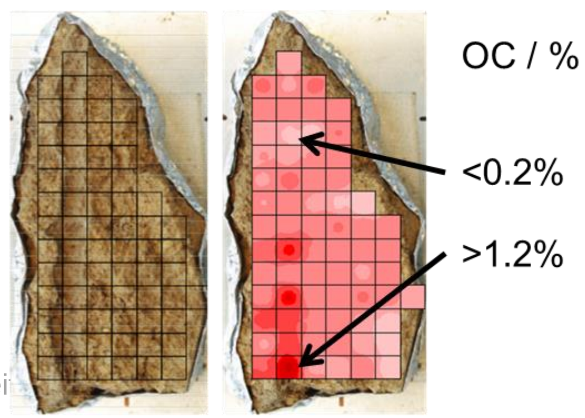


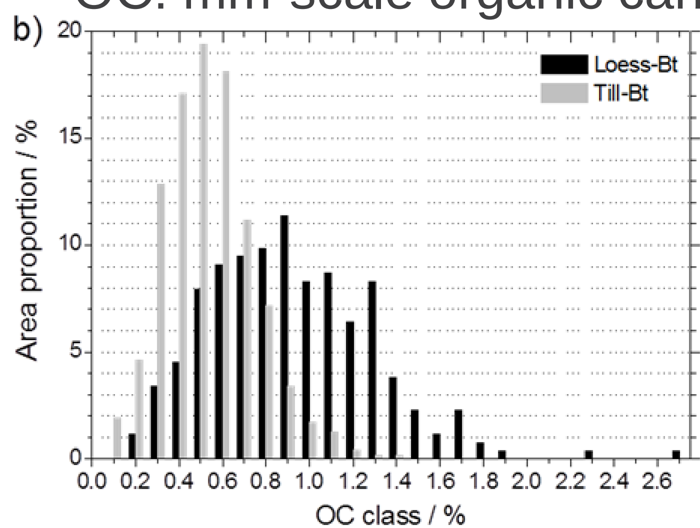
CEC distributions predicted by

- PLSR and total DRIFT spectra (middle)
- linear regression using signal intensity at WN 1246 cm^{-1} (right).

Leue et al. 2018

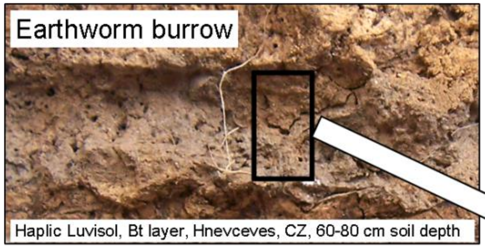
OC: mm-scale organic carbon distribution

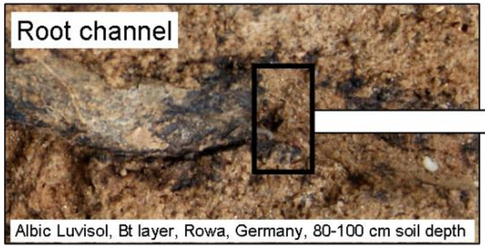


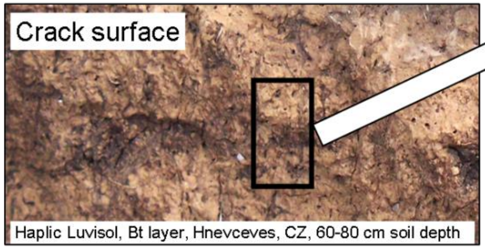


Leue et al. (2013) Eur. J. Soil Sci. 64:757-769

Classification: macropore types



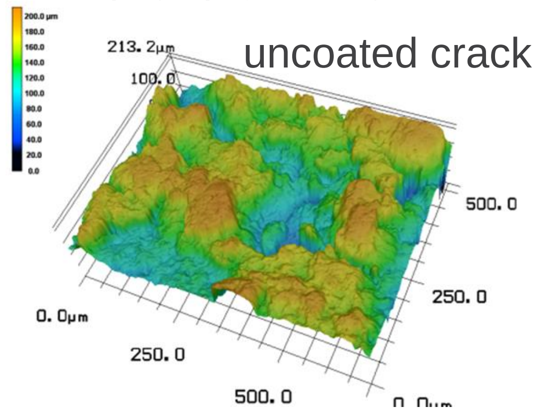


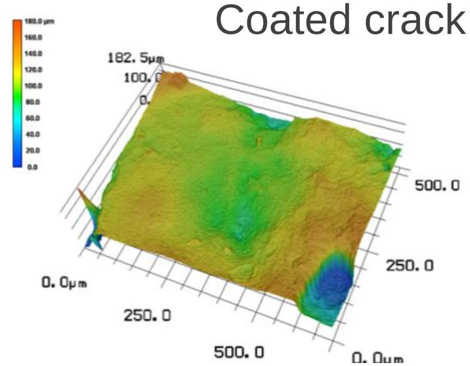


Differences in

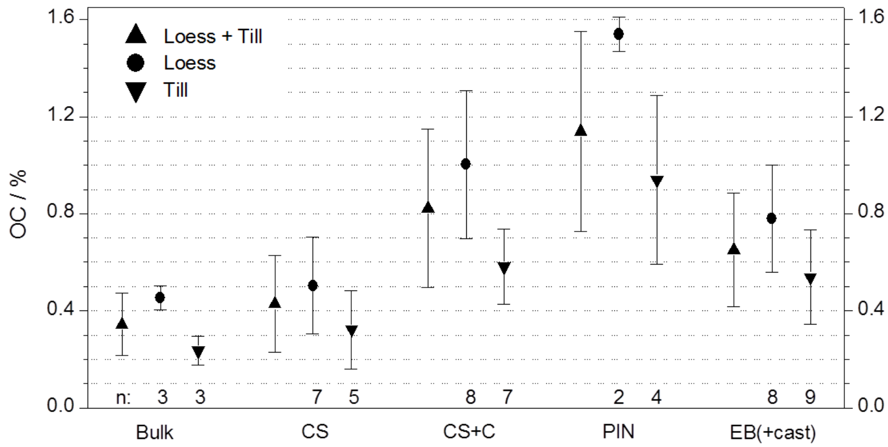
Sorption & wettability

Microtopography & roughness



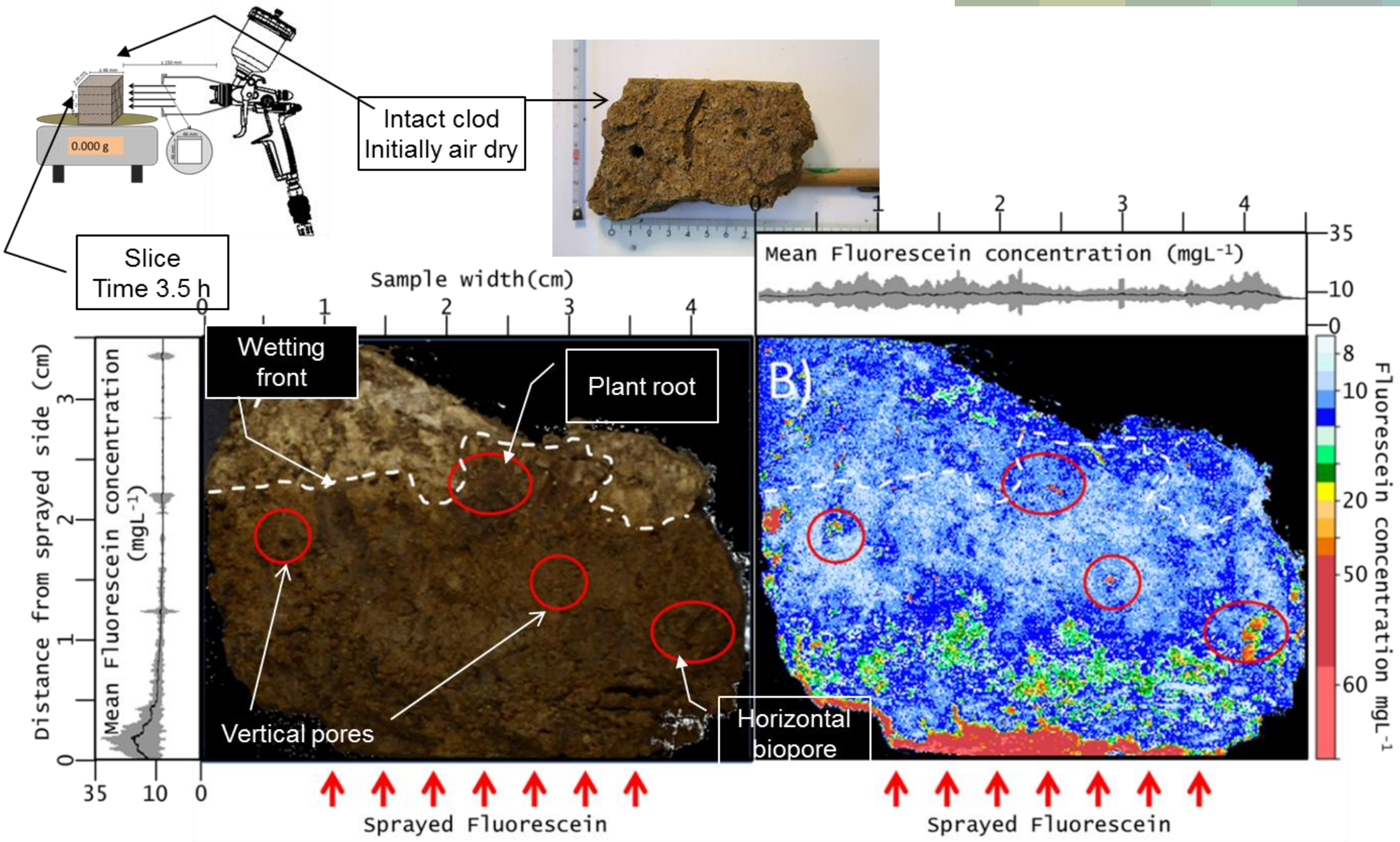


Leue & Gerke (2016) JPNSS 179:529-536



Leue et al. (2017) Soil Till. Res. 176:1-9.

Mass exchange experiment



photo

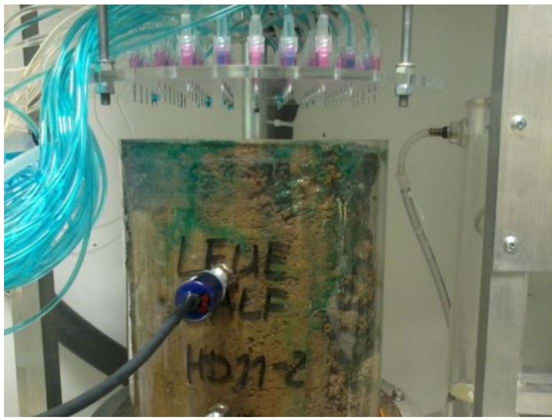
Applied fluorescein concentration: 60 mg/L,
≈10 mL sprayed for 3.5 hours (0.9 mg/s).

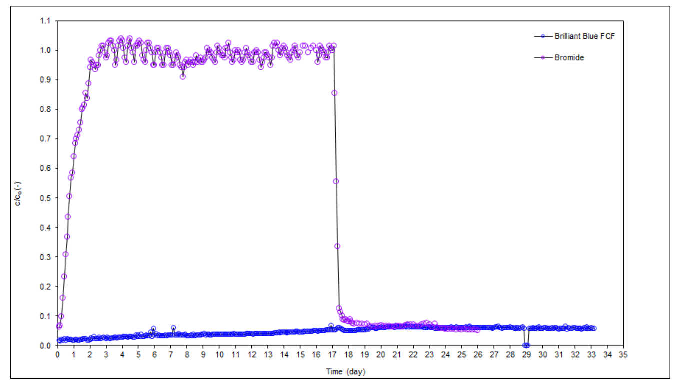
calculated concentrations

Picture : C. Haas, ZALF; Haas et al. Geoderma 2020

Percolation: Bromide and BB

A) Steady-state flow, bromide Brilliant Blue FCF (BB)
→ Local equilibrium conditions





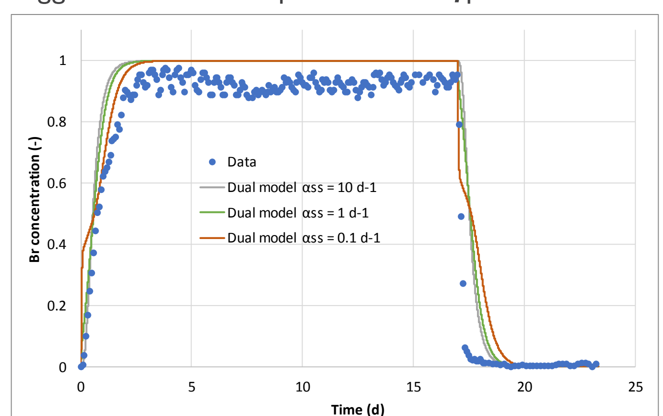
Transport parameters, only bromide q = 11.5 cm d^{-1}

Single domain model: λ = 2 cm;

Dual: λ_f = 10 cm, λ_m = 2 cm, α_{ss} = 10 d^{-1}, w_f = 0.04, q_f = 142 cm d^{-1}

→Effect of α_{ss} on bromide BTC shape

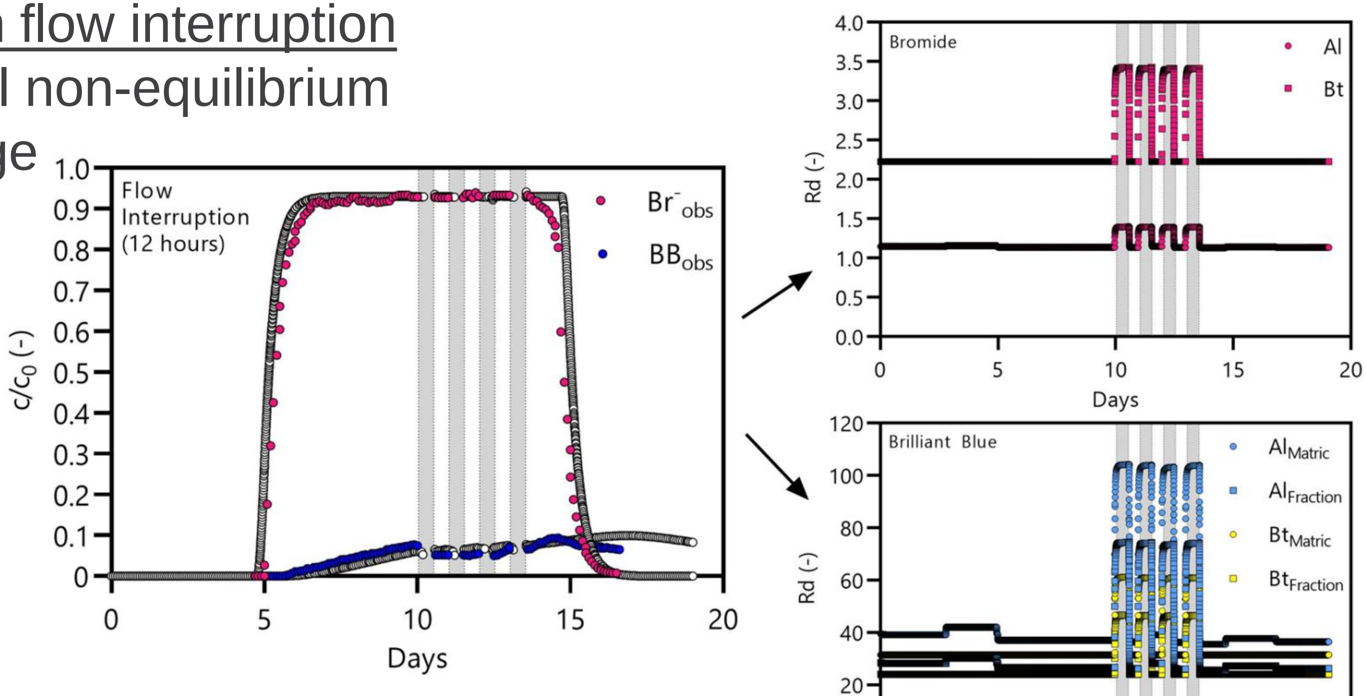
at CTU Prag



Percolation: Bromide and BB

B) Percolation with flow interruption

→to stimulate local non-equilibrium and mass exchange



Retardation factor **Rd=1+Kd*ρb/θ**

Discussion & Conclusions

- Local macropore structural properties are characterized: texture, organic matter, micro-topography, bulk density, chemical sorption,…
- Numerical modelling based on small-scale distributed maps of OM composition as proxy of OM sorption properties.
- Simulation of reactive tracer breakthrough curves in undisturbed soil columns possible with two-domain model.

Open questions remain:

How is mass exchange affected by sorption along macropore walls during reactive solute transport

Acknowledgements

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