A short history of research at GRS concerning bentonite re-saturation

Klaus-Peter Kröhn, GRS

Meetings for knowledge exchange

10th and 11th September 2015, Jyväskylä and Espoo

Overview

Arriving at an alternative conceptual model

Increasing complexity

Latest activities

Open questions

Summary

Arriving at an alternative conceptual model

History of modelling re-saturation

Early 1980s

- empirical “diffusion”-model for isothermal water uptake atmospheric pressure

Early 1990s up to now

- coupling of balance equations for
  - (T) heat
  - (H) mass of water
  - (M) mechanical forces
- established state

First GRS-project on bentonite re-saturation: 2000 - 2003

- reproduce state-of-the-art modelling
- find simplifications for integrated modelling
- accompanying water uptake tests

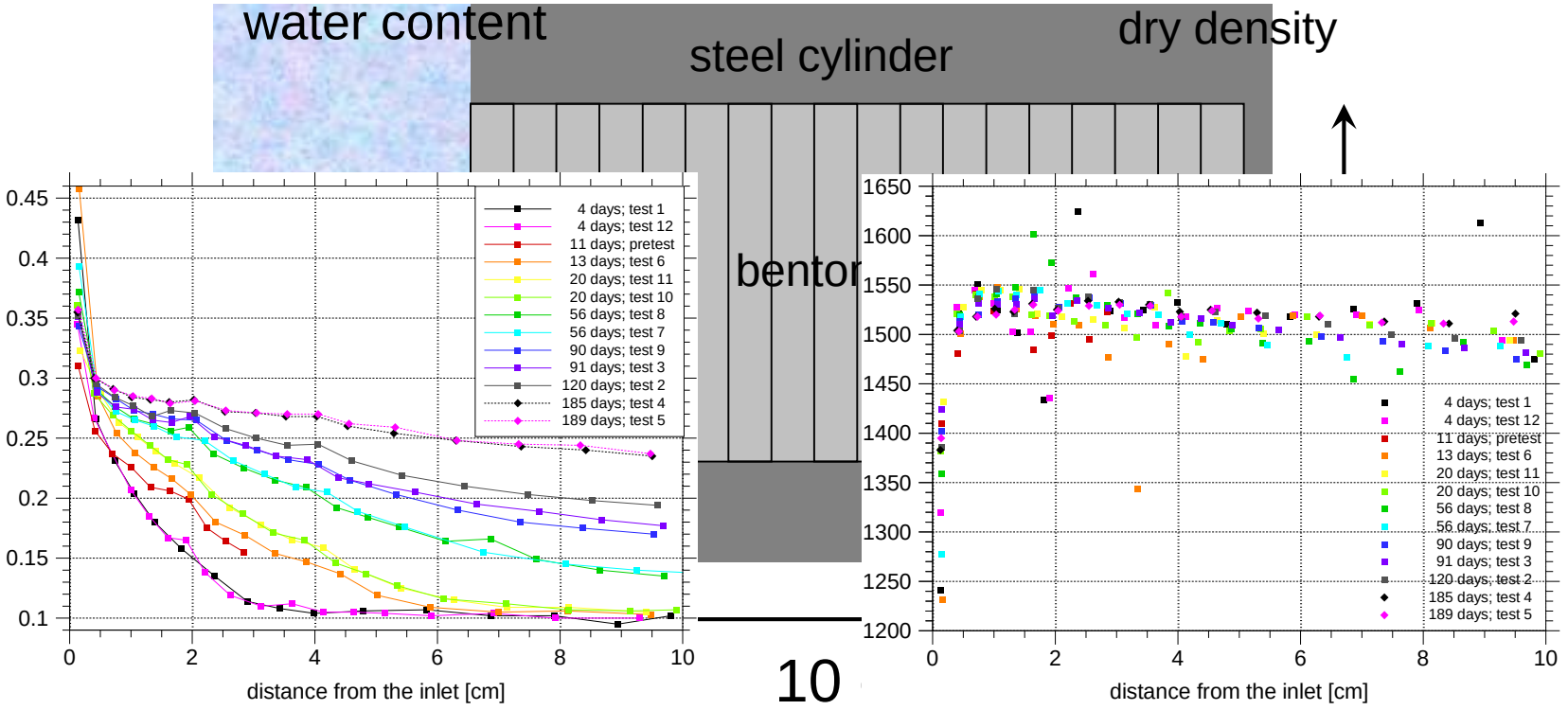
Difficulties with the state-of-the-art THM-modelling

Concept of two-phase flow for water movement

- no difference between hydrated water in the interlamellar space and free water in the pore space
- the retention curve replacing the Capillary-Pressure-Saturation relation represents suction and not capillary forces
- the concept of relative permeability developed for rigid porous media does not apply to re-saturating bentonite
- relative permeability for water cannot be measured directly

Water uptake

1-D experiment (report GRS-199)



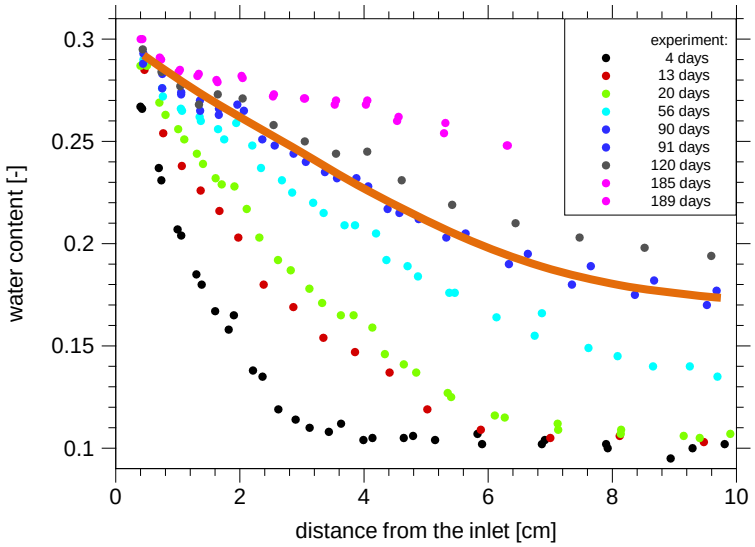
Water uptake

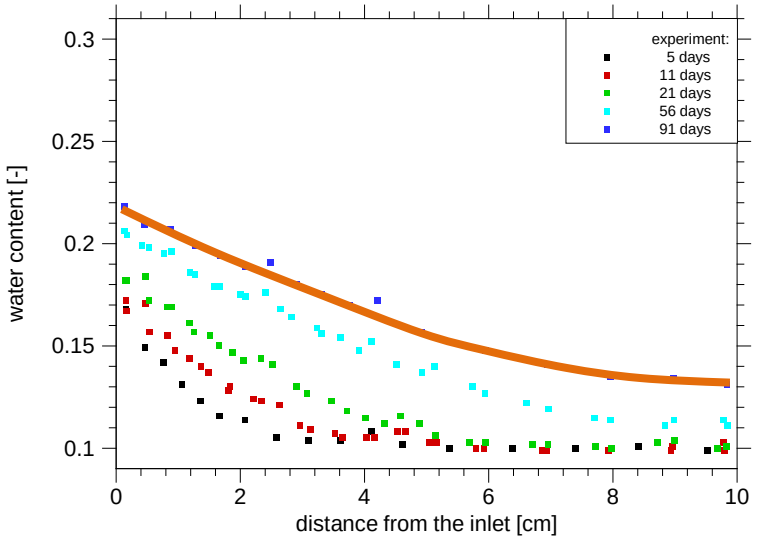
1-D experiment (GRS-199)

water

water vapour

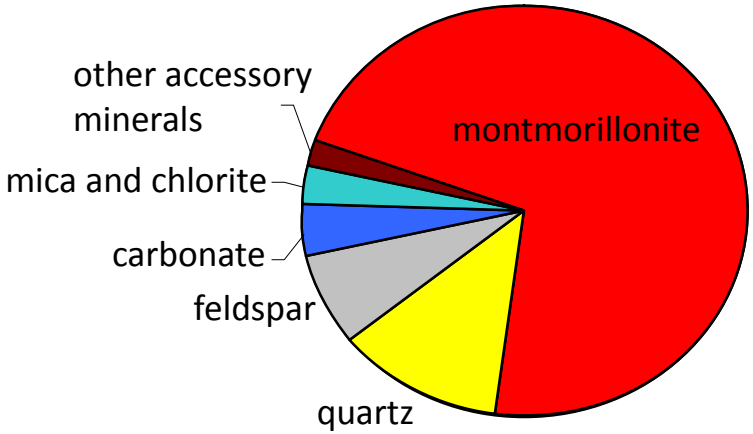
distribution of water content after 90 days



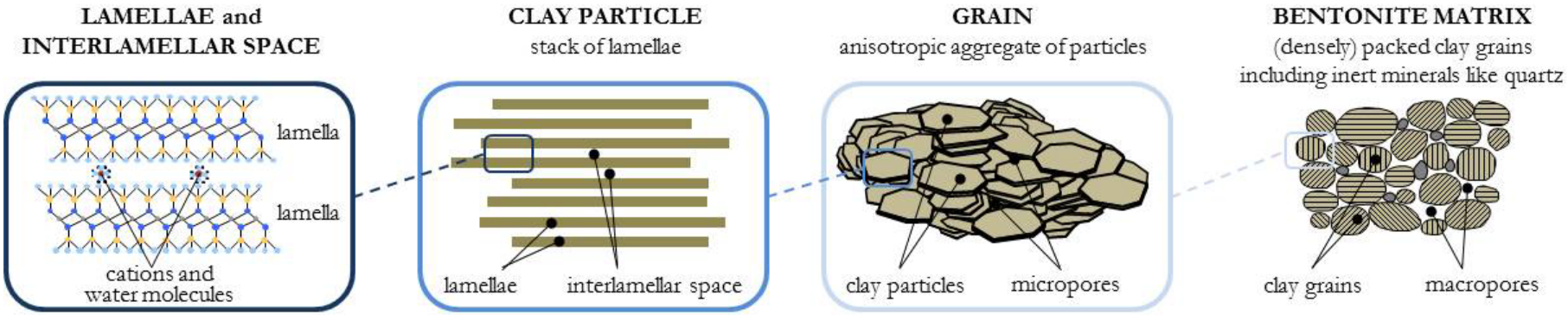


Bentonite structure

Composition

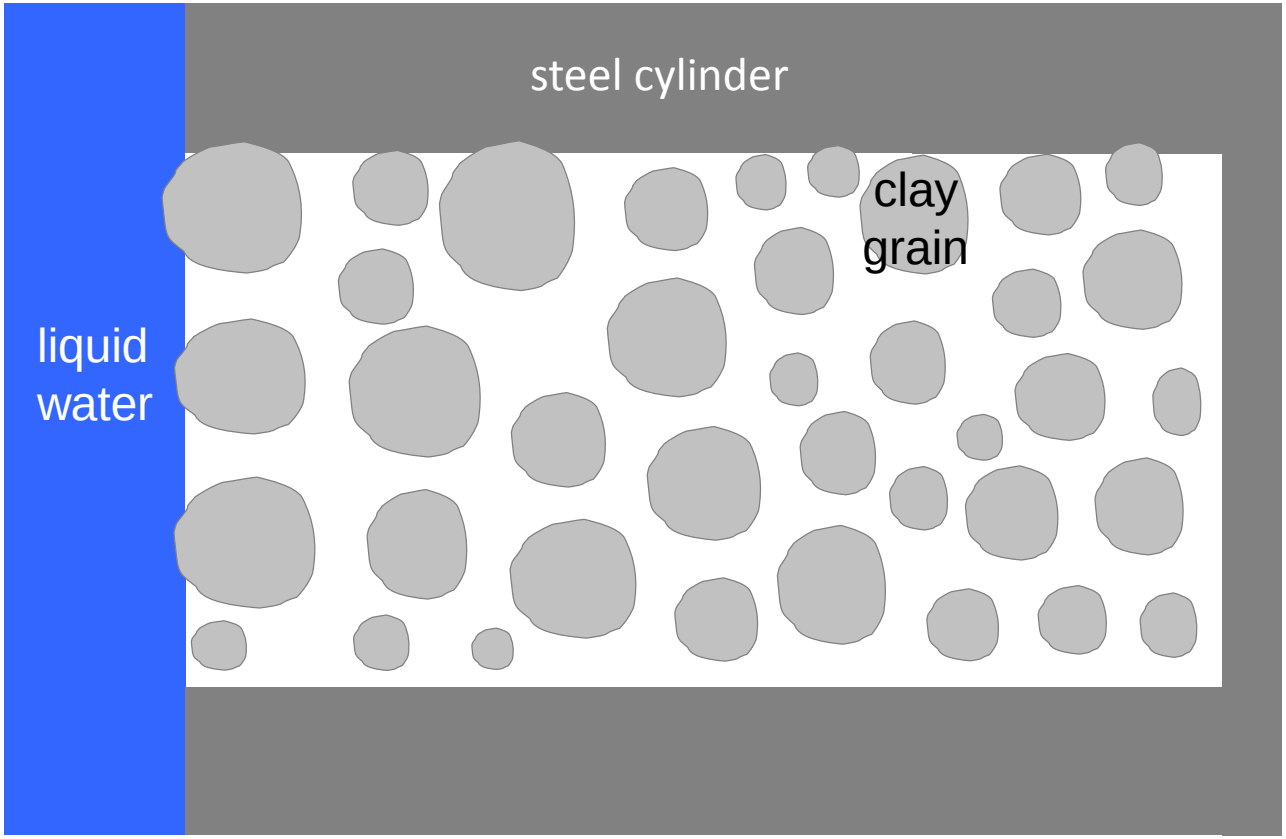


Microstructure of montmorillonite



Conceptual model for bentonite re-saturation

Pre-stage: uptake of liquid water by capillary forces



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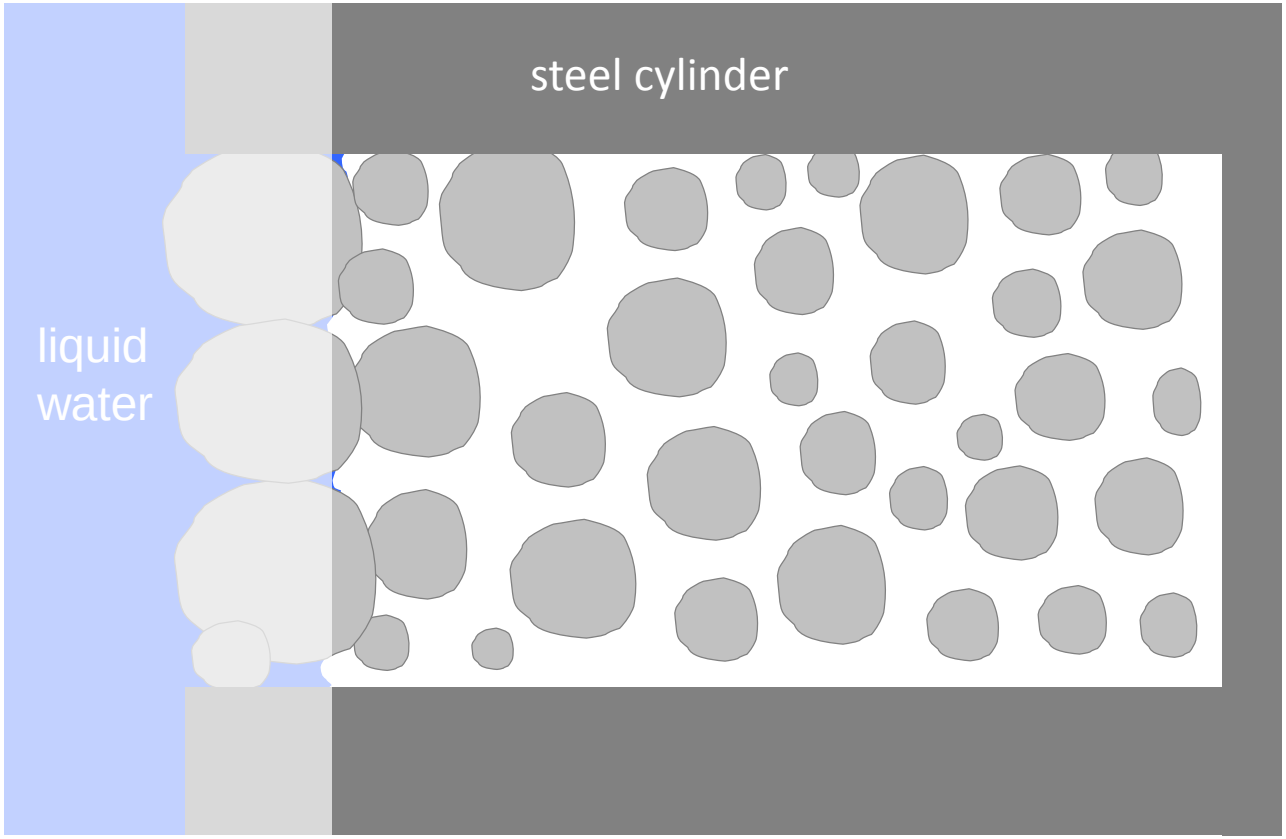
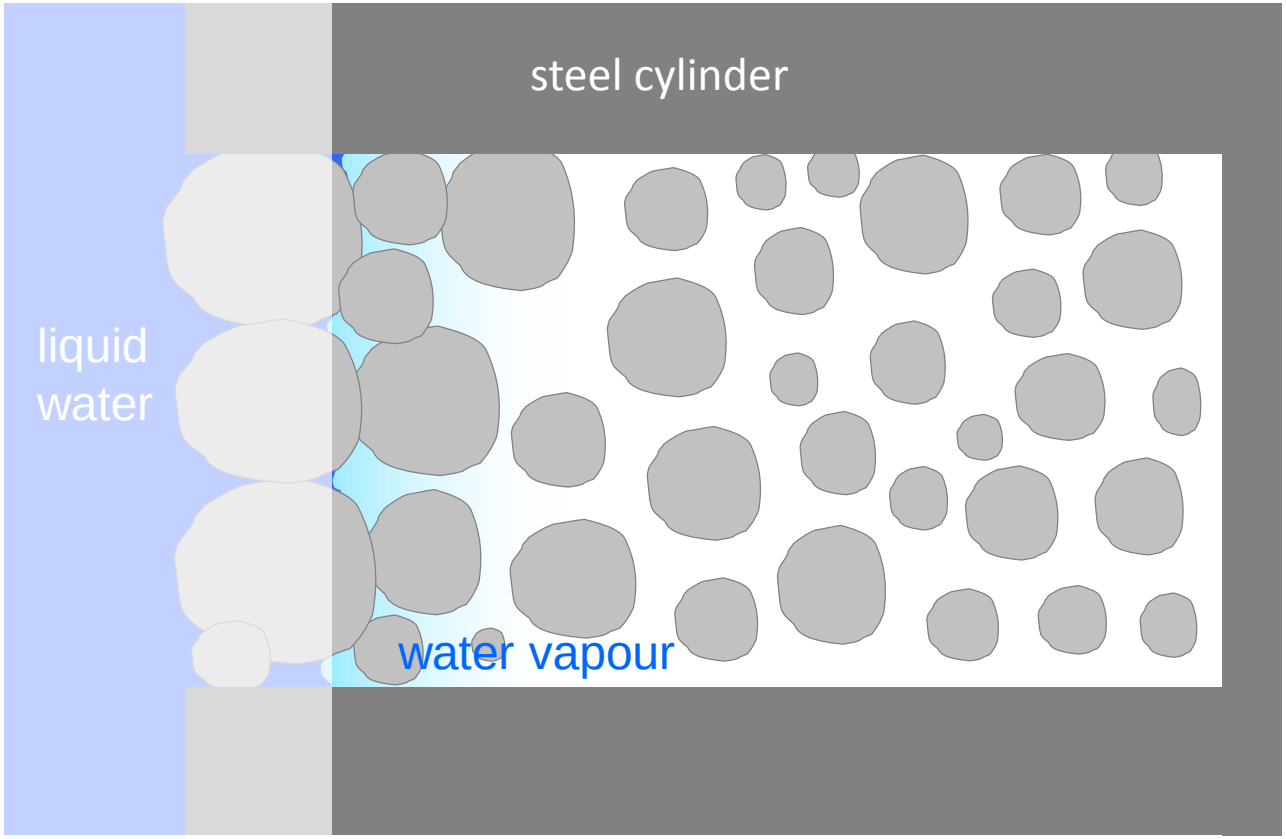


Main stage: re-saturation via water vapour



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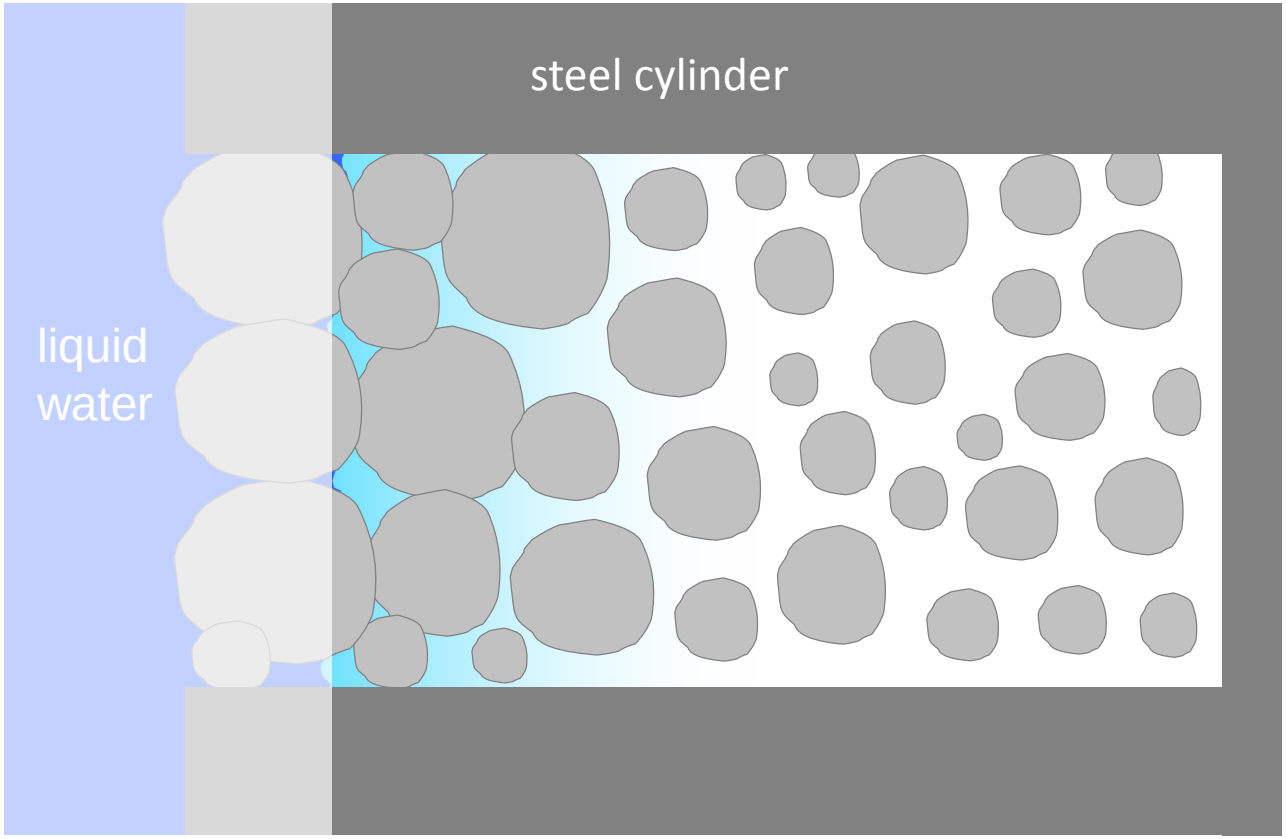

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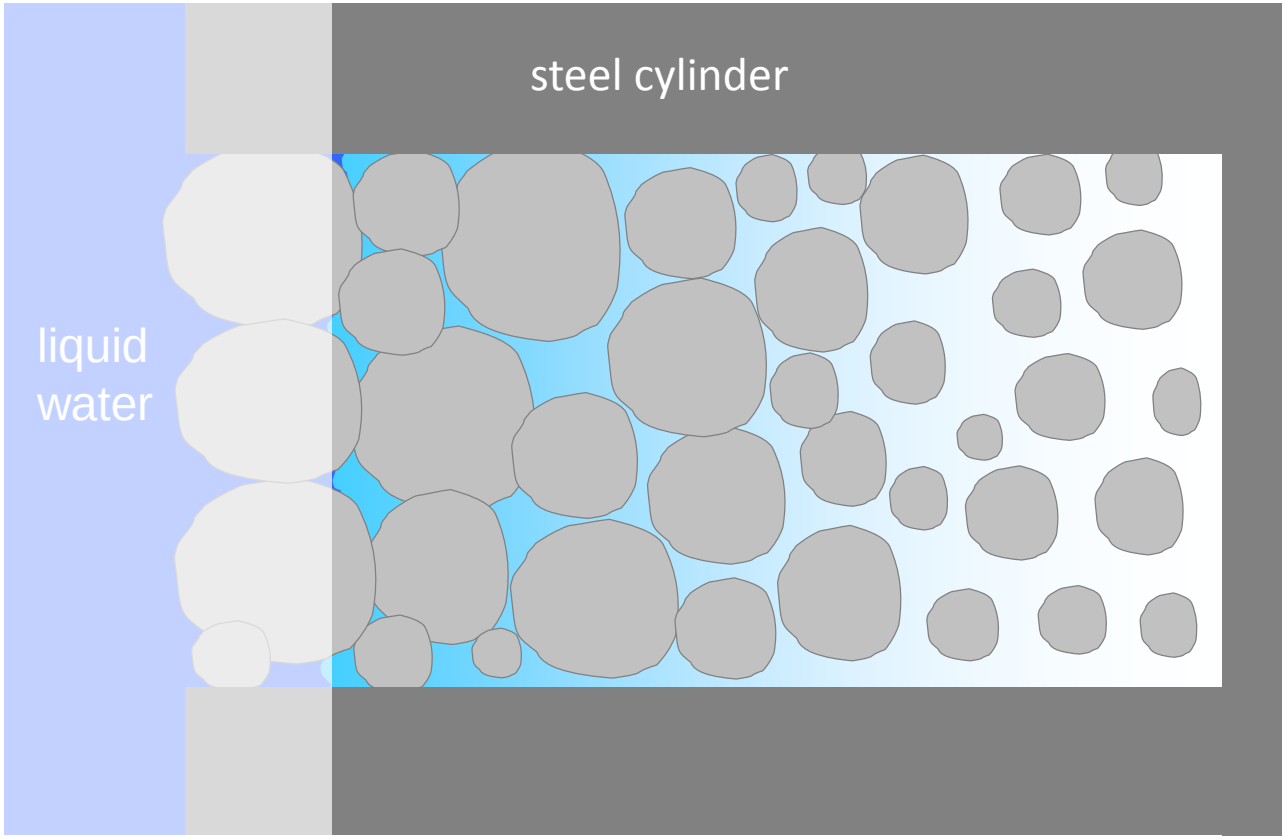
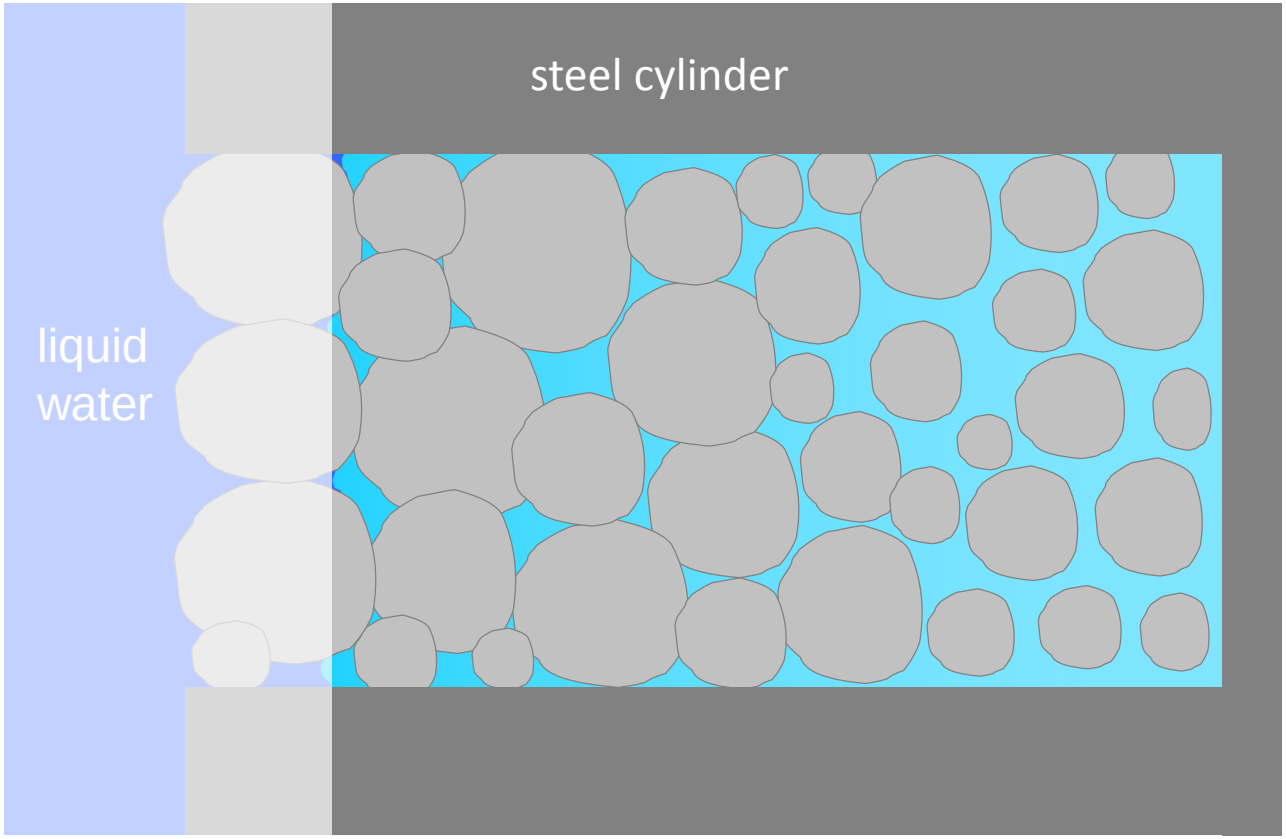


Main stage: re-saturation via water vapour



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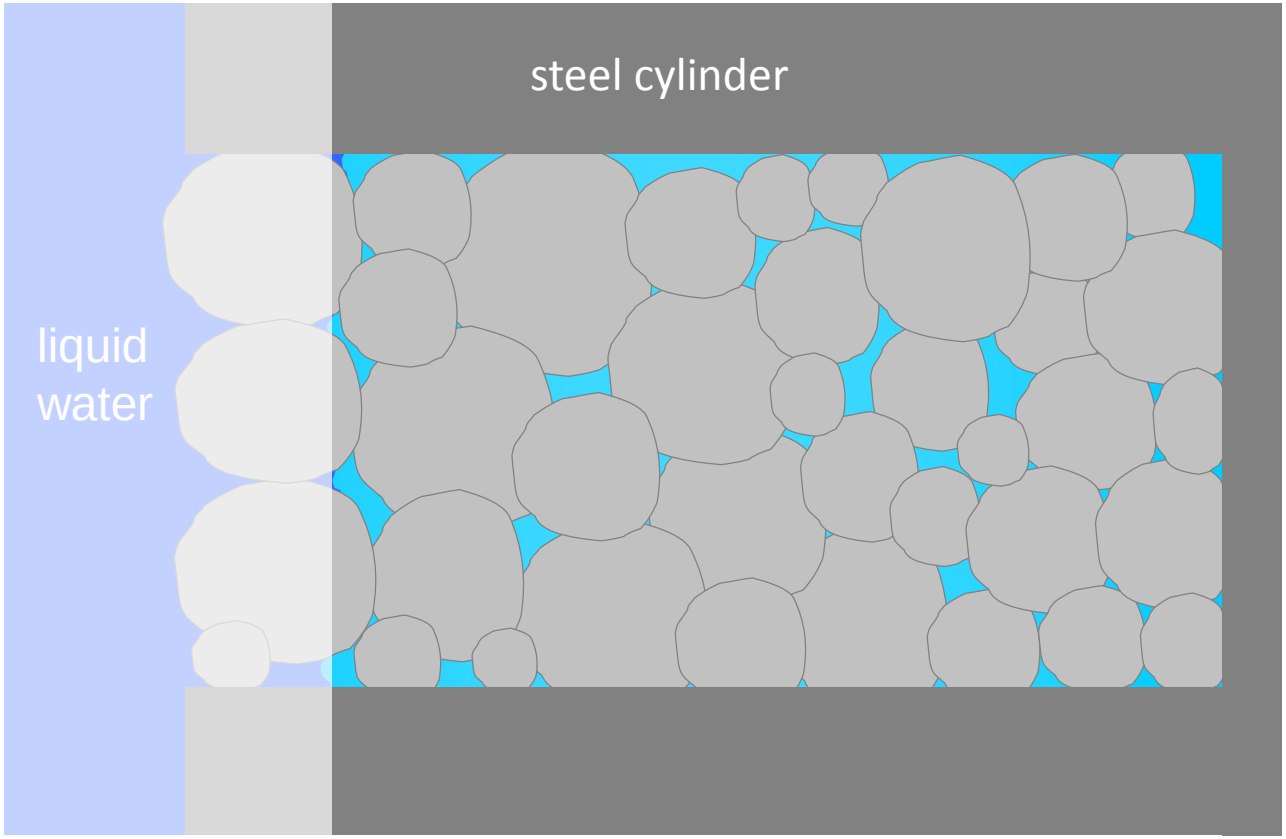
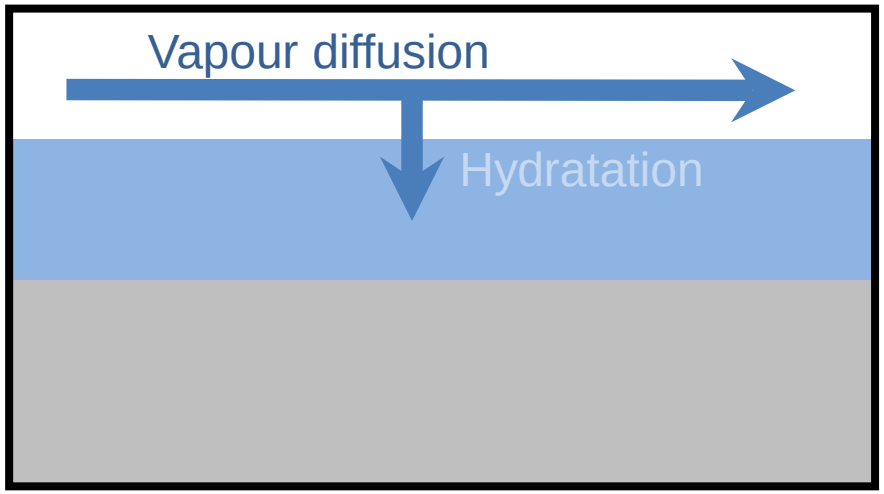


Relevant processes

Volumes

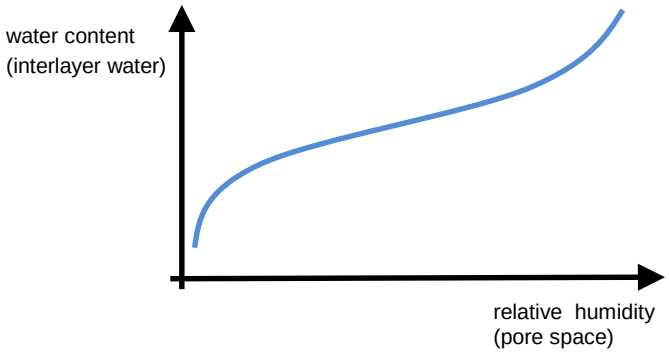
Physical processes



Equilibrium of

- humidity in the pore space
- water content in the interlayer

→ isotherm



Modelling

Balance equation

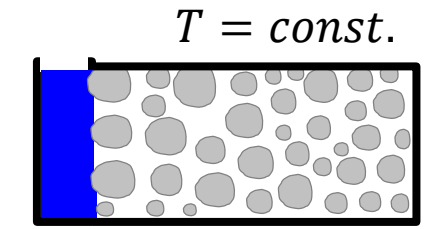
- for vaporous plus hydrated water
- requires almost exclusively established textbook data
- → little room for model calibration
- explained the empirical „diffusion“ coefficient quantitatively (Engineering Geology, Vol. 82 (2005)

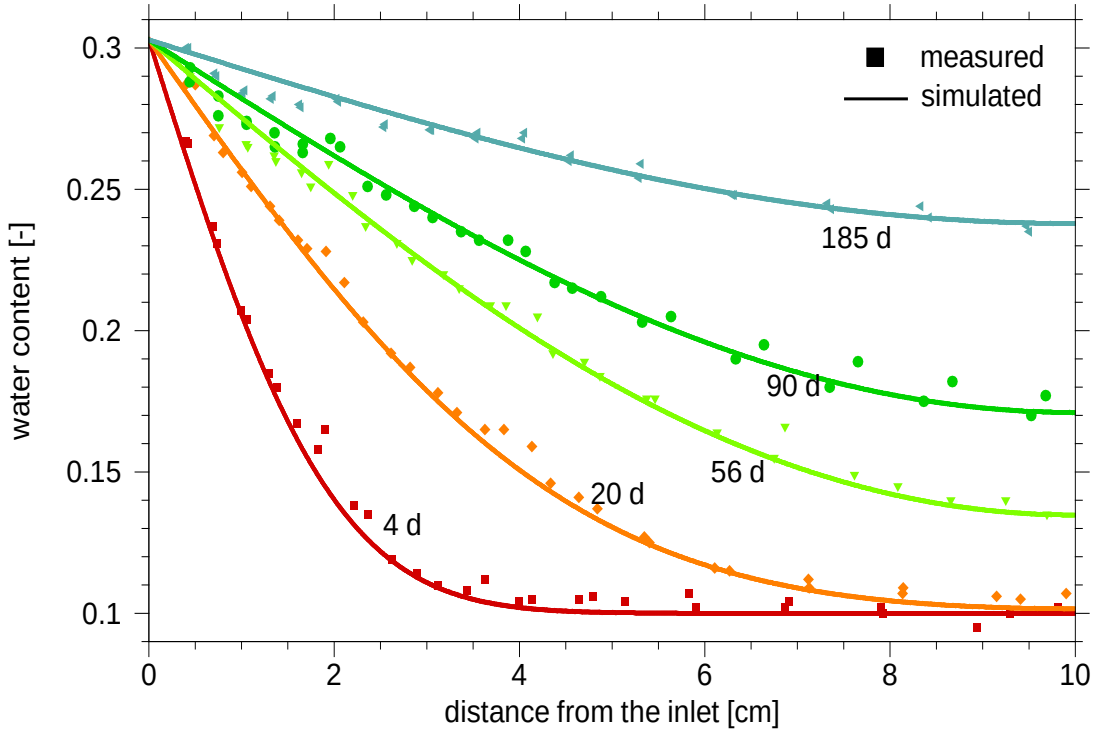
Code development

- Finite Element Equations in 1d; later also 1d axial-symmetric elements
- → experimental code VAPMOD; now **VIPER**

Increasing complexity

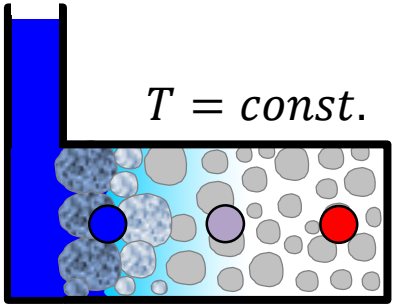
Re-saturation under ambient conditions



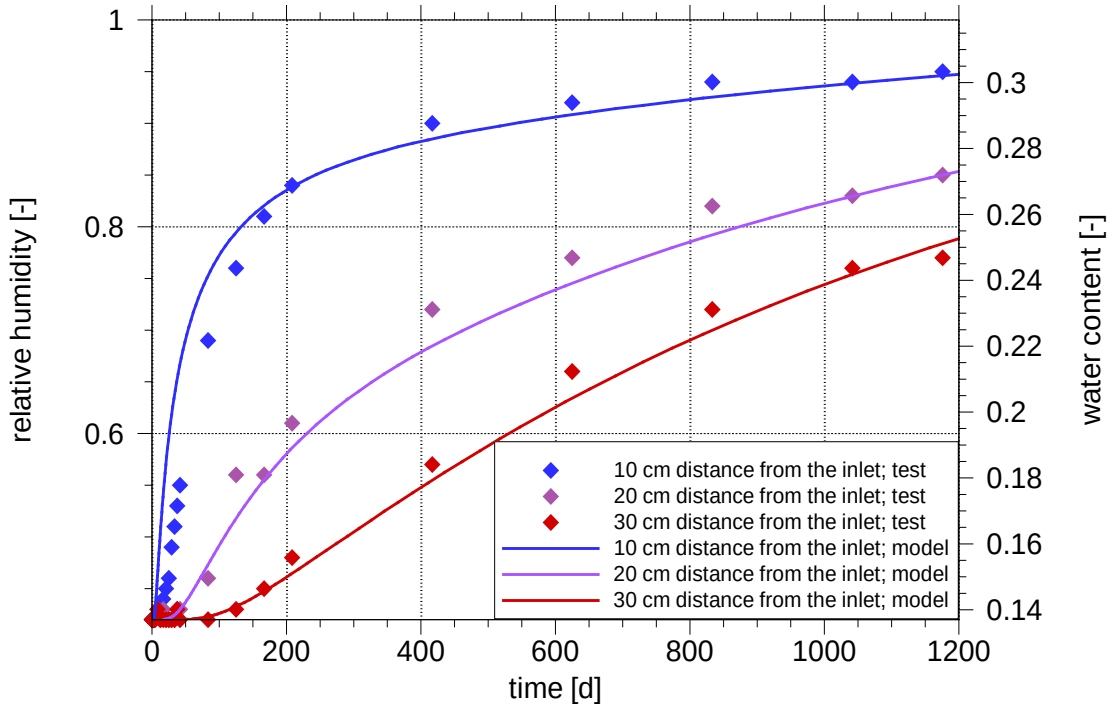


Report GRS-199 (2004); Engineering Geology, Vol. 82 (2005)

Re-saturation at increased hydraulic pressure



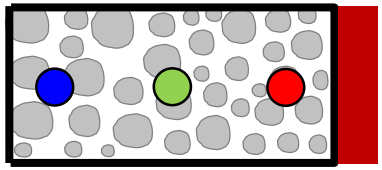
$p = 1{,}2\ MPa$



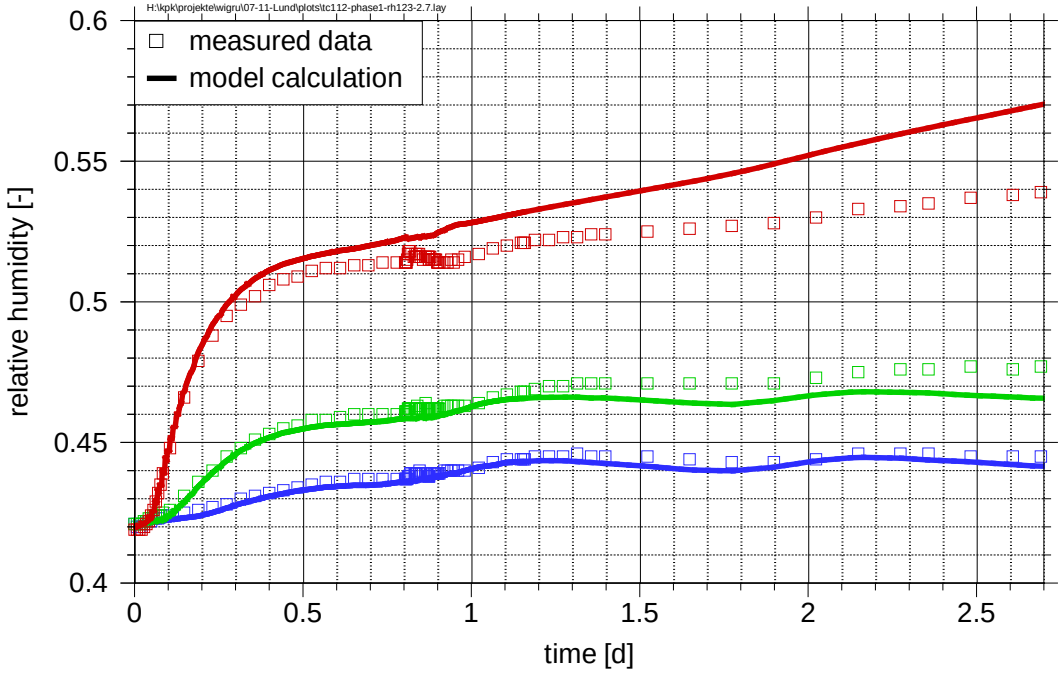
Report GRS-222 (2006)

Moisture redistribution under a thermal gradient

$25\,°C < T < 90\,°C$

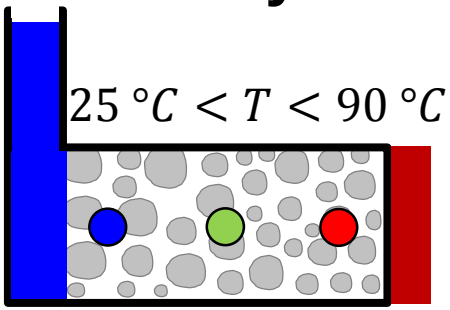


$p = p_0$

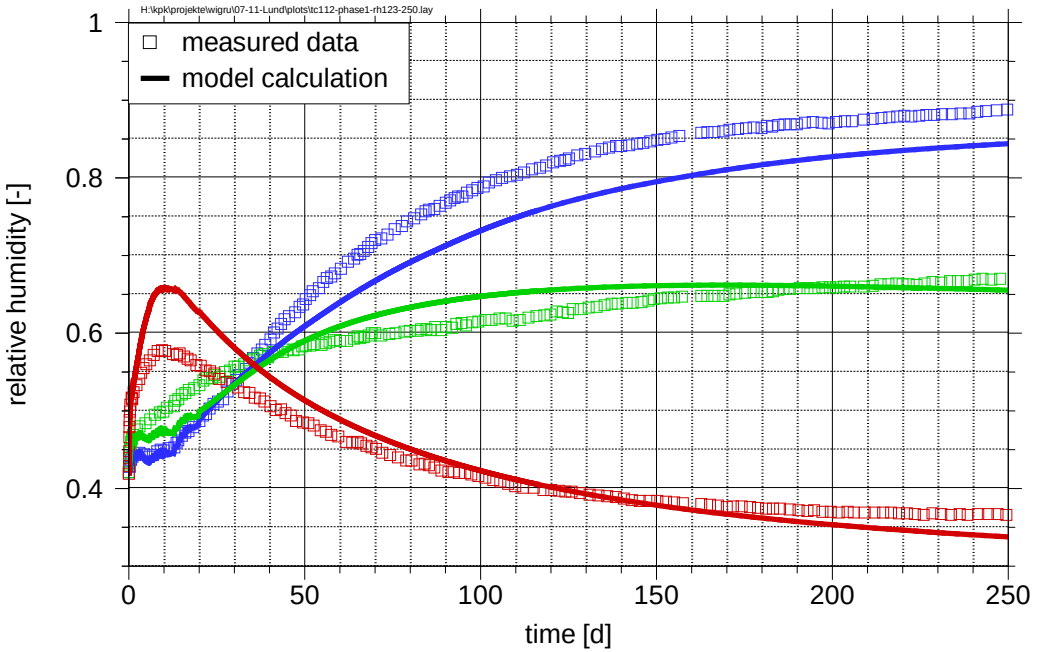


Applied Clay Science, Vol. 47 (2010)

Increased hydraulic pressure & thermal gradient



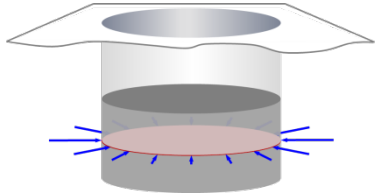
$p = 1{,}2\ MPa$



Applied Clay Science, Vol. 47 (2010)

Re-saturation of a bentonit-sand-mixture (ITT-Test, URL, Canada)

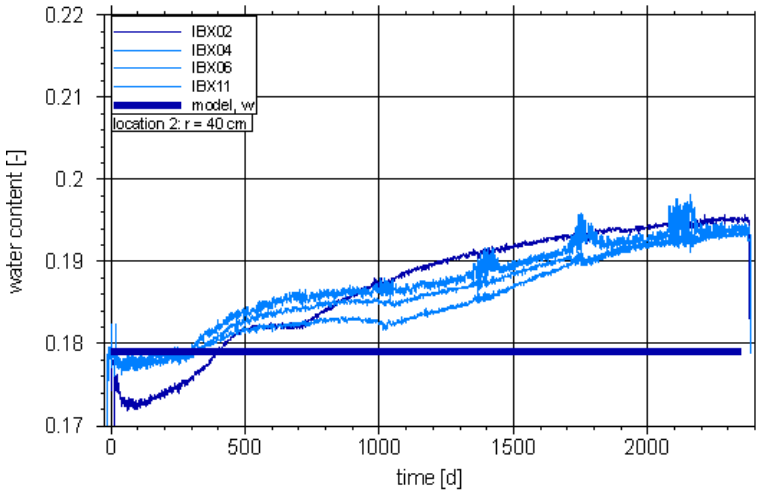
$T = const.$



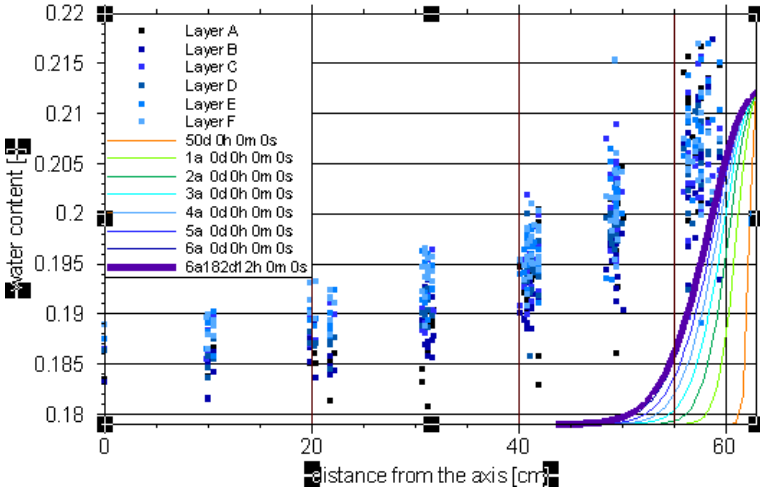
$p \sim p_0$

only vapour diffusion

breakthrough



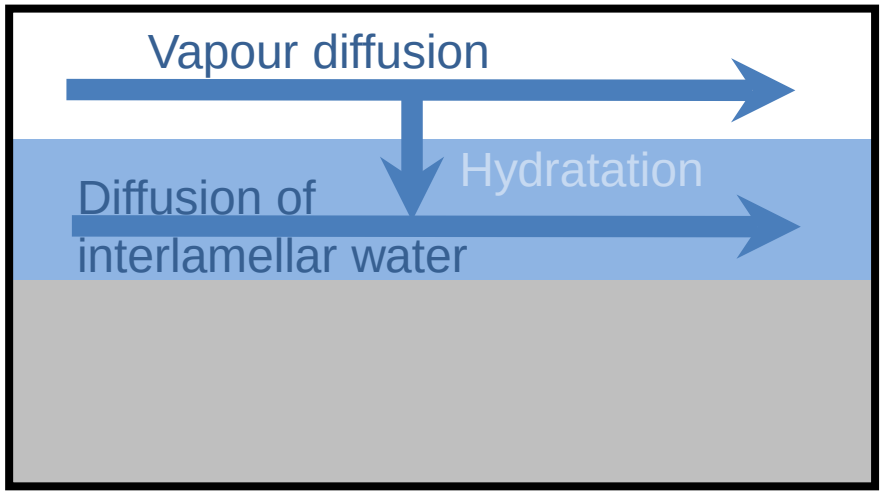
end-of-test distribution



Relevant processes

Abstraktion of volumes

Physical processes



Equilibrium of

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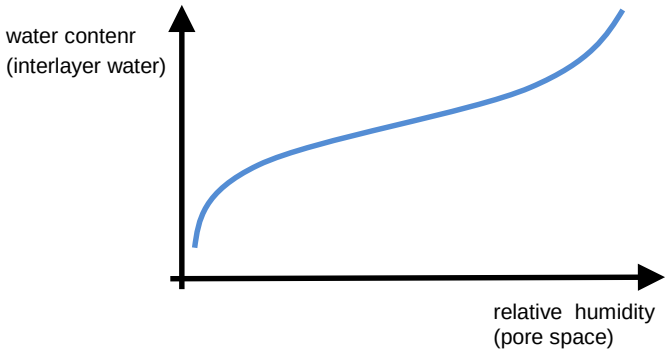
→ isotherm



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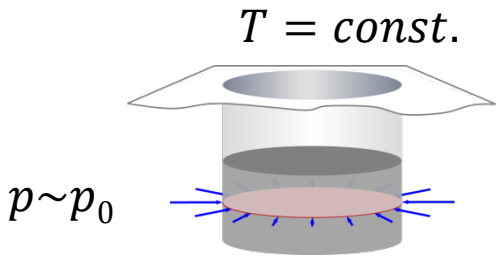
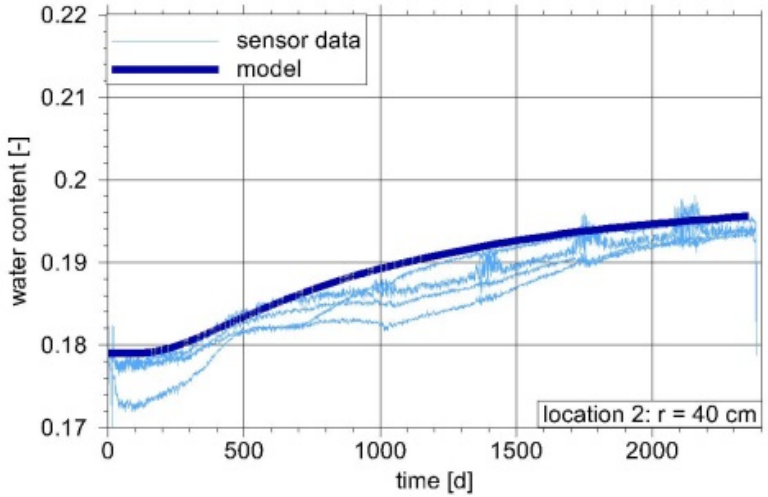
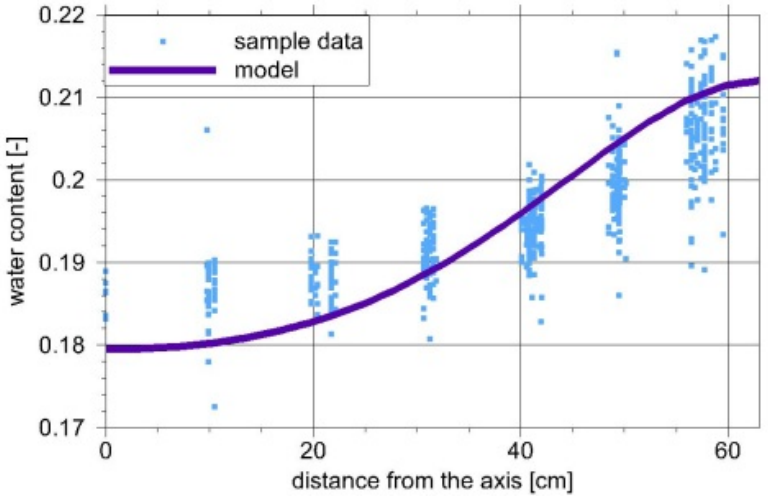


Extended vapour diffusion model

breakthrough



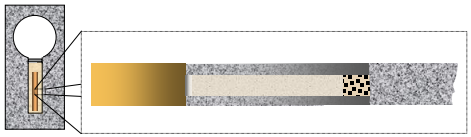
end-of-test distribution



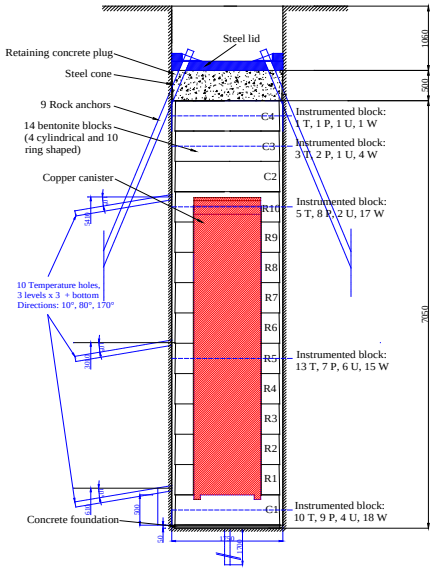
Report GRS-269 (2011)

Re-saturation in-situ under a thermal gradient (Canister Retrieval Test, Äspö)

$$90\ °C > T > 8\ °C$$



$$p = \sim 0{,}3\ MPa$$


Steel lid
Retaining concrete plug
Steel cone
9 Rock anchors
14 bentonite blocks (4 cylindrical and 10 ring shaped)
Copper canister
10 Temperature holes, 3 levels x 3 + bottom Directions: 10°, 80°, 170°
Concrete foundation
Instrumented block: 1 T, 1 P, 1 U, 1 W
Instrumented block: 3 T, 2 P, 1 U, 4 W
Instrumented block: 5 T, 8 P, 2 U, 17 W
Instrumented block: 13 T, 7 P, 6 U, 15 W
Instrumented block: 10 T, 9 P, 4 U, 18 W
C4
C3
C2
R10
R9
R8
R7
R6
R5
R4
R3
R2
R1
G1
1000
600
4500
500
500

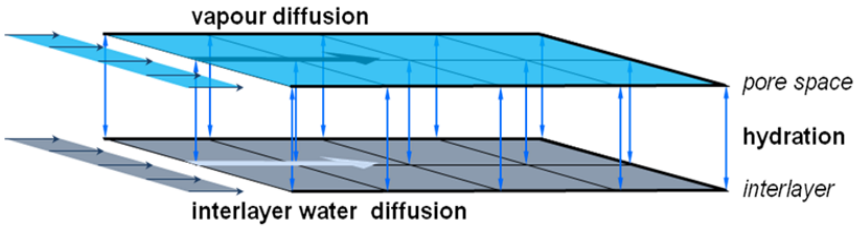
Present model concept

Extended Vapour Diffusion model

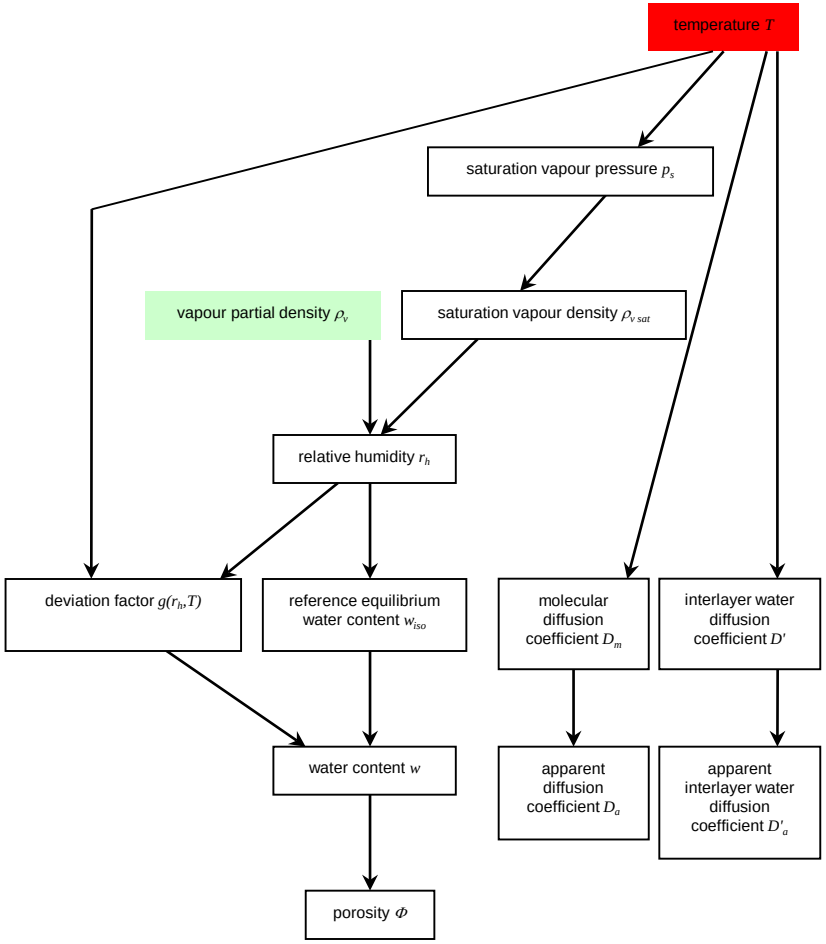
three processes

- binary vapour diffusion in the pore space
- diffusion of water in the interlamellar space
- exchange by hydration
  (controlled by an adsorption isotherm)

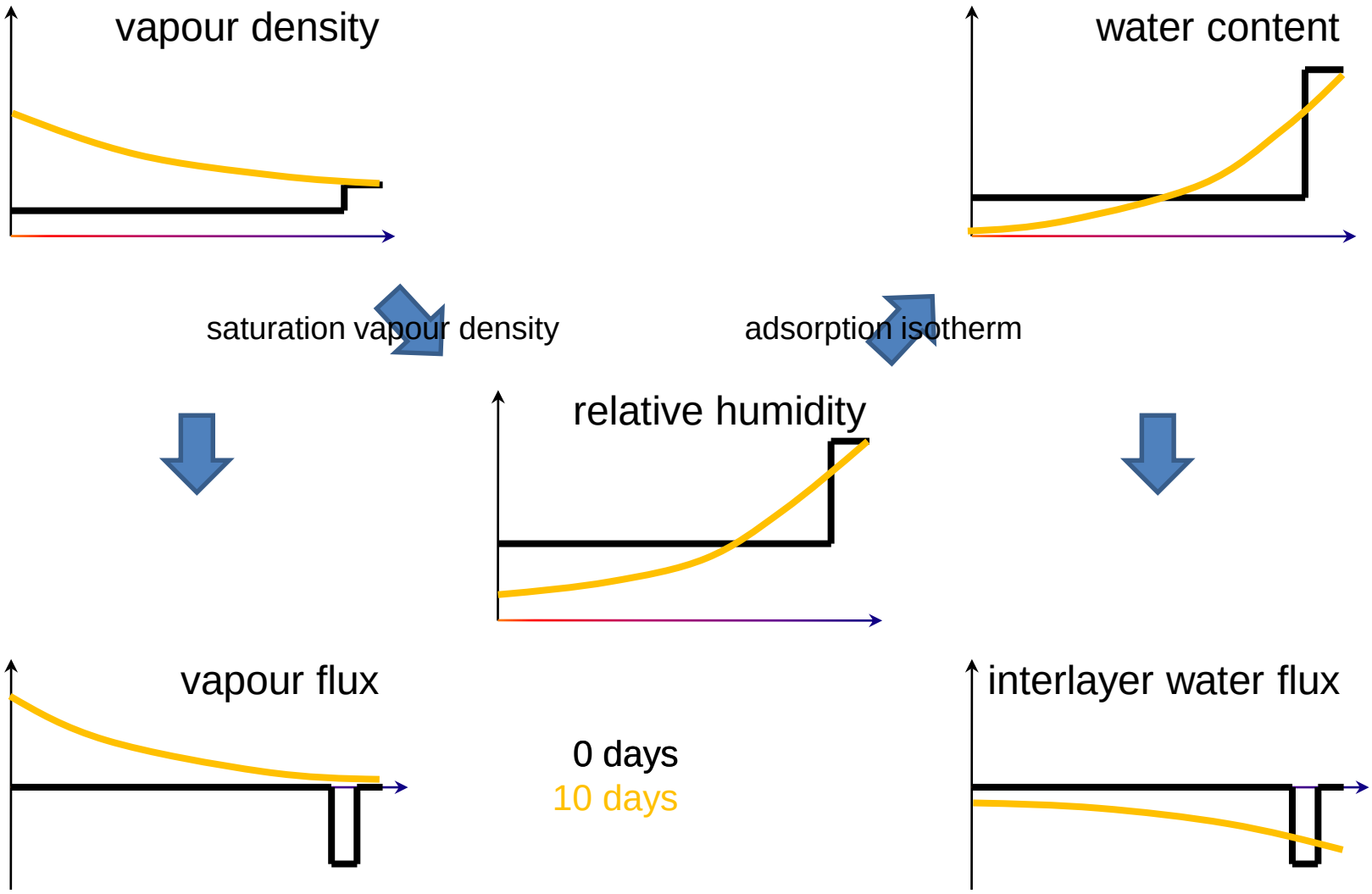
double-porosity model



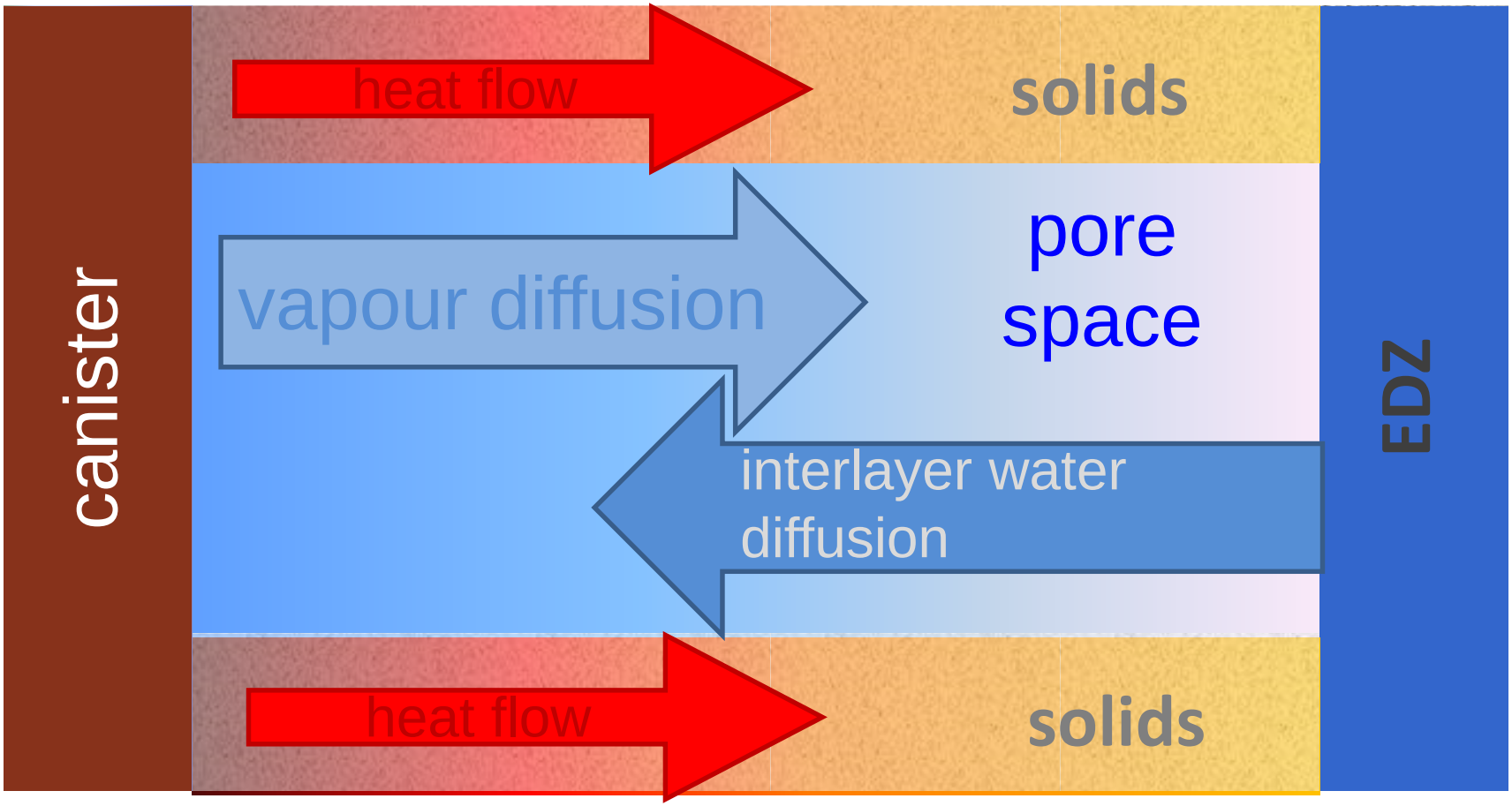
interplay of secondary variables



What happens in the CRT in principle?



In principle a counterflow system!



Latest activities

Formal comparison of mathematical models

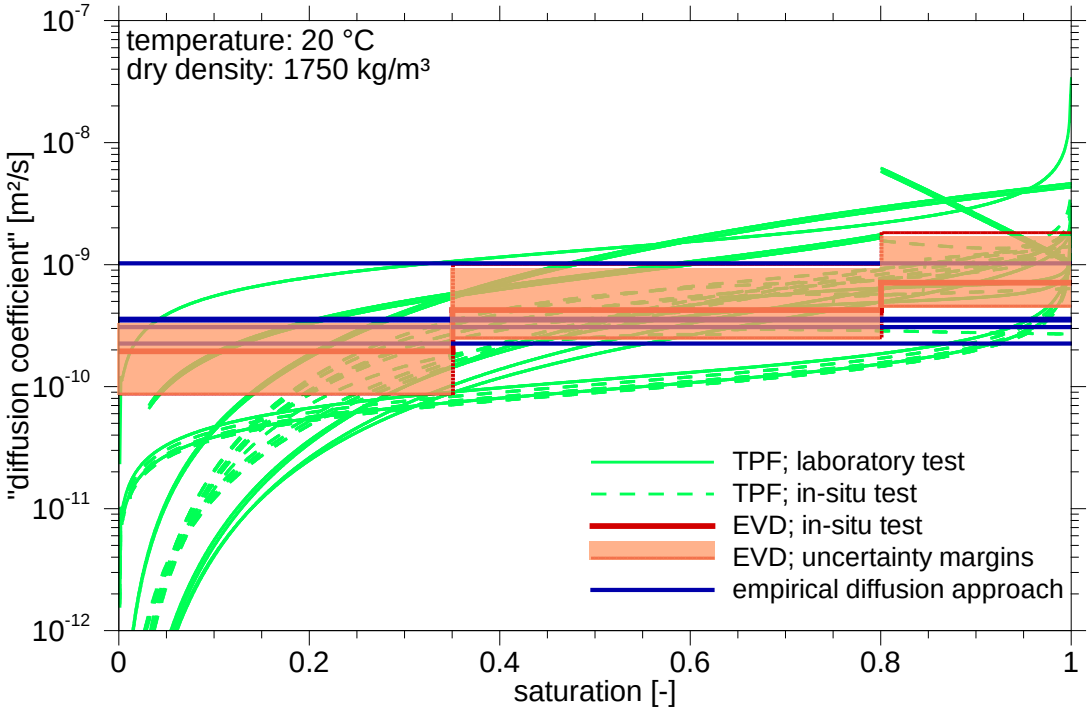
Qualitatively

- full set of two-phase flow balance equations $\frac{\partial(\Phi\, S_\alpha\, \rho_\alpha)}{\partial t} + \Delta\left(\rho_\alpha \mathbf{v}_f\right) - \rho_\alpha q_\alpha = 0$
- → Richards equation $\frac{\partial S_w}{\partial t} + \frac{\partial}{\partial x}\left(\hat{D}\frac{\partial S_w}{\partial x}\right) = 0$ $\hat{D}_{THM} = \frac{k}{\mu_w \Phi} \cdot k_{rw} \frac{\partial p_c}{\partial S_w}$
- Coefficient in VIPER model (linear isotherm) $\hat{D}_{VIPER} = \frac{\rho_{v\,sat}}{\rho_d w_e} \cdot D_a + D'$

Quantitatively

- EOS from several groups
  - for two non-isothermal experiments with MX-80 (one laboratory, one in-situ test)
  - at a dry density of ~1750 kg/m³

Comparison of “diffusion coefficients”



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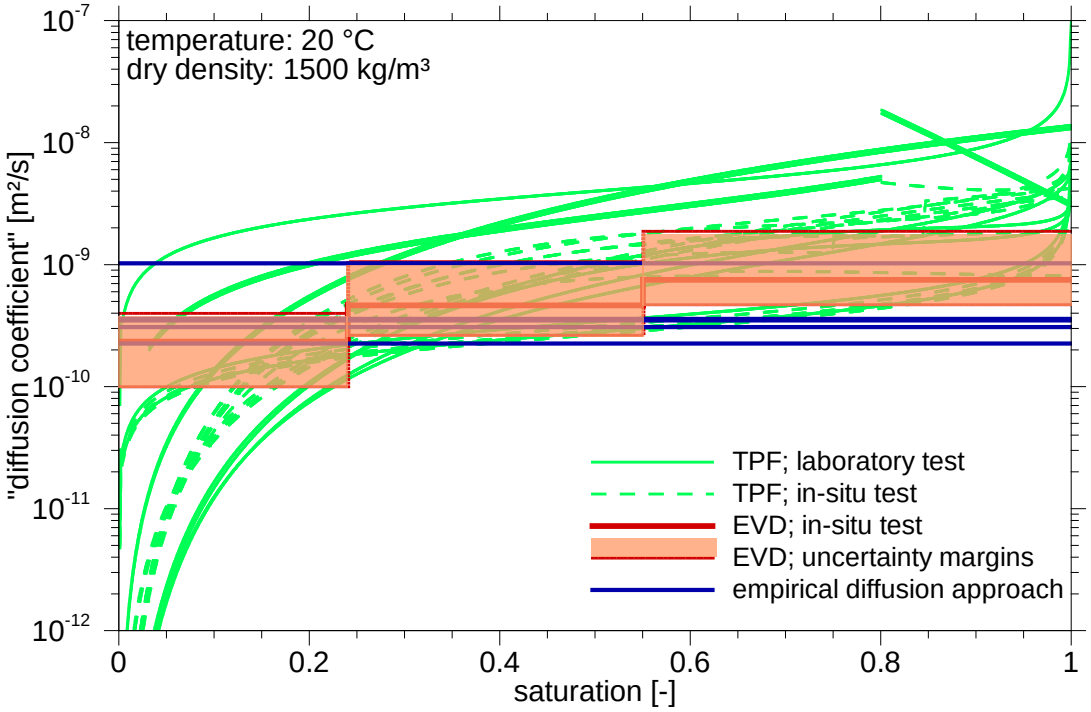

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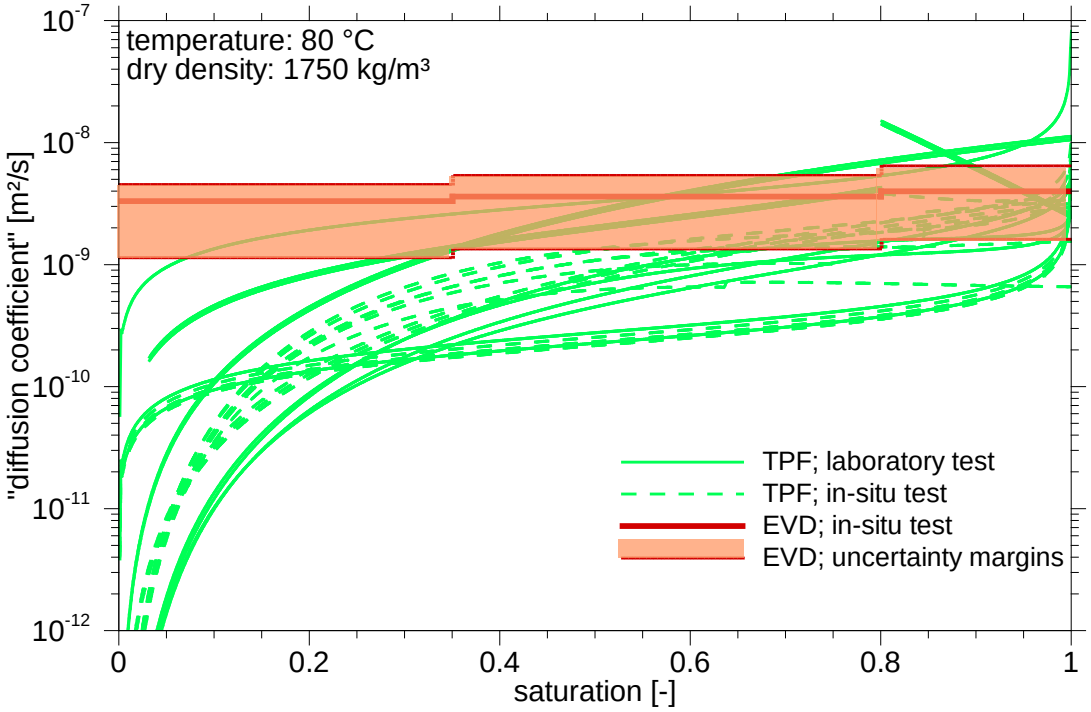
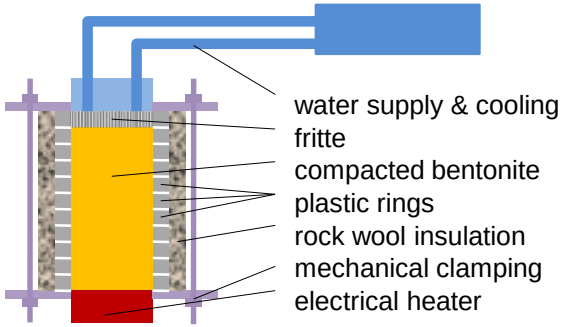


Submitted as a paper at the Clay Conference 2015

Ongoing laboratory tests

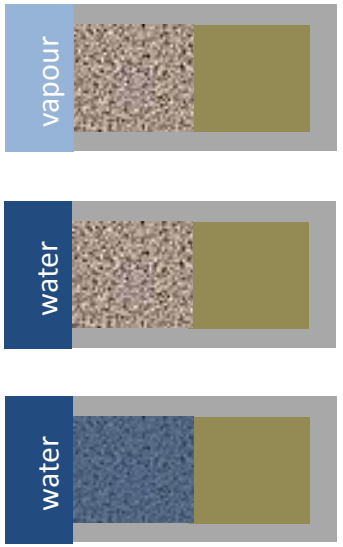
Non-isothermal water uptake test

- → what is the steady-state distribution of water?



Isothermal uptake tests with restricted water supply

- → what are the uptake dynamics inside the bentonite?



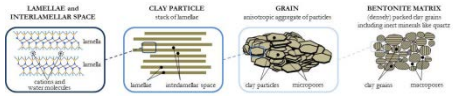
Non-isothermal water uptake test

- → dependency of the isotherm on temperature

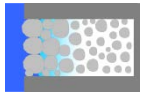
Summary
and
open questions

Summary

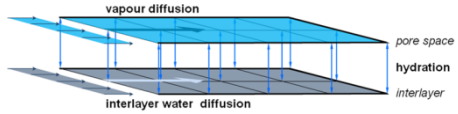
Bentonite is a complex material

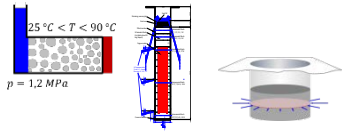


Alternative concept for buffer re-saturation under constraint conditions

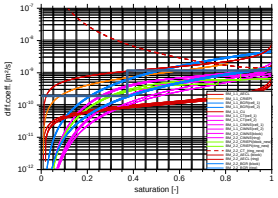


- Based on simple well-known physical processes
  → little leeway for calibration
- Qualified for
  - Non-isothermal uptake in the laboratory and in the field
  - Bentonite-sand mixtures
- Economic in terms of computational effort
- Formally comparable to the two-phase flow hydraulics used in classic THM-codes

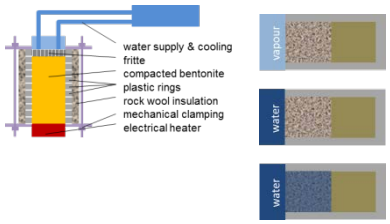




$$\frac{\partial S_w}{\partial t} + \frac{\partial}{\partial x}\left(\hat{D}\frac{\partial S_w}{\partial x}\right) = 0$$



Several ongoing laboratory tests



Open questions, concerning …

… the thickness of the narrow highly saturated zone at the water inlet:

- Dependency on the hydraulic pressure?
- Dependency under low inflow rates?
- Change with time?

… the steady-state distribution of water

- under ambient conditions (pressure and temperature), especially in case of entrapped air?
- under a temperature gradient?

… the uptake dynamics under restricted access to water?

… the isotherm for bentonite:

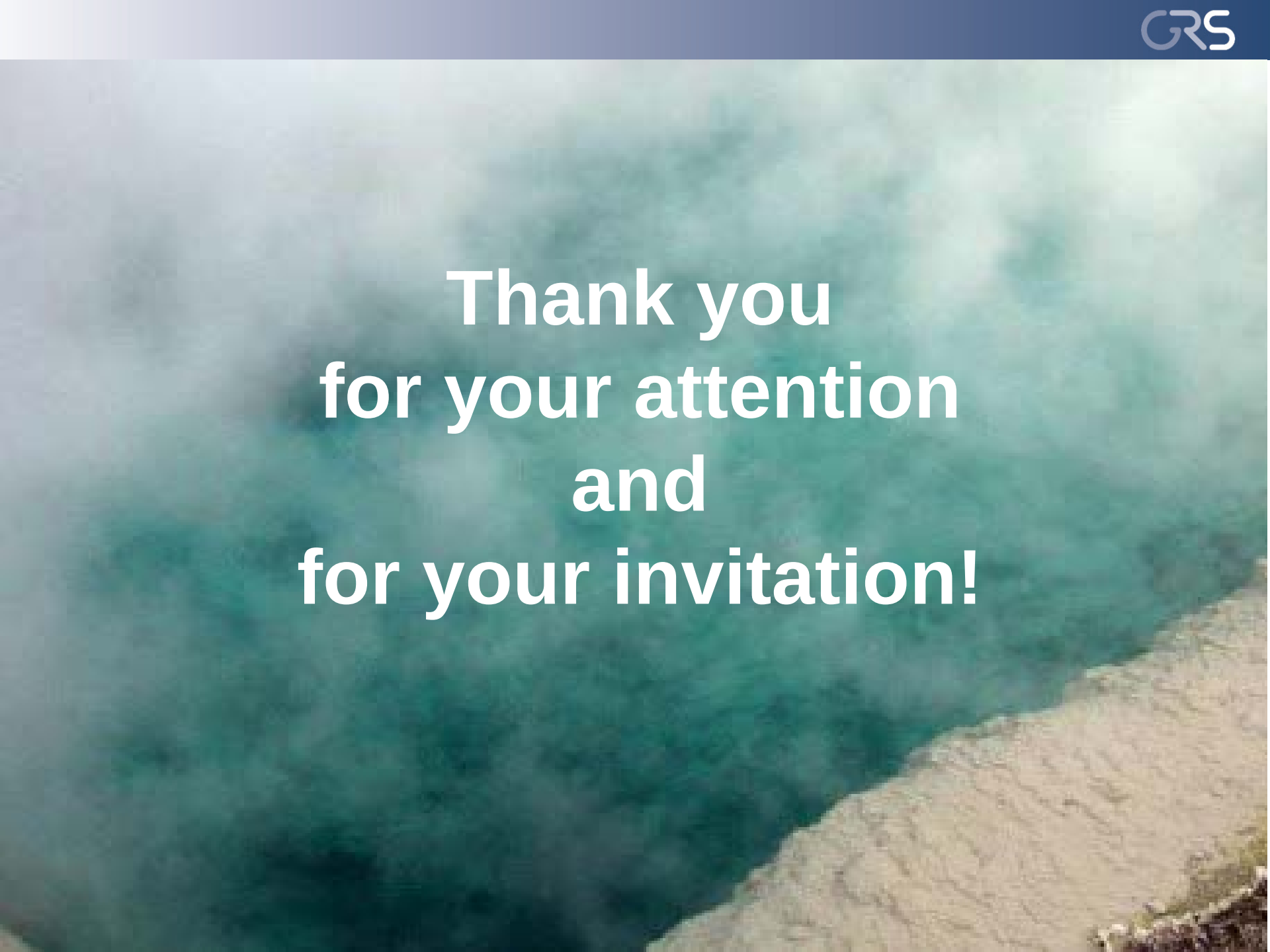
- Dependency on temperature
- Hysteretic behaviour under different wetting/drying histories?

… the process of hydration:

- Kinetics?

… 3d-modelling:

- Transfer from VIPER to COMSOL?


Thank you
for your attention
and
for your invitation!