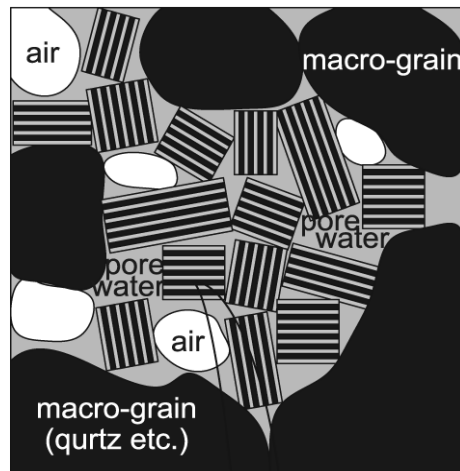



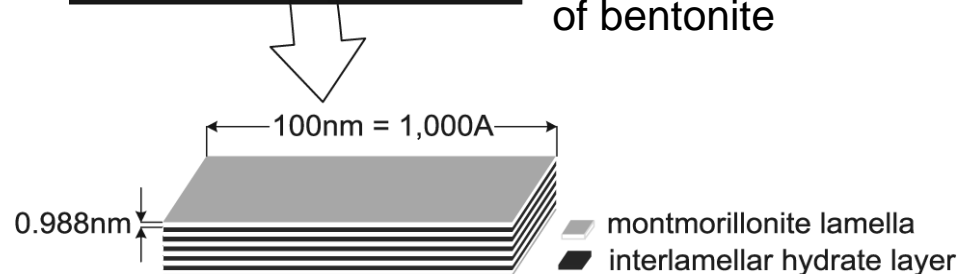
Colloid Stability of Dispersions of Calcium Dominated Bentonites

Longcheng Liu, Luis Moreno, Ivars Neretnieks



 A stack of montmorillonite lamellae

Microscopic structure of bentonite



BELBAR WP4

- MX-80 (Na-bentonite)
- Deponit CA-N (Ca-bentonite)



Objectives

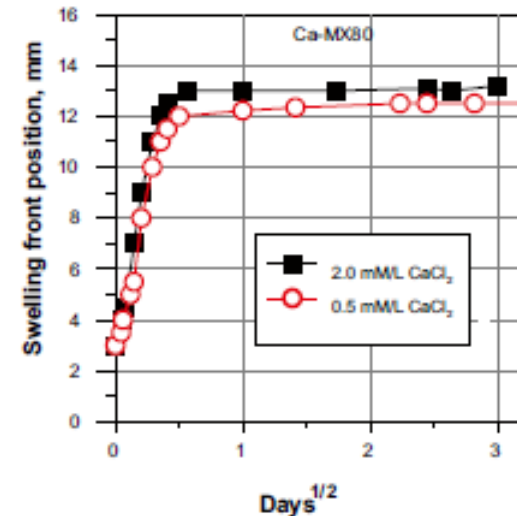
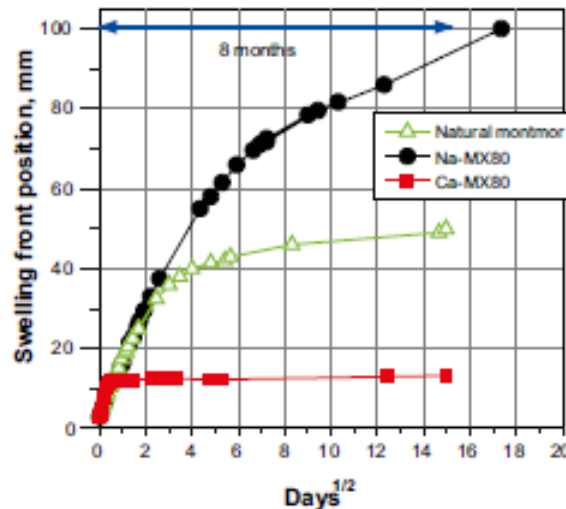
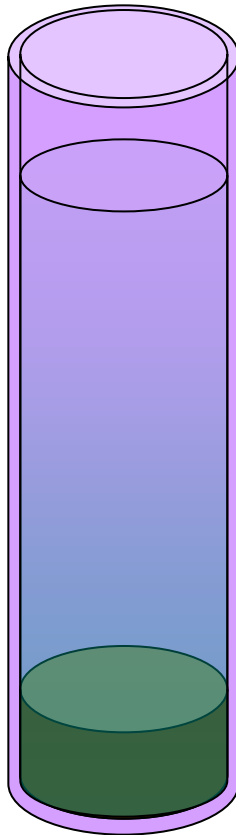
To understand the mechanisms and to develop models that govern or account for

- Stack formation and properties**
- Swelling behavior and properties**
- Rheological behavior and properties**
- Impact of water chemistry**
- Impact of accessory minerals**

Motivation

Dvinskikh & Furó, 2009

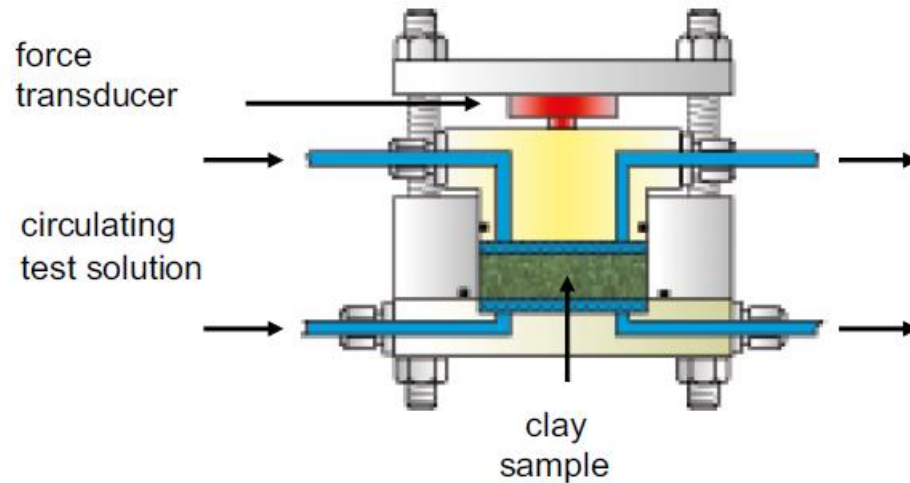
$\Delta V/V \approx 300\%$ for Ca-bentonite compacted



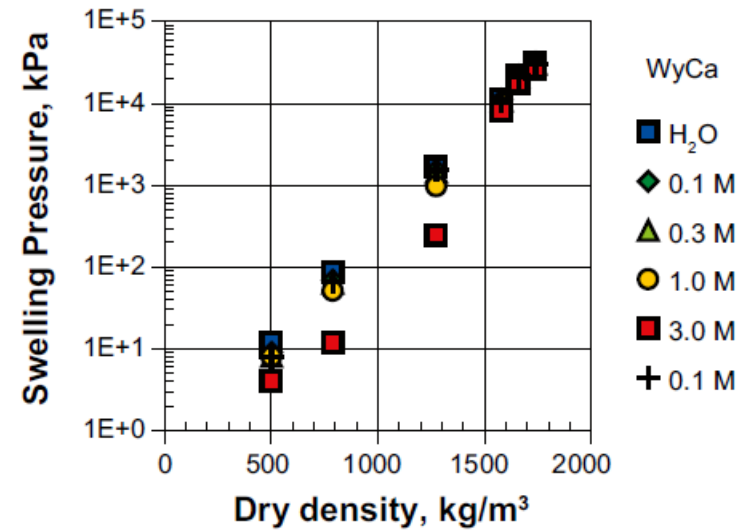
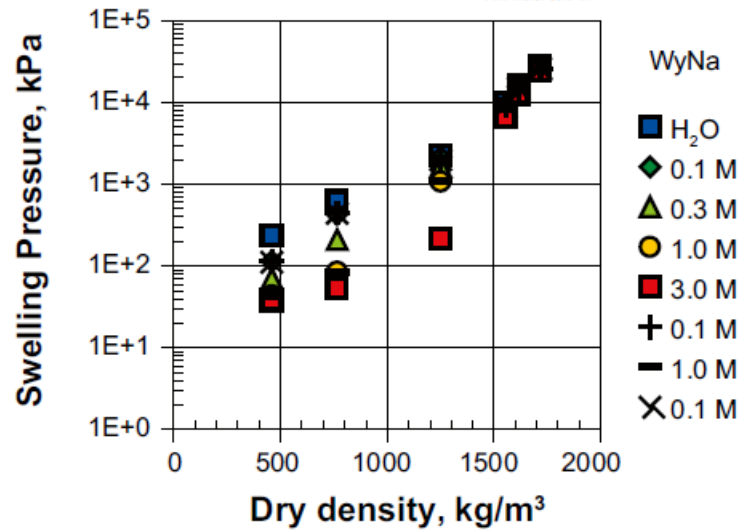
Mielenz & King, 1955

$\Delta V/V \approx 45 \sim 145\%$ for Ca-bentonite in powder

Motivation



Karnland et al., 2006

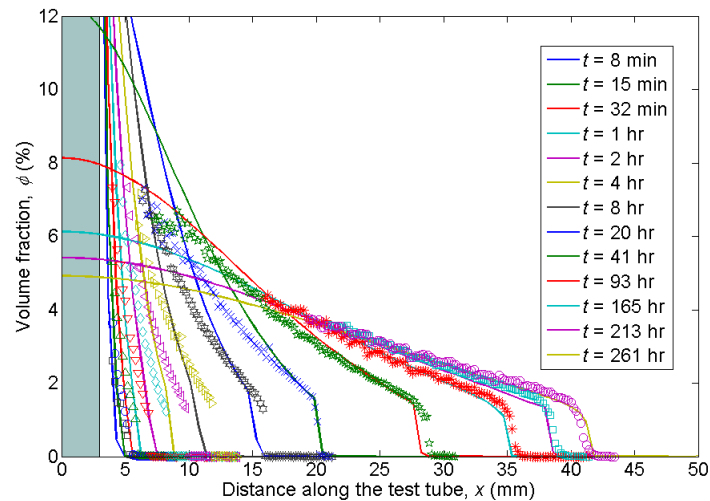


Motivation

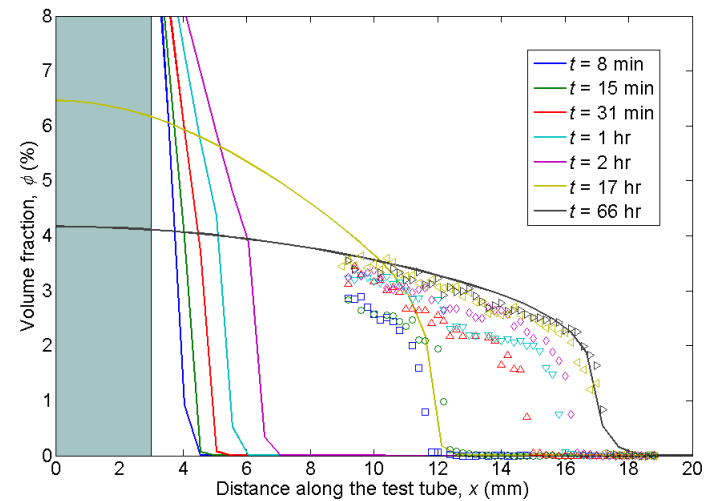
A force balance model (Liu et al., Langmuir, 2009)

$$\frac{\partial \phi}{\partial t} = \frac{\partial}{\partial x} \left\{ -\phi \left(F_s \frac{\phi}{f} + D_F \frac{\partial \phi}{\partial x} \right) \right\}$$

$$D_F = \frac{k_B T}{f} - \frac{\delta_p \phi_{\max}}{f} \left(\frac{\partial F_A}{\partial \phi} - \frac{\partial F_R}{\partial \phi} \right)$$



Na-bentonite in distilled water

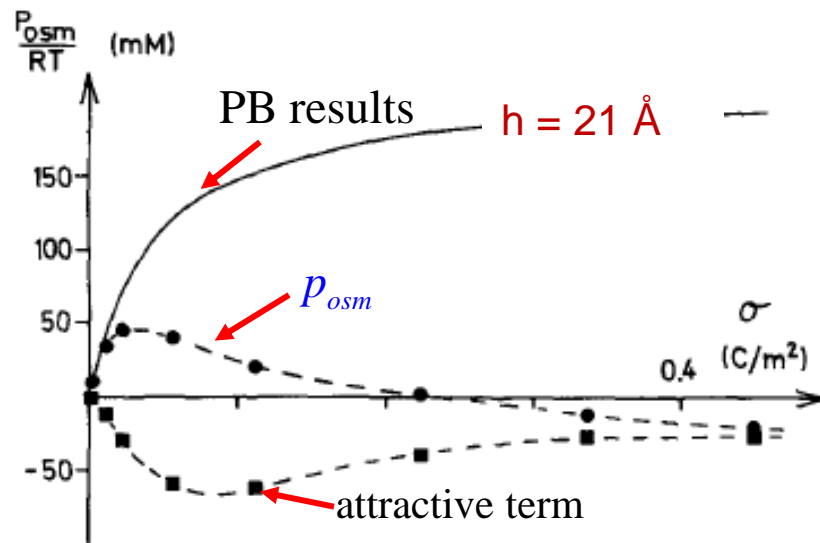


Ca-bentonite in distilled water

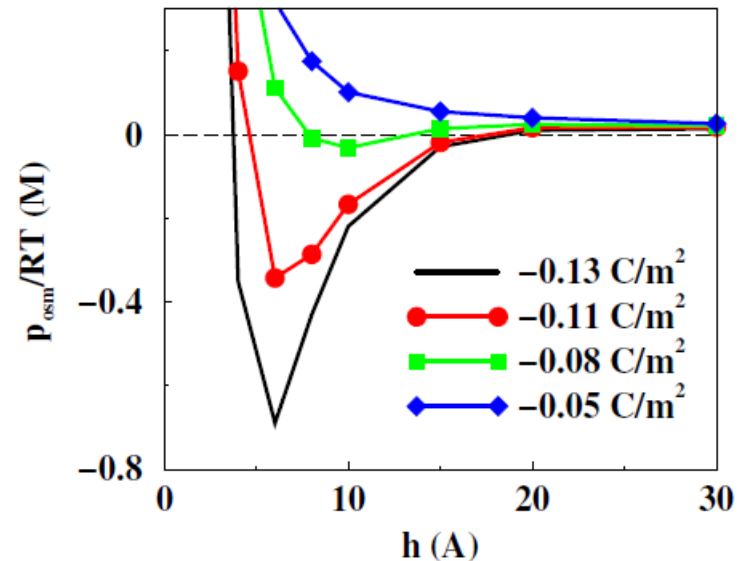
Motivation

Interaction between two lamellas – MC simulations

In salt free system



Guldbrand et al., 1984

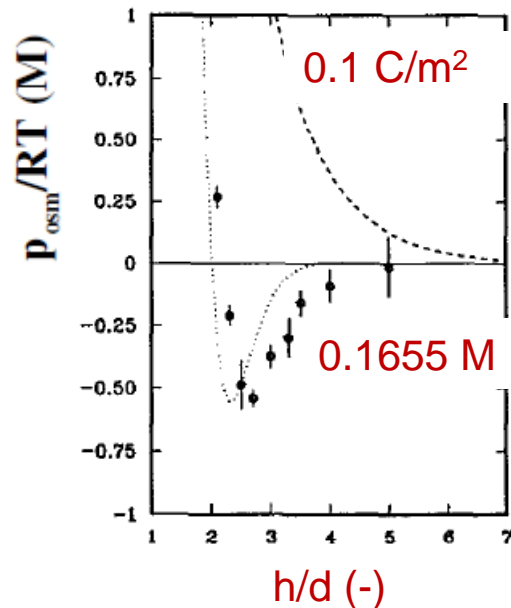


Segad et al., 2010

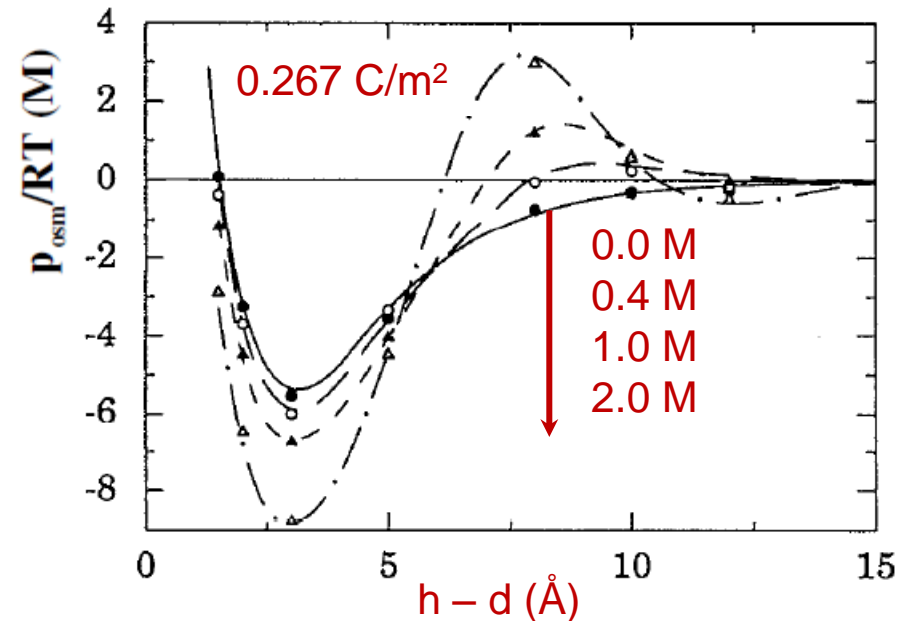
Motivation

Interaction between two lamellas – Theoretical studies

In 2:2 salt system



Tang et al., 1992 (DFT)



Kjellander et al., 1992 (AHNC)

Swelling behavior

To develop

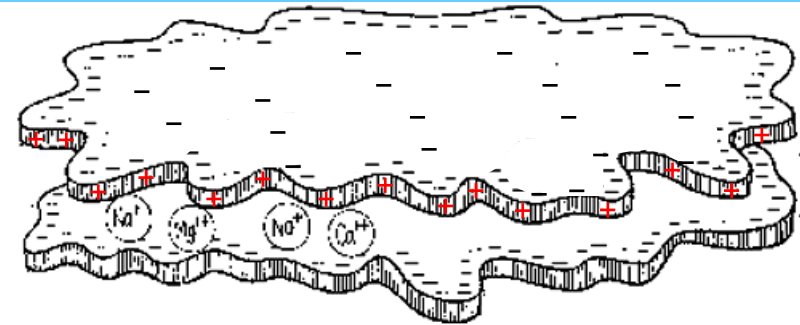
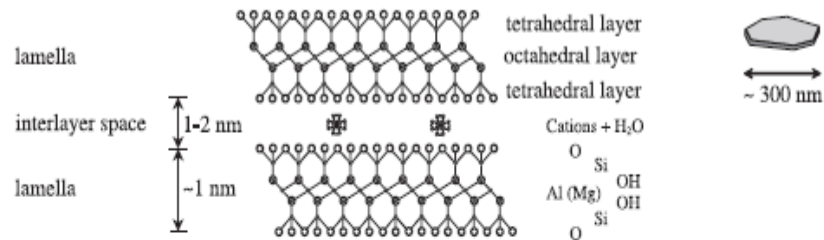
- A simple DLVO-based model by taking the particles as stacks of collapsed lamellas

To understand

- The cohesive/expansive properties
- The effects of mixed electrolytes
- The effects of particle arrangements
- The effects of dimensional heterogeneity

Stack Formation

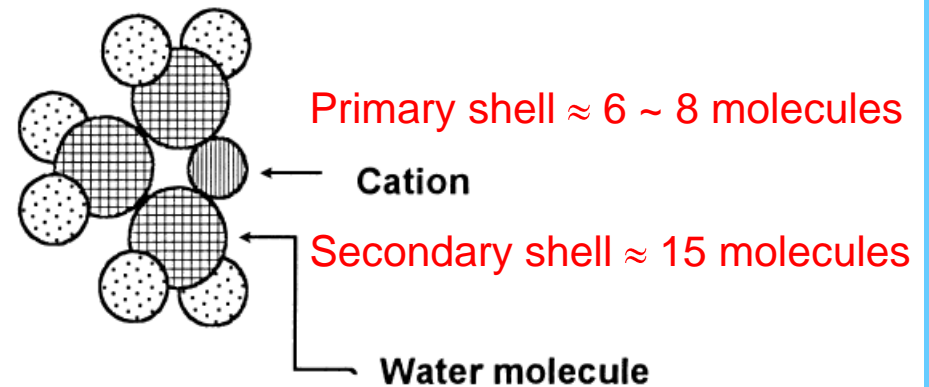
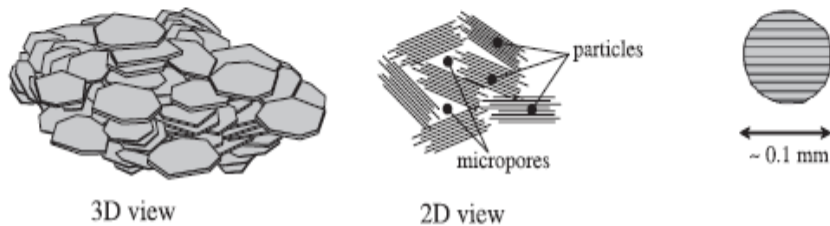
PARTICLE: stack of lamella



$d(001) \approx 1.89 \text{ nm}$ when fully saturated

$N(\text{lamella}) \approx 6 \sim 16$ per particle

GRAIN: anisotropic aggregate of particles

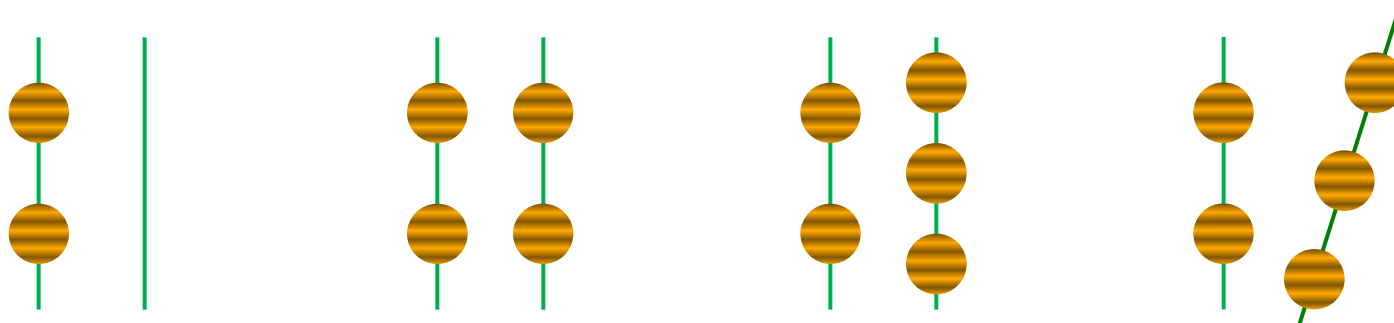


Stack Formation

Surface charge distribution



Surface arrangement



Stack Formation

To investigate the effects of

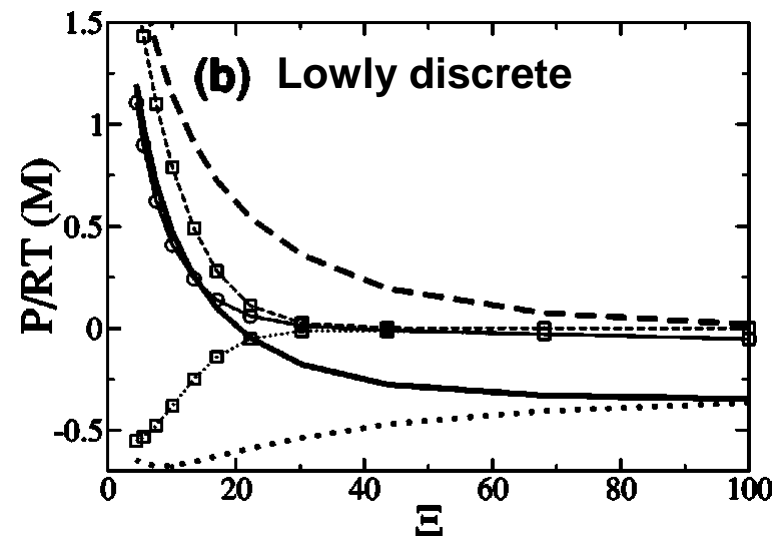
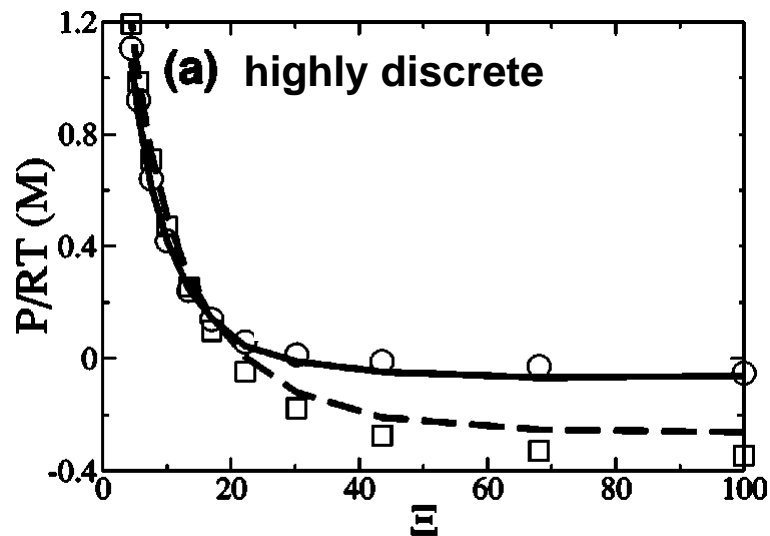
- Surface charge heterogeneity**
- Surface arrangement**
- Ionic sizes**
- Hydration shells**
- Mixed electrolytes**

by both Monte-Carlo simulations and the Weighted

Correlation Approach of the Density Functional Theory

Stack Formation

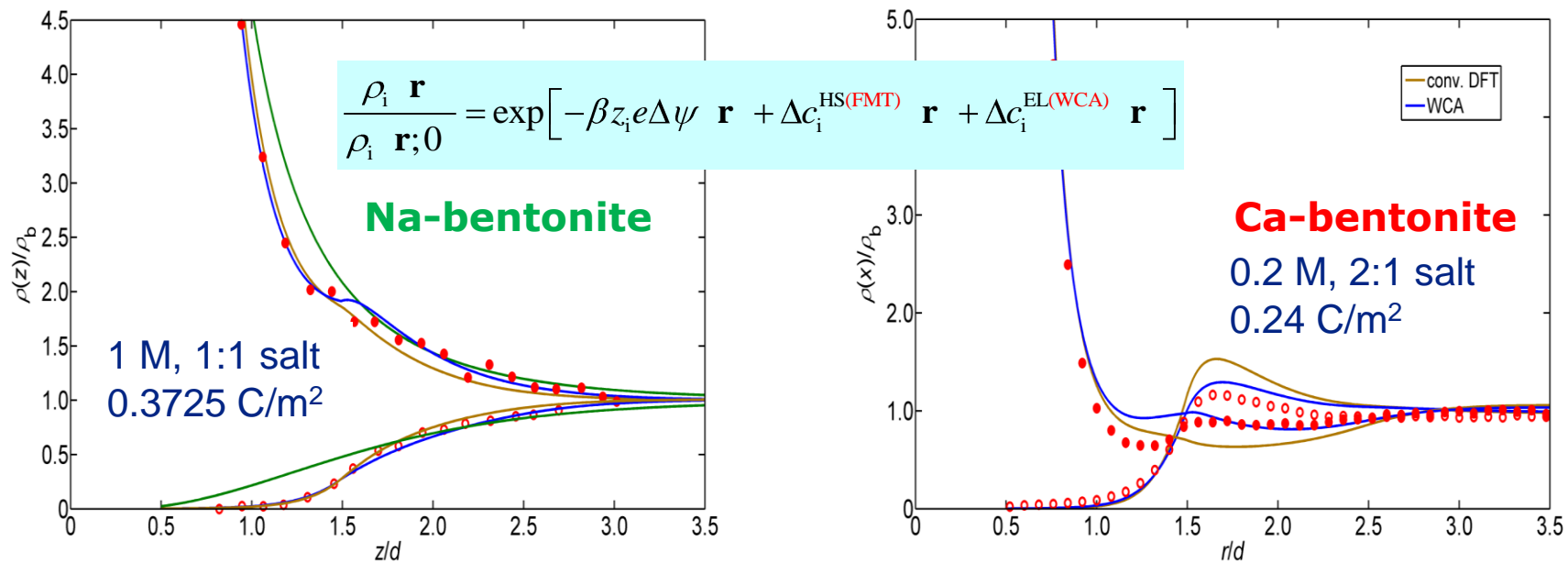
Monte Carlo simulations – discrete σ



□ The attractive force is weakened and can even be
truned into a repulsive force $z \propto z^3 \sigma$

Stack Formation

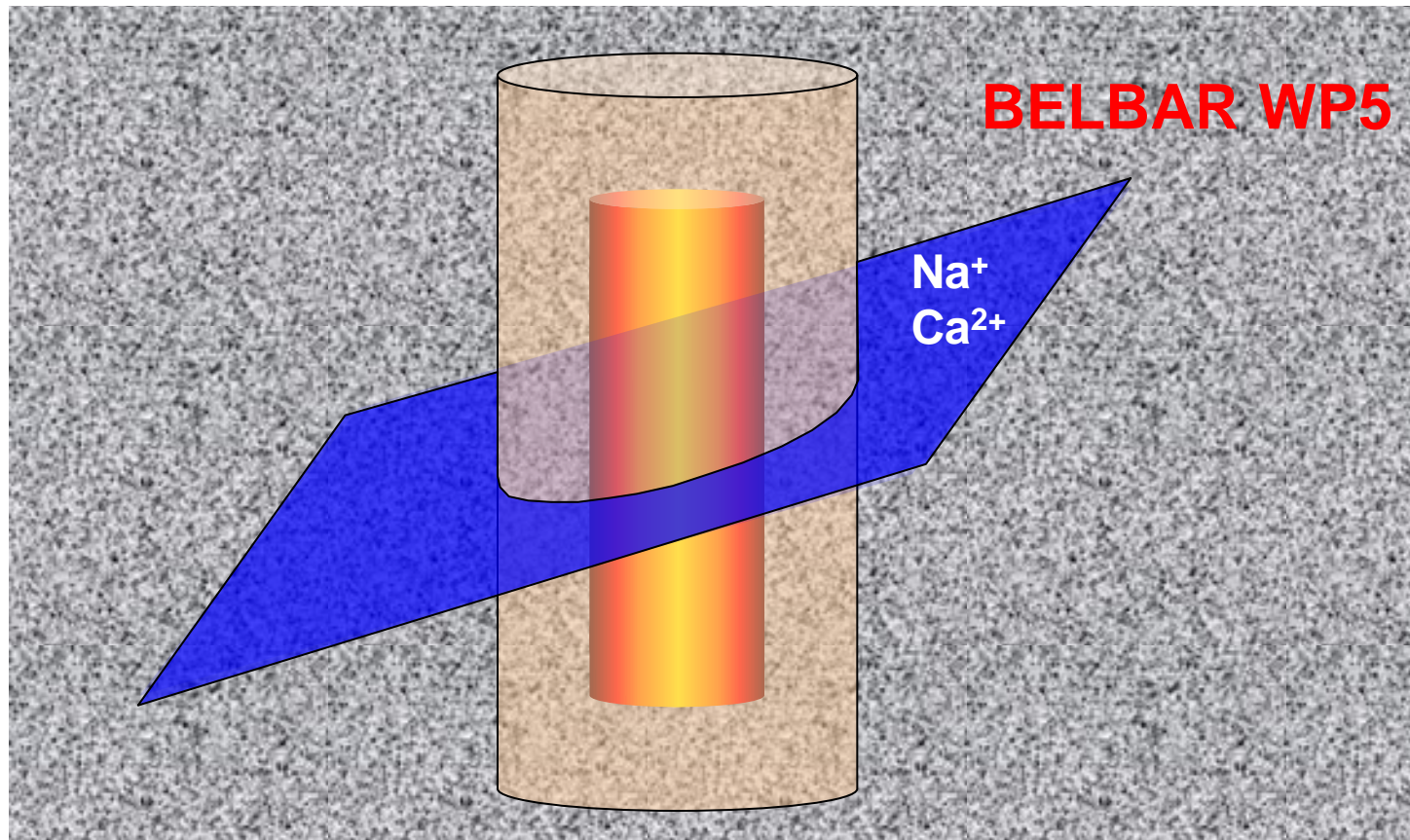
Weighted Correlation Approach



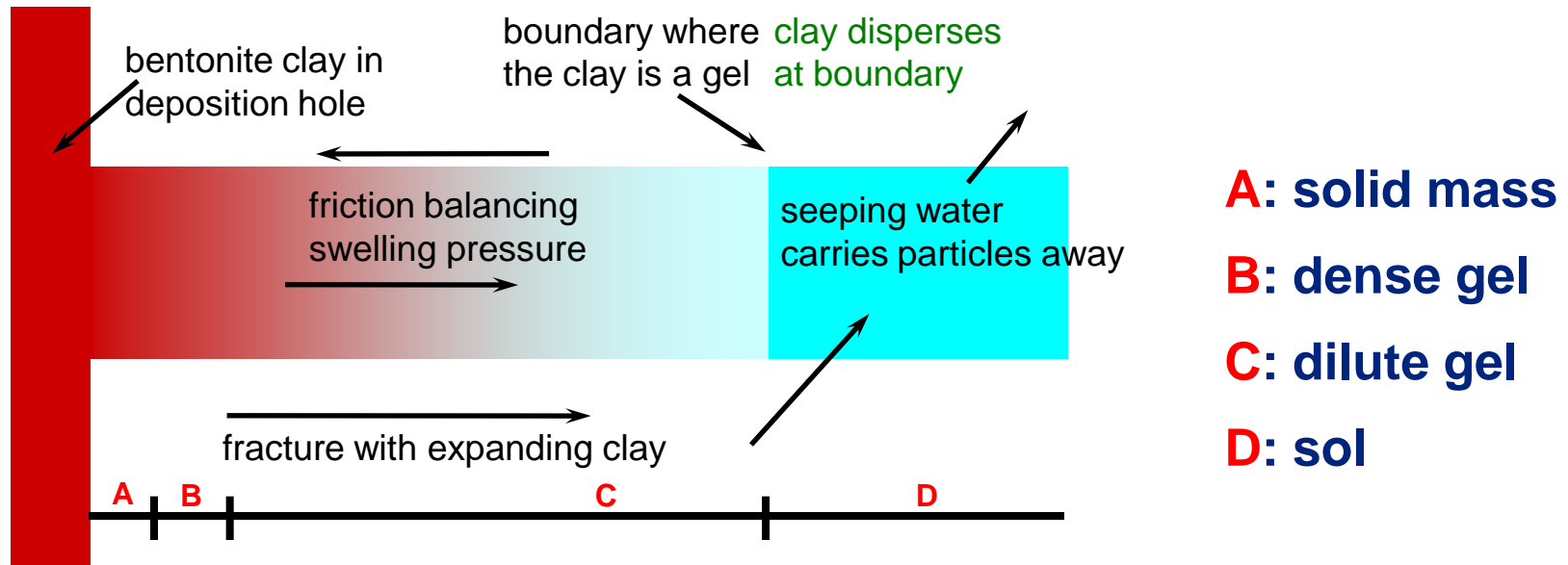
- ❑ To develop simple expressions for swelling pressure
- ❑ To gain insight into ion-ion correlations and other effects

Development of Conceptual and Mathematical Model for Bentonite Erosion under Repository Conditions

Longcheng Liu, Luis Moreno, Ivars Neretnieks



Transport Processes



To assess the rate of bentonite erosion

➤ MX-80 (Na-bentonite)

➤ Non-saline groundwater ($c \ll C.C.C$)

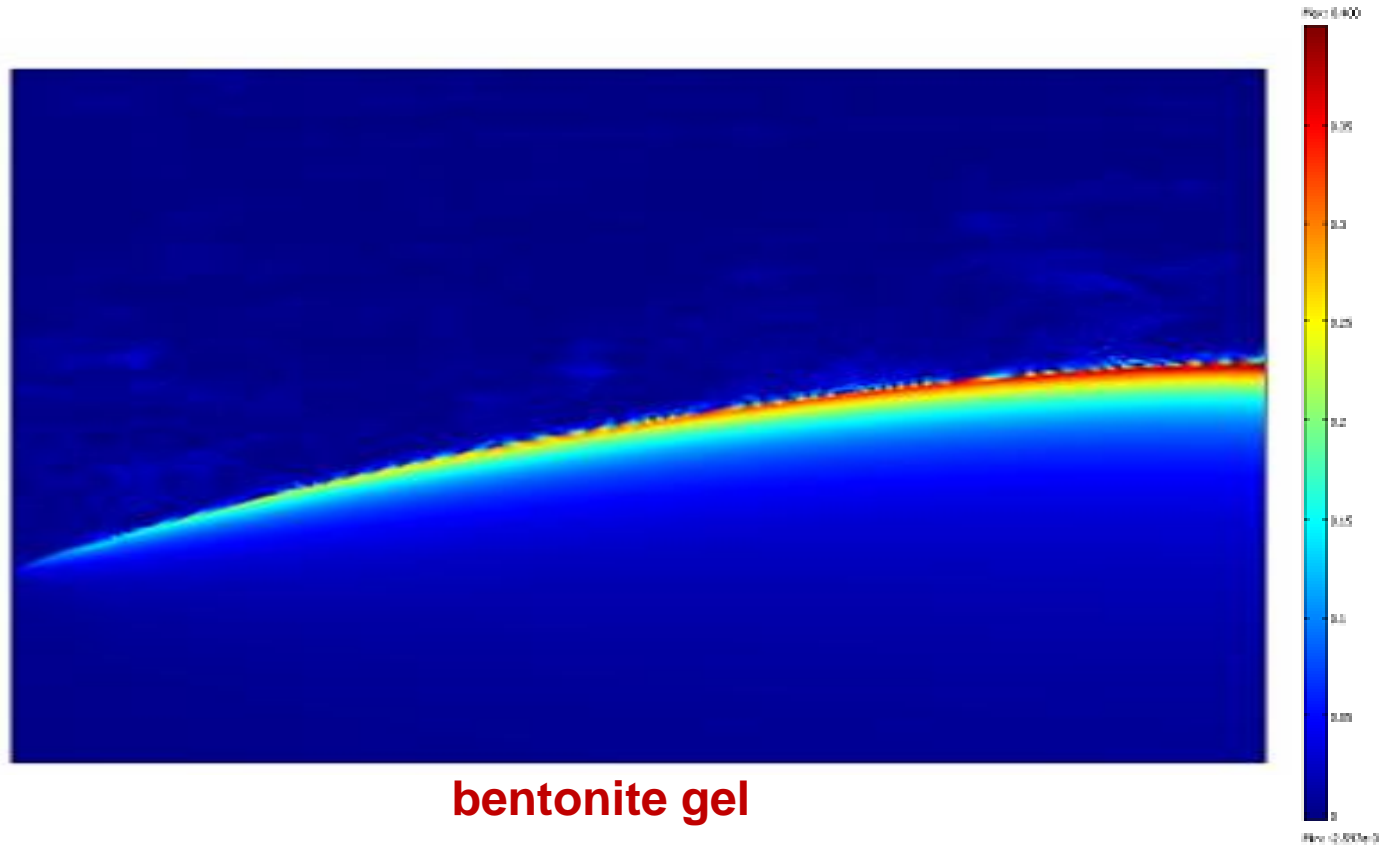
{ glacial melt water
 fresh meteoric water

Motivation

To improve/validate the transport model developed previously that accounts for

- The swelling behavior (a force balance model)
- The rheological behavior (a viscosity model)
- The ionic diffusion (impact of water chemistry)
- The volume-fraction dependence of diffusion
- The water seepage (Darcy's law)

Release Flux Distribution



bentonite gel

Objective

To investigate the effects of

- Chemistry evolution of pore water**
- Mass transfer of solutes at gel/sol interface**
- Release of colloids and stacks to flowing water**
- DDL properties of Ca rich system**
- Variable aperture fractures**

by refining/simplifying the model against experimental evidences, to make it running fast and stable

What do we need

To understand important mechanisms involved and to validate/refine the models

□ Experimental results on swelling behavior

□ Experimental results on bentonite erosion

□ Experimental results on chemical evolution

□ Experimental results on gel visvosity

Look forward for co-operation with groups working in experiments, as we will not make extensive experiments