SPP 1315 Biogeochemical Interfaces in Soil

Quantification of active interfaces with respect to dissolved chemicals in unsaturated structured soil

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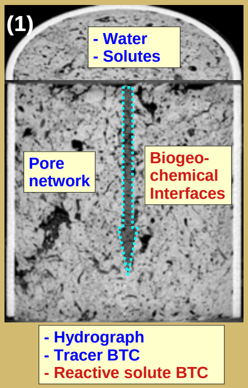
Hypotheses

1. **Pore structure** governs **water** & **tracer movement**

2. **BGI** control **solute retardation**



Objectives

1. **Predict** **hydraulic functions** & **tracer transport** based on **pore structure characterization**

2. **Predict** **adsorbed chemical transport** based on:
a) macroscopic sorption data (batch tests)
b) distribution & properties of **BGI**

Introduction

The main obstacle for a reliable prediction of chemical displacement in soil is the inherent heterogeneity of the material which is structured at multiple scales. Soil structure invokes a heterogeneous flow regime depending on saturation and driving forces. Additionally, biogeochemical interfaces provide local reaction zones for dissolved chemicals resulting in macroscopic retardation of transport. We study the effects of soil pore structure and biogeochemical interfaces on relevant soil functions, such as hydraulic properties and solute transport behavior.

Methodical Approach

1. Measure pore network

2. Quantify morphological properties

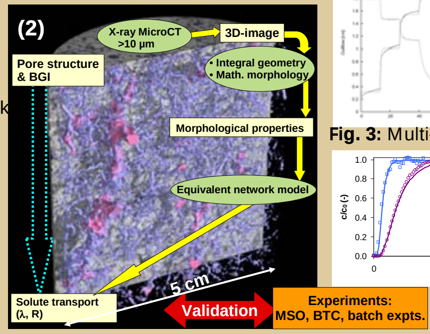
3. Set up equivalent network model

4. Predict tracer transport

5. Estimate adsorption

6. Predict react. transport

- Validation experiments -



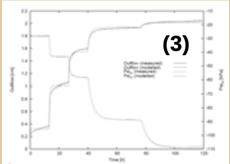


Fig. 3: Multi-step outflow

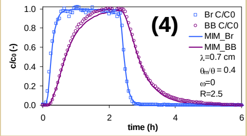


Fig. 4: Br⁻ and BB-FCF breakthrough

Some experimental data of Fuhrberg sand used for inferring hydraulic parameters (Fig. 3) and transport parameters (Fig. 4), respectively. This information is subsequently used for validation of network model prediction.

First Achievements. A) Structure Analysis

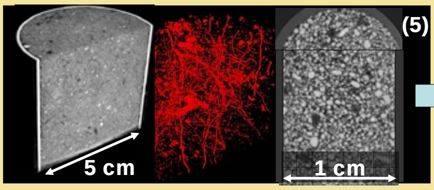


Fig. 5: Images obtained by µCT of Fuhrberg sand samples at two different scales.
A root system and organic constituents are present in some samples.

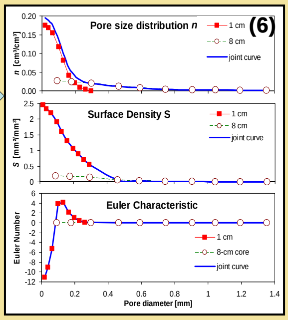


Fig. 6: Minkowski functions

Hierarchical image analysis at different scales allow us to include a large range of pore sizes, while maintaining optimal resolution (Figs. 5, 6).

B) Network Modelling ← → Experiments

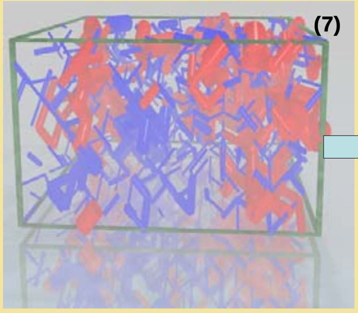


Fig. 7: Pore Network Model based on Minkowski functions (see Fig. 6)

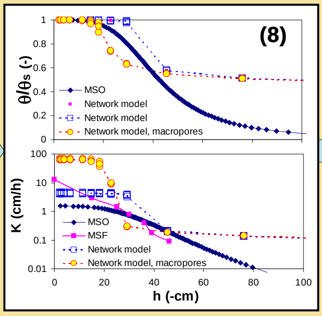


Fig. 8: Experimental soil hydraulic functions (MSO, MSF) of Fuhrberg sand and network model predictions

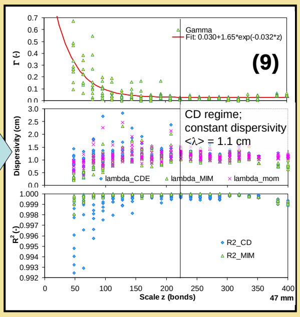
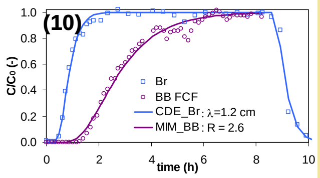


Fig. 9: Scale dependence of network predicted transport parameters for Fuhrberg sand

Computational cost makes real size network simulation often prohibitive. Comparison between experimental and model results then requires analysis of the transport regime tending asymptotically towards convection dispersion (Fig.9). The Br⁻ tracer dispersivity λ obtained by 1D-CDE fitting (λ =1.2 cm; Fig. 10) compares favorably to the network model prediction (λ =1.1 cm; Fig.9) for Fuhrberg sand.

Fig. 10 (right): Experimental Br⁻ & BB-FCF BTC for Fuhrberg sand for unsaturated flow (-15 hPa), and corresp. 1D-CDE fits



Discussion and Contributions to SPPs Grand Goals

- Two morphological functions - pore size distribution and Euler characteristic - permit network model prediction of tracer transport for unsaturated conditions.
- Local percolation probability is an additional connectivity criterion relevant for macropores.
- Adsorbed solute displacement in unsaturated soil can be reasonably predicted if an accurate estimate of sorption is available.
- Further improved prediction of retardation is contingent upon information on (spatial distribution) of reactive surface properties.

CONTRIBUTION TO SPP 1315 GRAND GOALS

- Improve mechanistic understanding of how physical and chemical processes operative at the pore scale of biogeochemical interfaces are reflected by the fate of chemicals at the soil column to pedon scale (in cooperation with TG 4 - Bridging Scales).
- Development of a tool to evaluate the macroscopic effect of microscopic heterogeneity of physicochemical interface properties (Fig. 11) (in cooperation with TG3 - Imaging).

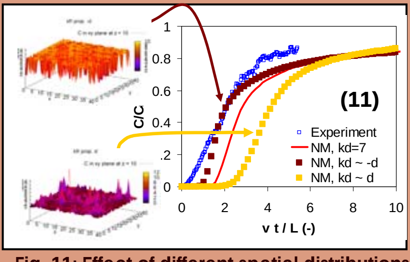


Fig. 11: Effect of different spatial distributions of adsorption coefficients on the predicted BTC

Manuscripts

- **Vogel, H.J., Schlüter, S., Weller, U., Quantification of soil structure based on Minkowski Functions, Computers & Geosciences**
- **Schlüter, S., Weller, U., Vogel, H.-J., Thresholding of X-ray microtomography images of soil using gradient masks, Computers and Geosciences.**
- **Weller, U., Vogel., H.-J., Ippisch, O., Köhne, J.M., direct measurement of unsaturated hydraulic conductivity in soil including temporal dynamics and hysteresis, Vadose Zone Journal**

Acknowledgement

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