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
1D vertical

Water flow: 2 Richards-equations

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

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

Water transfer, \( \Gamma_w \):

\[ \Gamma_w = \alpha_w (h_f - h_m) \]

\[ \alpha_w = \frac{\beta}{a^2} \gamma_w K_a(h) \]

Solute transport: 2 CDE

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

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

Solute transfer, \( \Gamma_s \):

\[ \Gamma_s = (1 - d) \Gamma_w c_f + d \Gamma_w c_m + \alpha_s (1 - w_f) \theta_m (c_f - c_m) \]

\[ \alpha_s = \frac{\beta}{a^2} D_s(\theta) \]

Two-domain concept

Structured soil

SM domain

PF domain

Mass Transfer

\( w_m \)

\( w_f = 1 - w_m \)

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

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

\[ \alpha_s = \frac{\beta}{\bar{a}^2} D_a(\theta) \]

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

Intact, DRIFT

Mapping

Separation

Destructive

Mixed Prop.

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

Classification: macropore types

Differences in Sorption & wettability

Microtopography & roughness

Coated crack

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

Mass exchange experiment

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: $\lambda = 2$ cm;
Dual: $\lambda_f = 10$ cm, $\lambda_m = 2$ cm, $\alpha_{ss} = 10$ d$^{-1}$, $w_f = 0.04$, $q_f = 142$ cm d$^{-1}$

→ Effect of $\alpha_{ss}$ on bromide BTC shape
B) Percolation with flow interruption → to stimulate local non-equilibrium and mass exchange
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
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