Business from technology

Microstructural studies of bentonite and modelling of erosion experiments

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Outline

Part I: Microstructural studies (Michał Matusewicz)

- motivation
- experimental methods
- first results
- uncertainties
- TEM images
- next

Part II: Modelling of erosion experiments (Veli-Matti Pulkkanen)

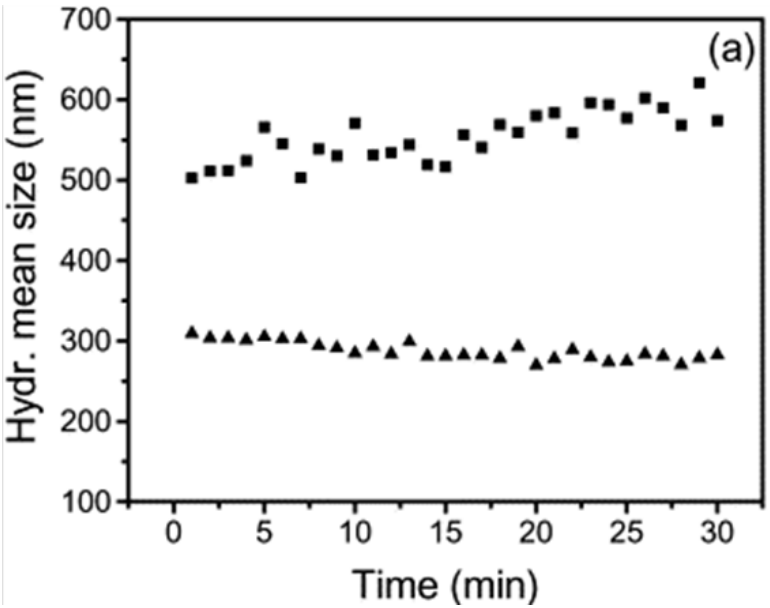
- modelling
- pieces of the model
- mechanical model
- wetting model
- effects of salinity

Part I: motivation

Bentonite breaks down on microstructural level in chemical erosion
→ a need to study microstructure when bentonite swells

colloids & larger particles

colloid sizes



Tiziana Missana et al.Generation and stability of bentonite colloids at the bentonite/granite interface of a deep geological radioactive waste repository, Journal of Contaminant Hydrology, Volume 61, Issues 1–4, March 2003,

Part I: experimental methods

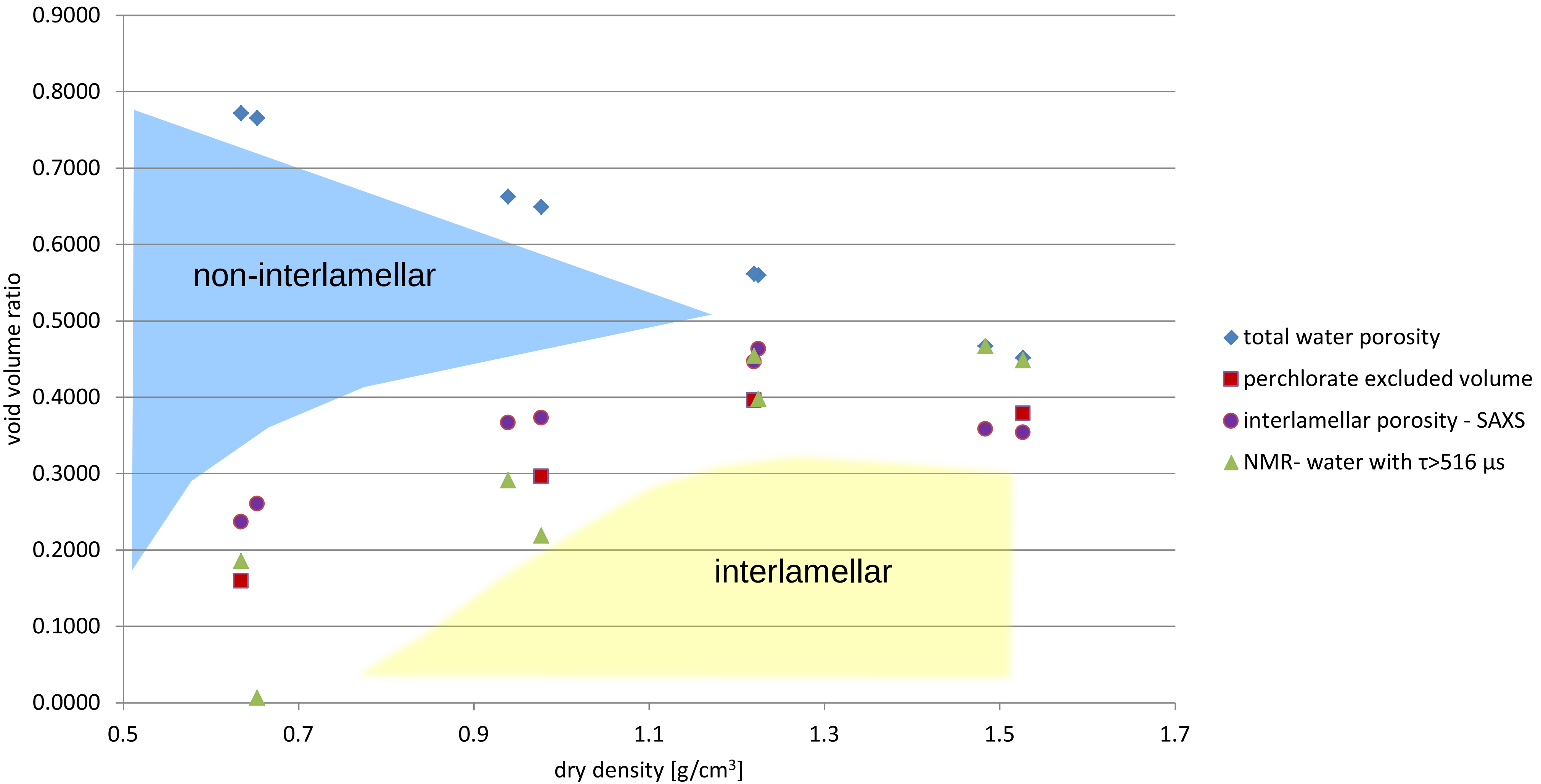
Methods

- SAXS – small angle x-ray scattering
  - “resolution” ≈ interlayer spacing
- NMR – nuclear magnetic resonance
  - hydrogen nuclei in different chemical (magnetic) environments
- also TEM and anion exclusion

First step: get the methods to work on water saturated, compacted samples

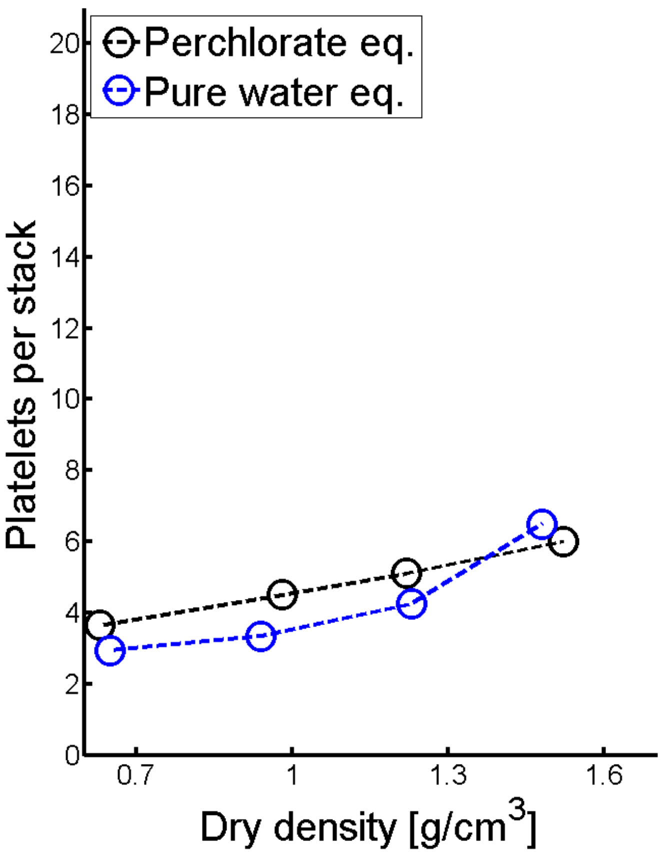
ρ_{dry} (g/cm^3)	MX-80	purified Ca-montmorillonite	purified Na-montmorillonite
0.7	autumn	done	spring
1.0	autumn	done	spring
1.3	autumn	done	spring
1.6	done	done	done

Part I: first results, Ca-montmorillonite

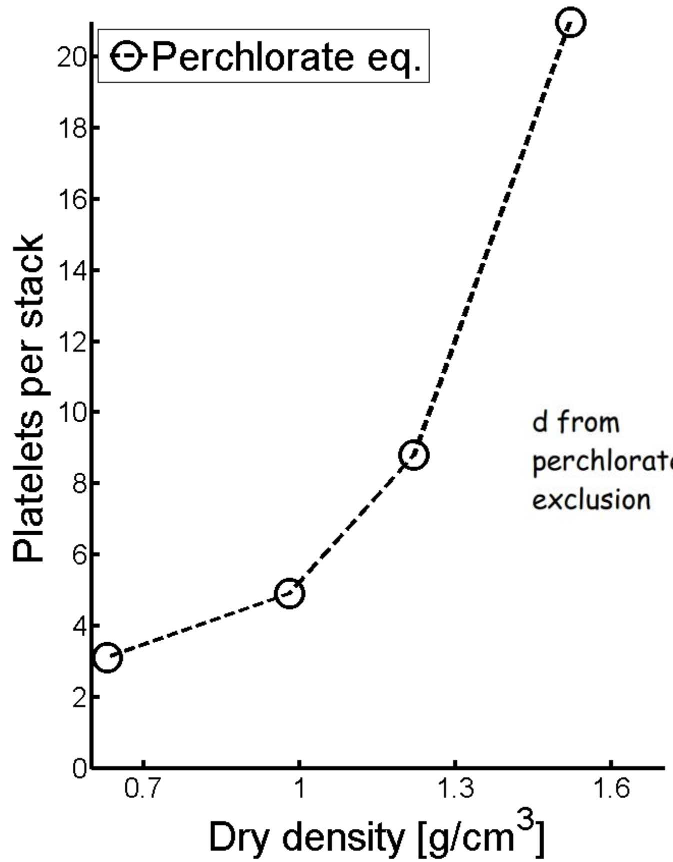


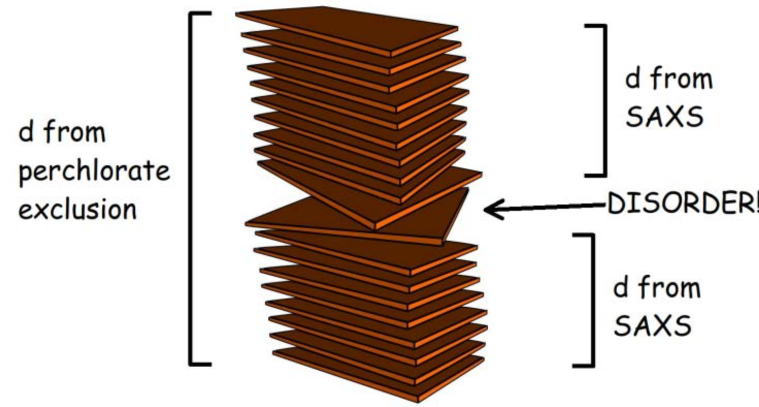
Part I: first results, stacking

Stack size estimation
(SAXS modelling)



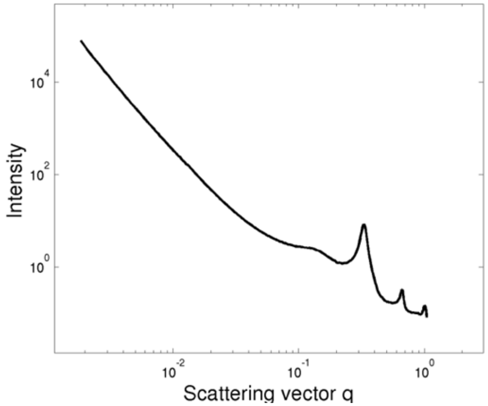
Stack size estimation (IE)
Perchlorate samples



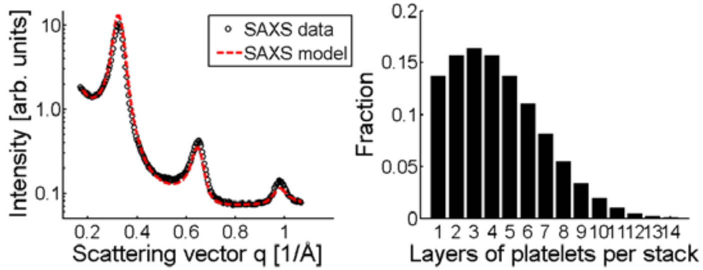


Part I: uncertainties (1)

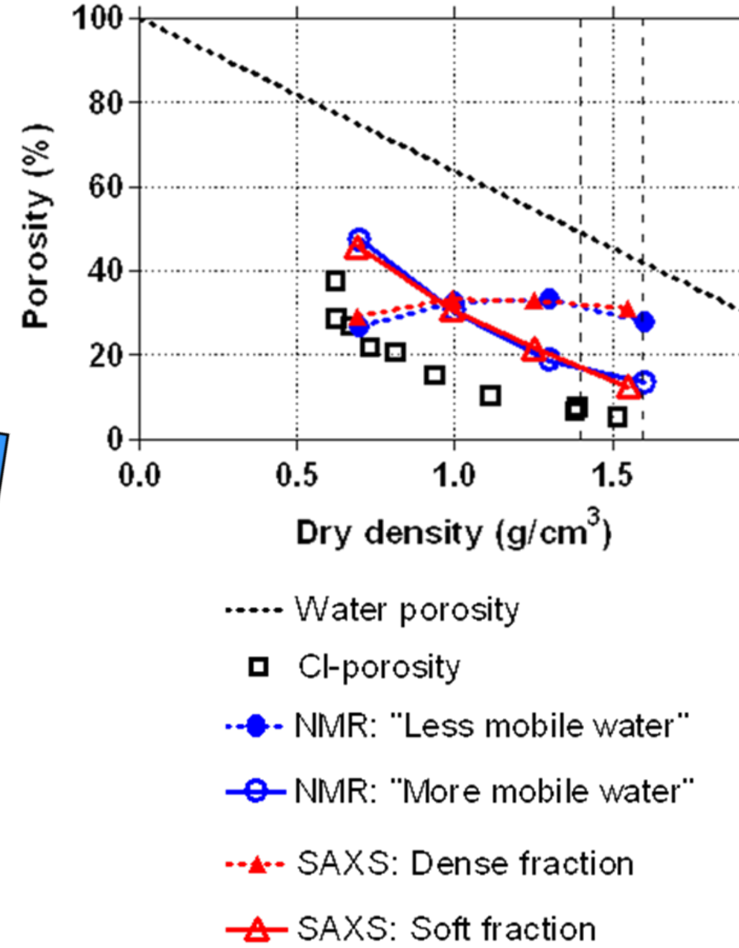
SAXS



structural model

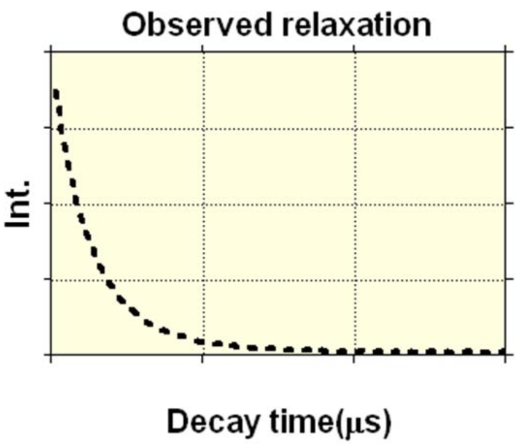


final results

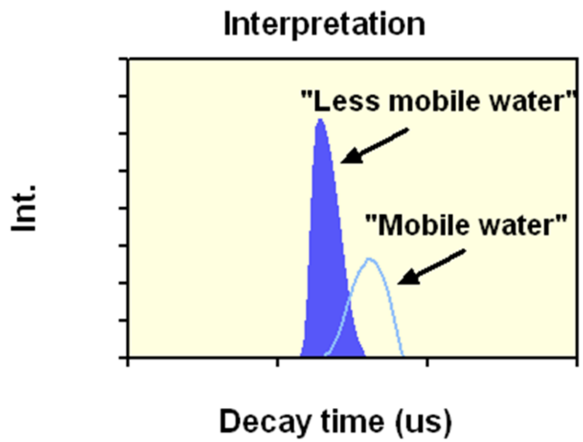


experiments

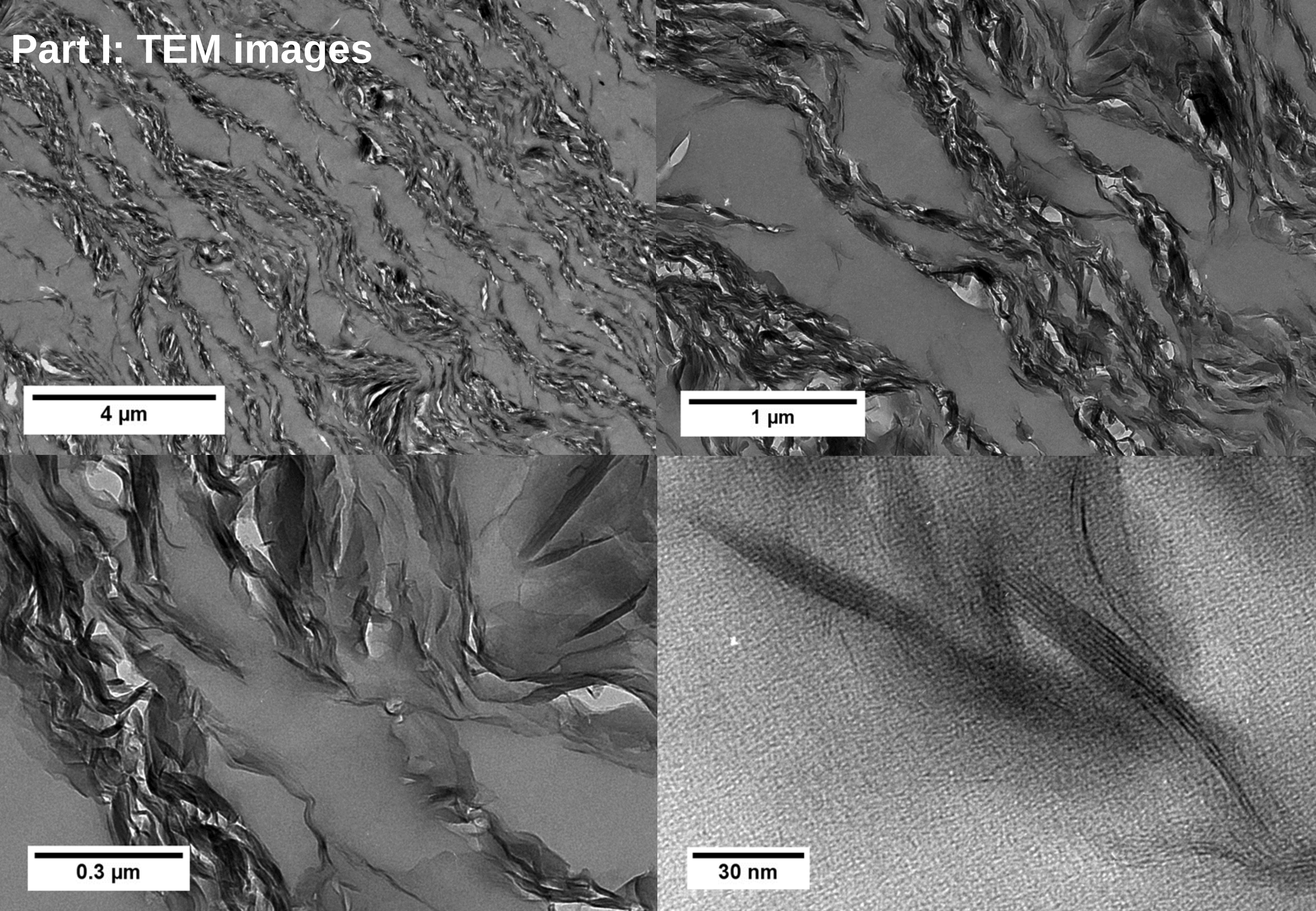
"model"



NMR



intrepretation of relaxation time


Part I: TEM images
4 μm
1 μm
0.3 μm
30 nm

Part I: uncertainties (2)

Artifacts due to the sample preparation

- opening a sample
  - → de-stressing
  - → changes in microstructure?
- drying of the samples

Part I: next

Same test program as earlier but samples prepared differently

- samples first compacted to ρ_{dry} = 1.8 g/cm^3 (emplacement density)
- let samples swell to target density
- why?
  - to see what happens in swelling
  - compacting = ”making intergranular space smaller”

Swelling sample: SAXS, XRD?

- mimicking slit experiments

Part II: modelling

Goal: model the slit experiments

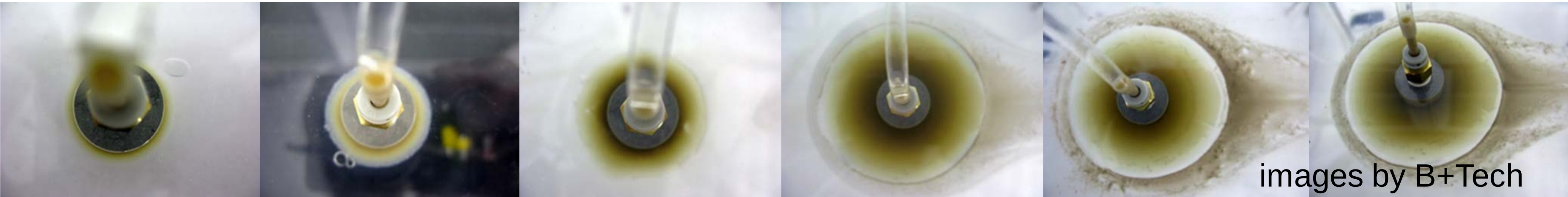
- why? comparison between model and reality

Problem: slit experiments are not only erosion experiments

- wetting
- swelling
- erosion

} at the same time

→ model has to be able to handle all these parts



images by B+Tech

Part II: pieces of the model

Mechanical model

- sets the geometry

Wetting model

Effect of salinity

- erosion

→all of them coupled

Part II: mechanical model

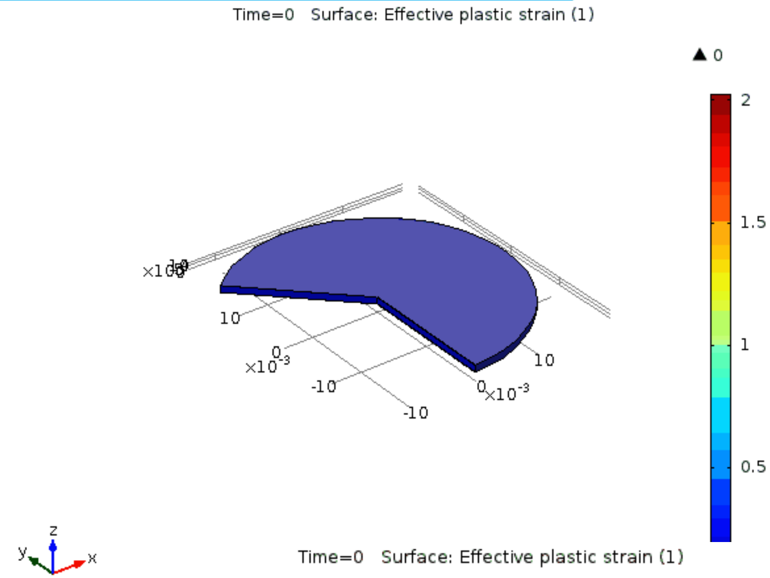
Elasto-plastic model (gel?)

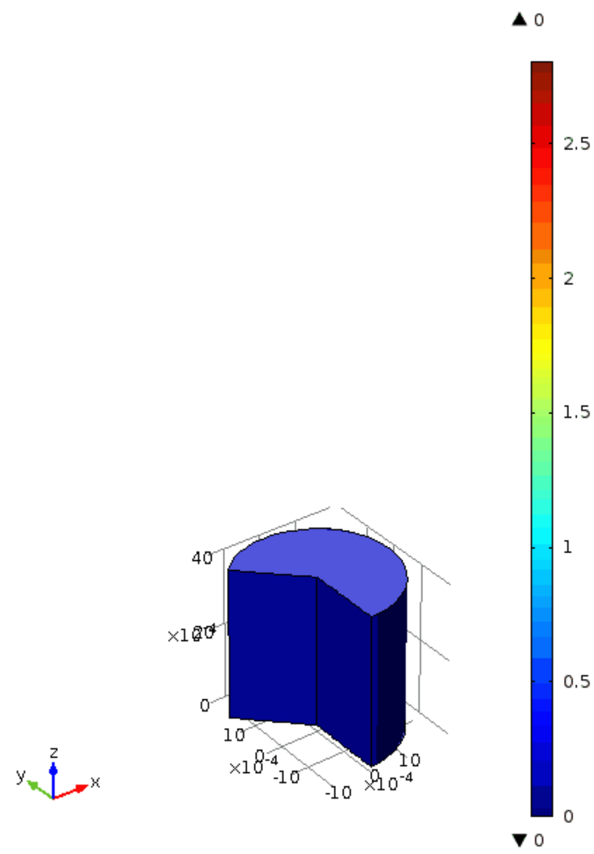
Sets the geometry

→ large deformations have to be included

Experimental work done at

- University of Jyväskylä (Markku Kataja et. al.)
- Claytech (Ann Dueck et. al.)
    - is it possible to have data (in numerical form) of e.g. TR-10-32?
- elsewhere?





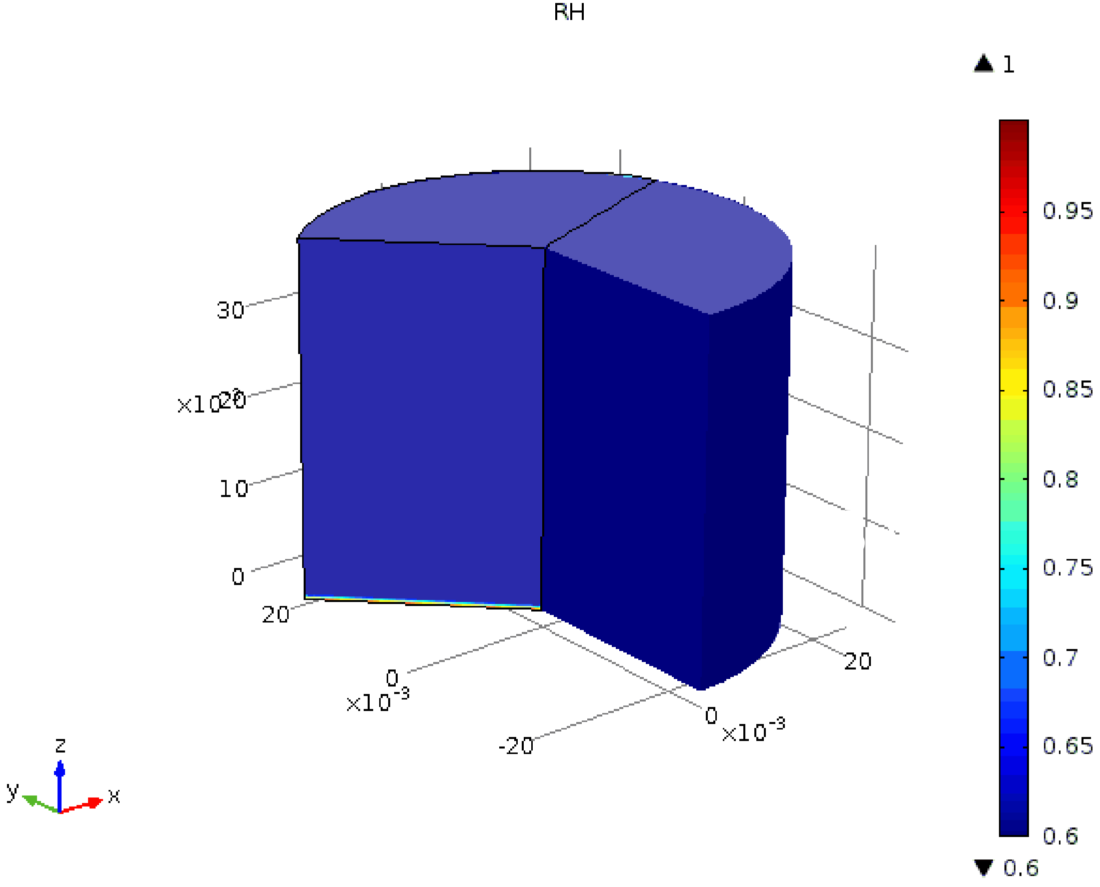
Part II: wetting model

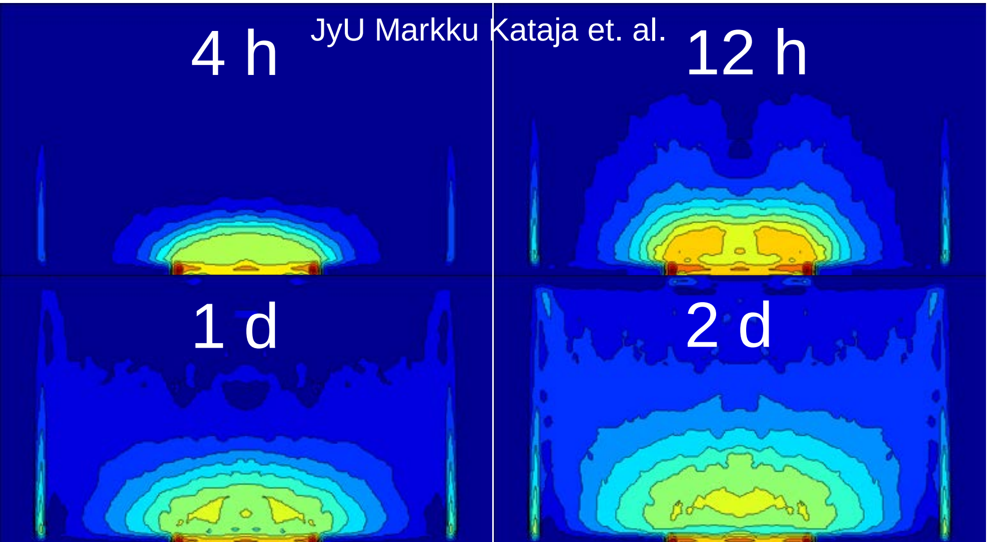
fast component

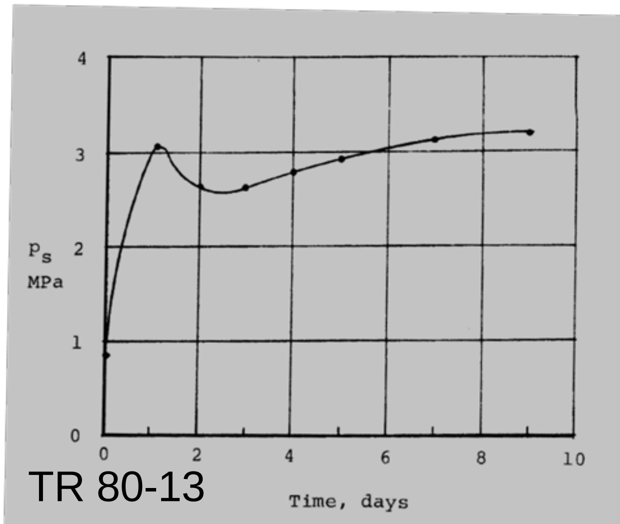
- vapour diffusion + absorption?
- absorption experiments at Claytech:
  - TR-10-55

slow component

- liquid water
  - salinity







TR 80-13

Part II: effects of salinity

Salinity of water and type of interlamellar cations affect

- rate of wetting
- rate of swelling
- swelling stress
- final chemical composition of bentonite (before erosion)
- cohesion of bentonite

    low salinity → erosion

Is time-dependent data from swelling stress experiments available? (p=p(t))

Thank you!