粘土の微視特性と巨視挙動

地盤工学会（広島）
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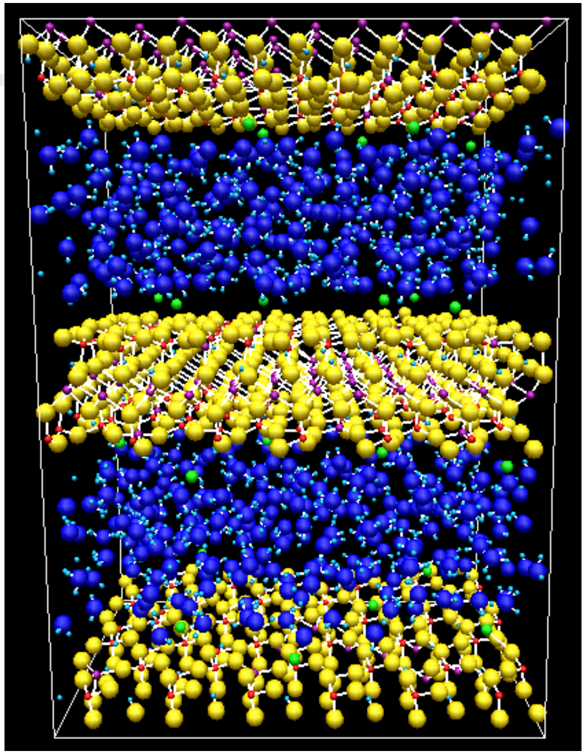
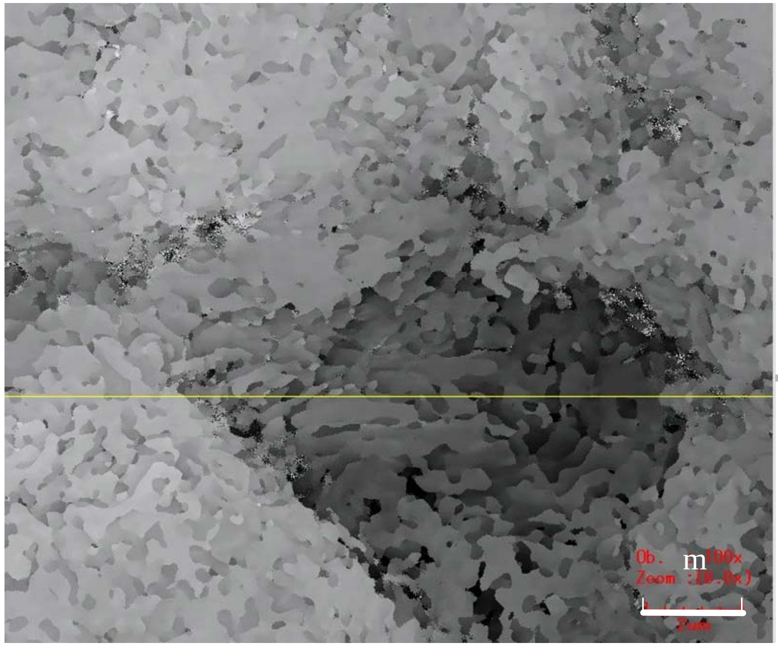


Montmorillonite Hydrate with 8.0 H_2O

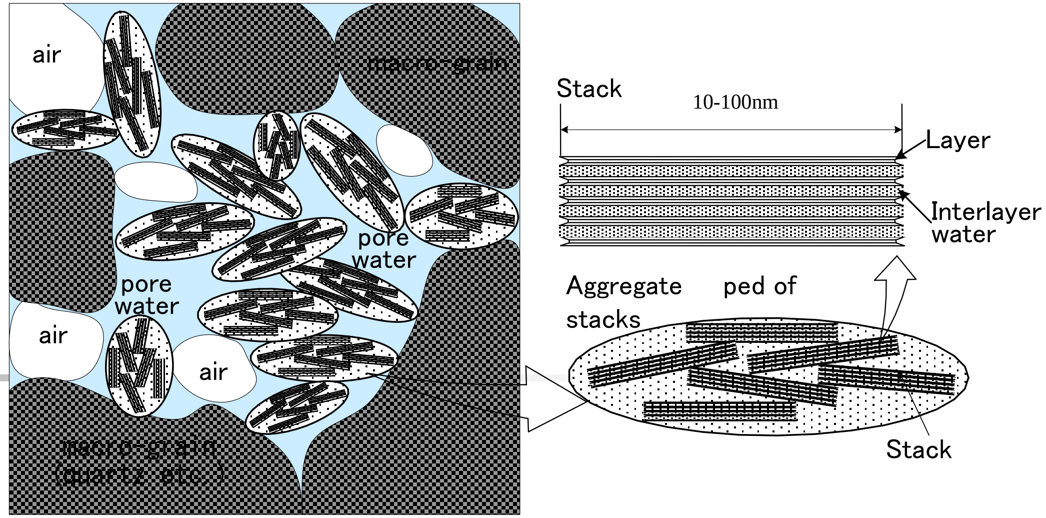
Aim of Research

Detection of the true mechanism of chemical process, water flow and deformation/fracturing based on

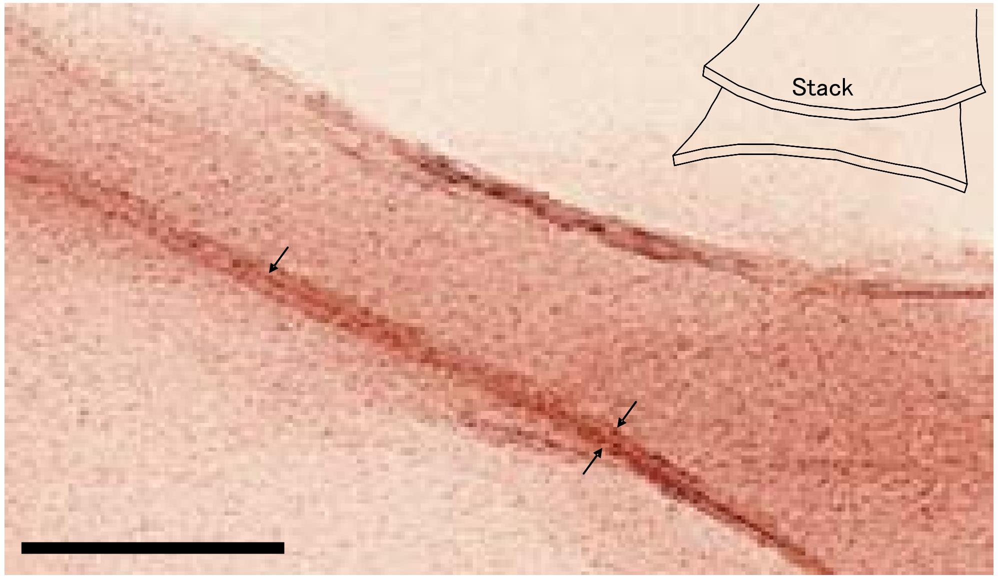
molecular simulation, and micro/macro multiscale homogenization analysis.



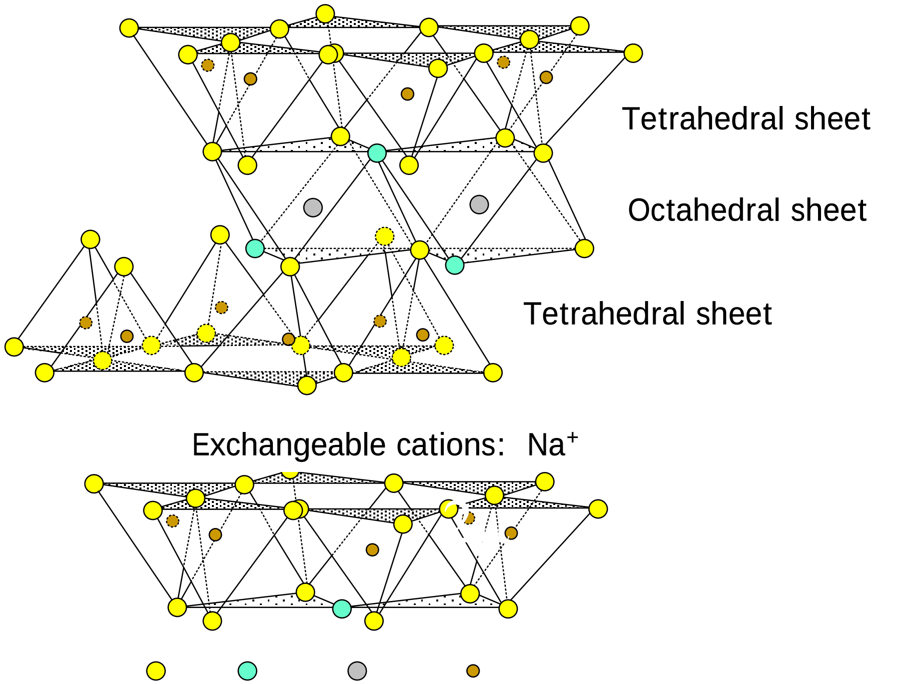
CLSM image



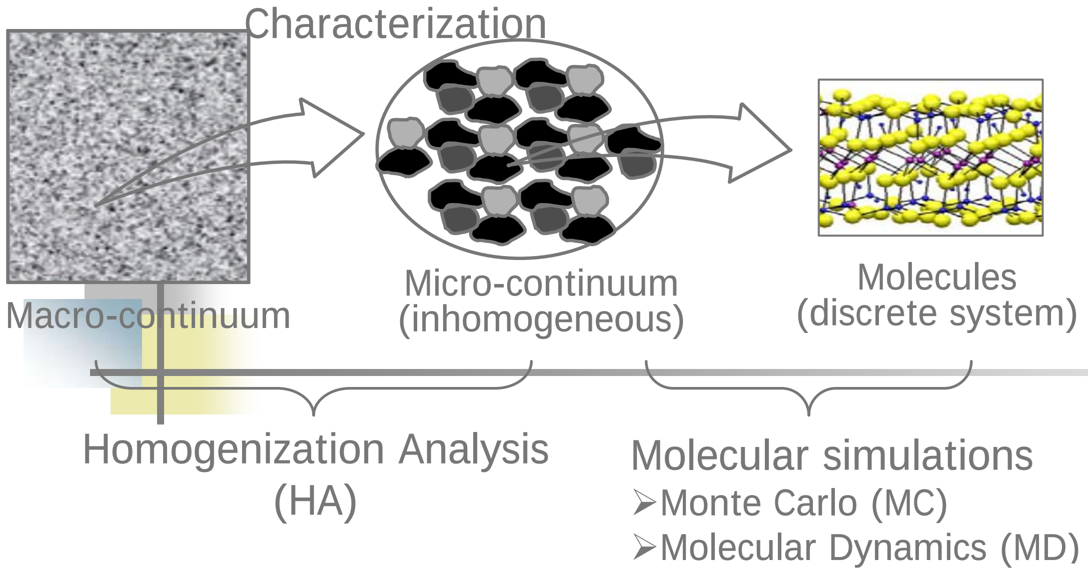
Schematic diagram of bentonite

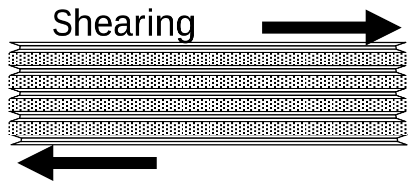


TEM image

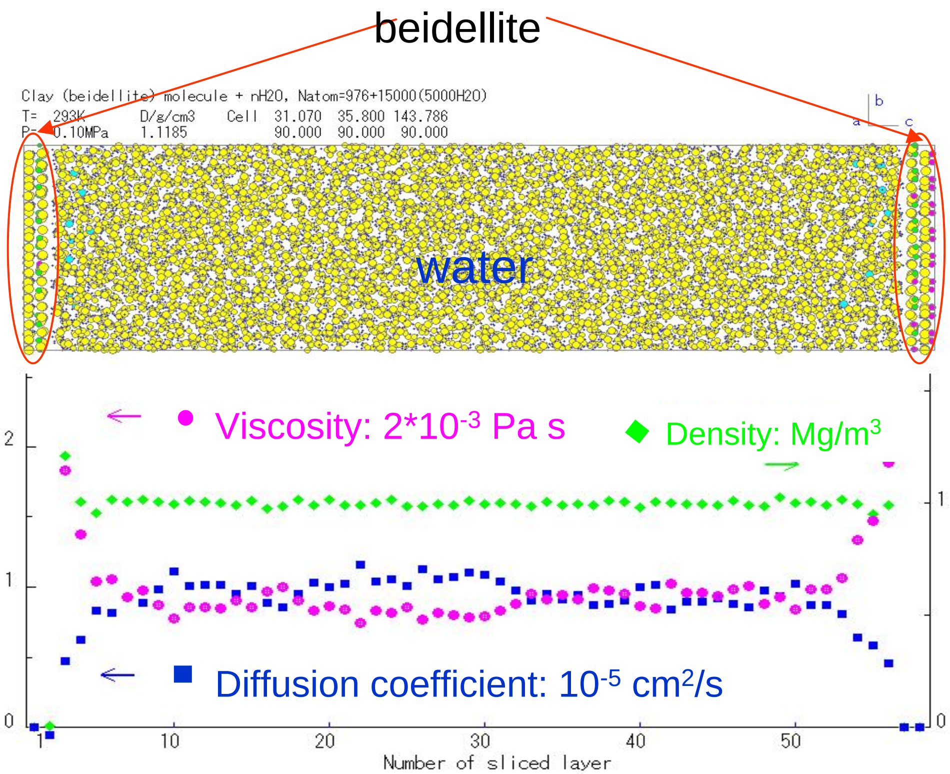


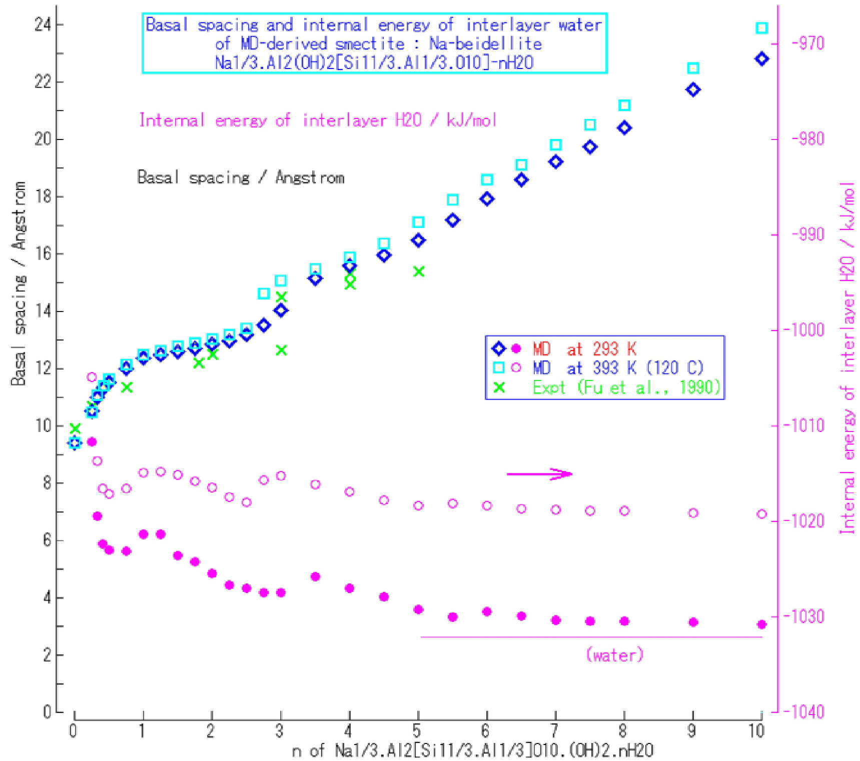
Atomic structure of smectite



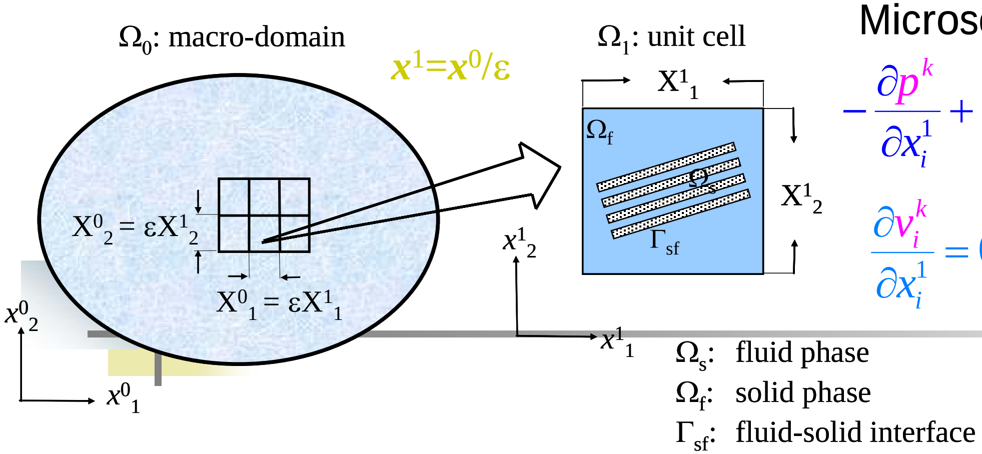


The viscosity of a stack (8x10^{-3} Pa s) is about ten times of water, which does not affect to a long-term deformation.





Swelling



Macroscale problem Microscale problem

Multiscale Homogenization Analysis (HA)

Microscale Equation

$$-\frac{\partial p^k}{\partial x_i^1} + \frac{\partial}{\partial x_j^1}\left(\mu \frac{\partial v_i^k}{\partial x_j^1}\right) + \delta_{ik} = 0$$

$$\frac{\partial v_i^k}{\partial x_i^1} = 0$$

By MD

HA-Daycy's Law

$$\tilde{V}_i^0(\boldsymbol{x}^0) = \langle V_i^0 \rangle = -K_{ij}\left(\frac{\partial P^0}{\partial x_j^0} - F_j\right)$$

$$K_{ij} = \langle v_j^i \rangle = \frac{1}{|\Omega_1|}\int_{\Omega_1} v_j^i \, d\boldsymbol{x}^1$$

Macroscale Seepage Equation

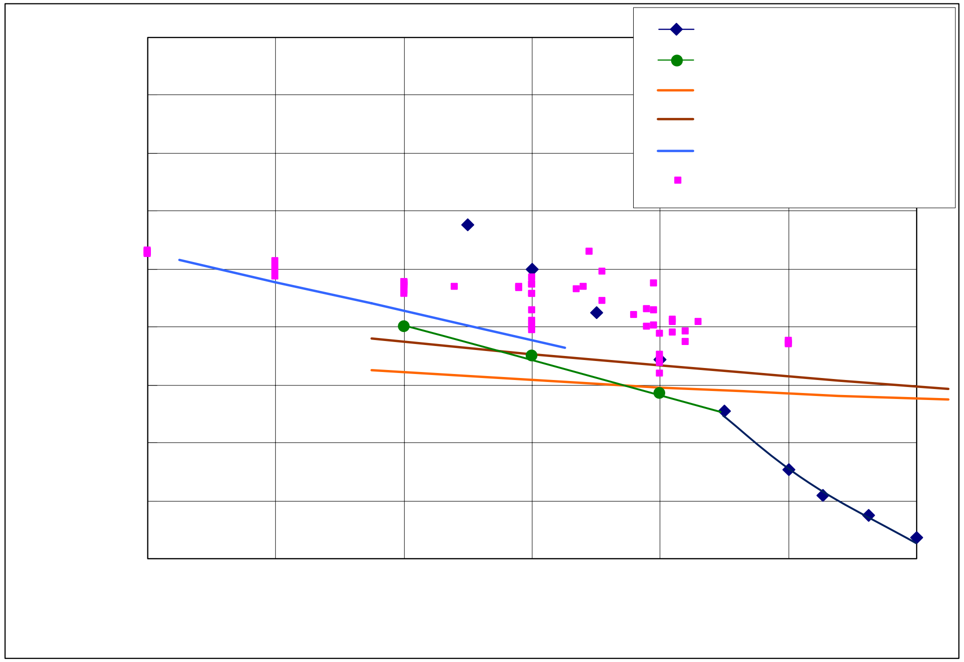
$$-\frac{\partial}{\partial x_i^0}\left\{K_{ij}\left(\frac{\partial P^0}{\partial x_j^0} - F_j\right)\right\} = 0 \quad \text{in } \Omega_0$$

True velocity and pressure

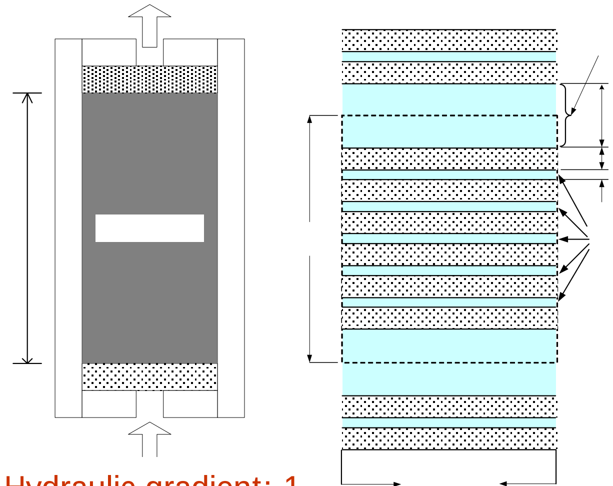
$$V_i^\varepsilon(\boldsymbol{x}) \cong \varepsilon^2 V_i^0(\boldsymbol{x}^0, \boldsymbol{x}^1), \qquad P^\varepsilon(\boldsymbol{x}) \cong P^0(\boldsymbol{x}^0)$$

Conventional vs HA-permeability

$$K_{ij}^* = \varepsilon^2 \rho g K_{ij}$$



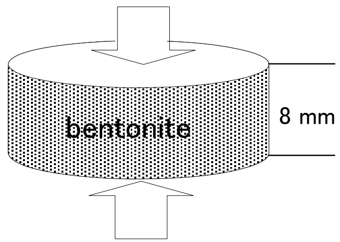
Seepage problem

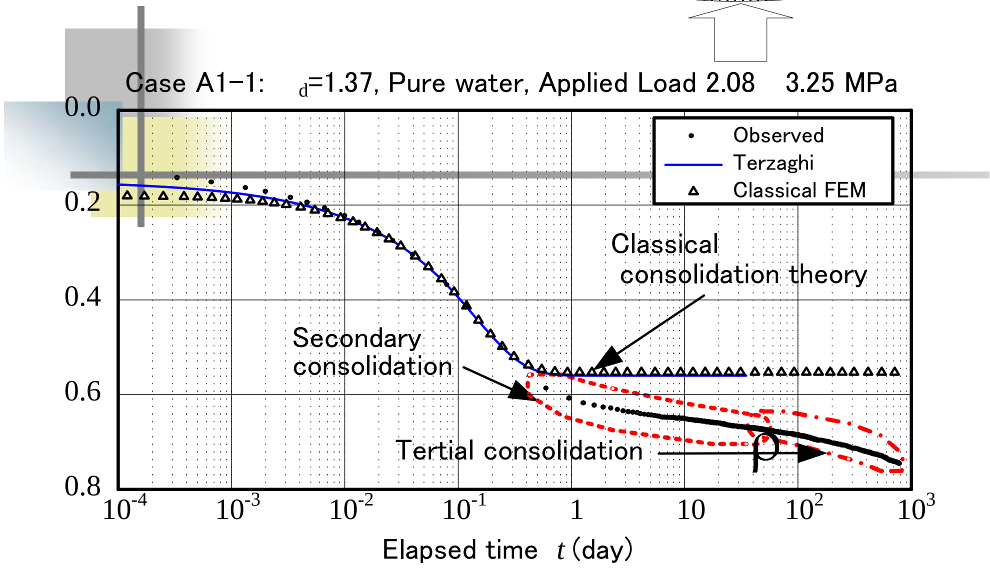


Hydraulic gradient: 1

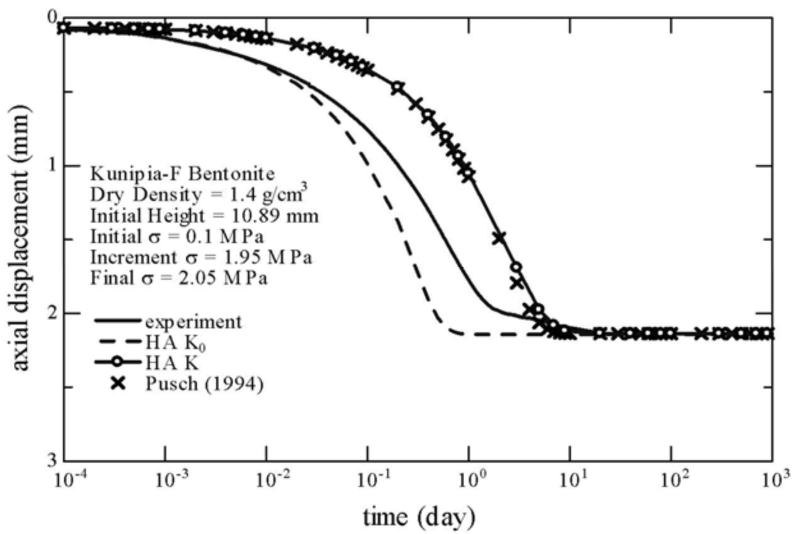
Peclet number: 0.14 – 1.34x10^{-14}

Long-term consolidation test

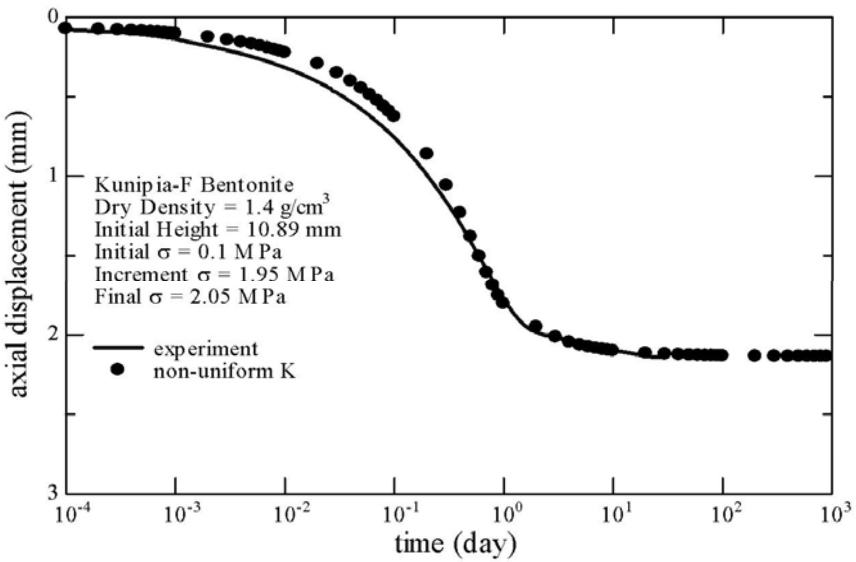


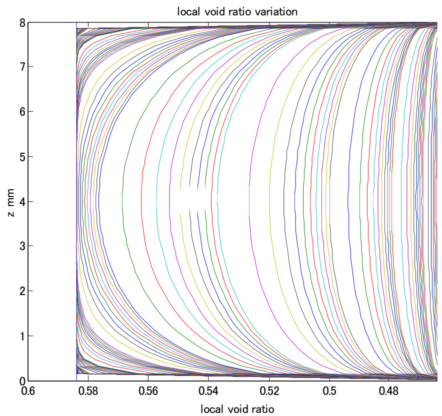


K: homogeneous

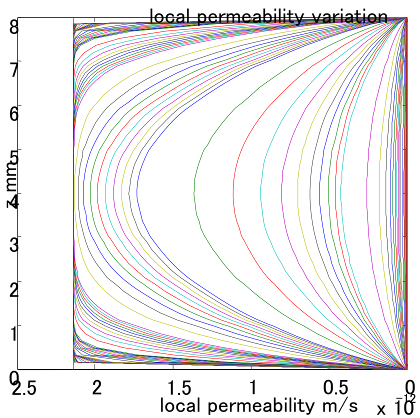


MD/HA



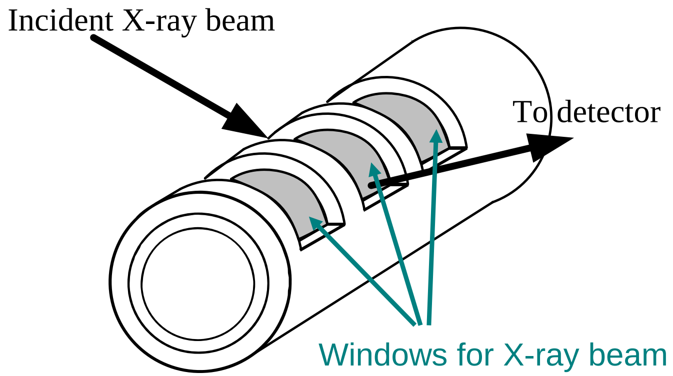


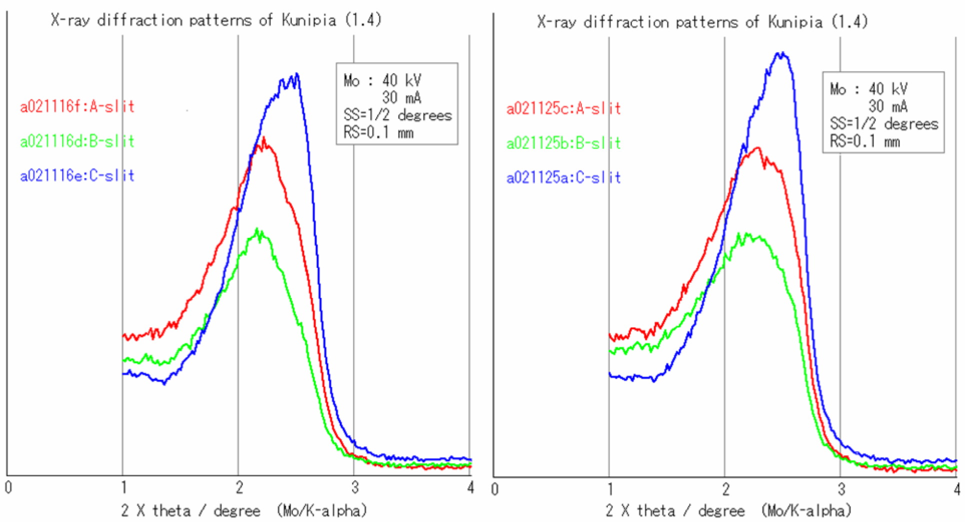
Time change of void ratio



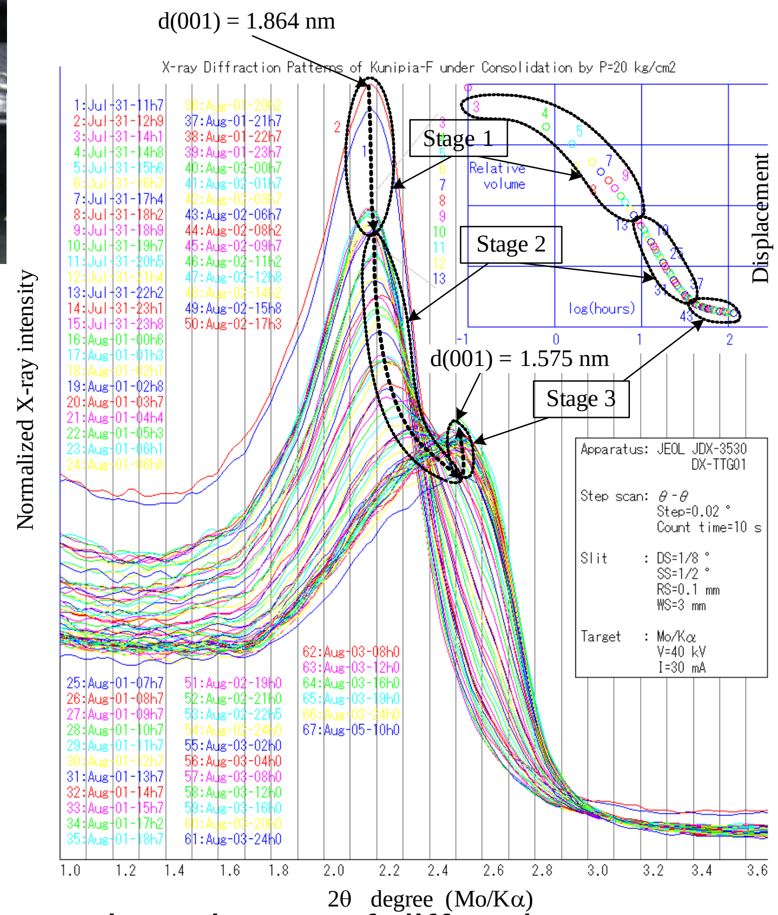
Time change of permeability

In-situ XRD Analysis





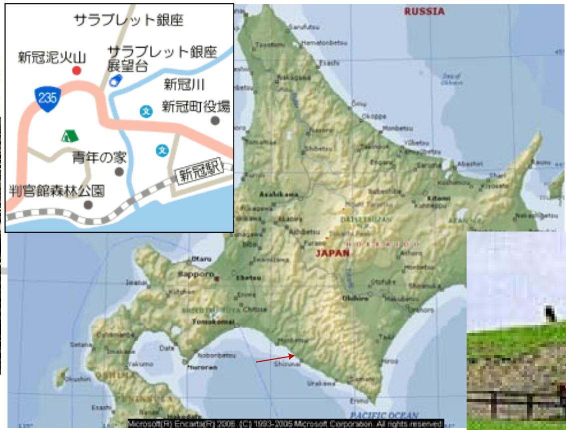
Diffraction patterns at different windows



Time-change of diffraction patterns

Mud volcano

Trinidad



Niikappu

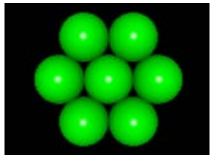
$$\frac{d\varepsilon_v}{dt} + \frac{\partial}{\partial x_j^0}\left(\varepsilon^2 \rho g K_{ij} \frac{\partial P^0}{\partial x_j^0}\right) = 0$$

Size of unit cell

Sand: 100μm-1mm

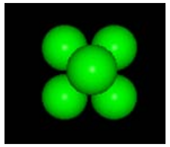
Clay: 0.1μm-1μm

Generating $d\varepsilon_v / dt$ due to dilatancy



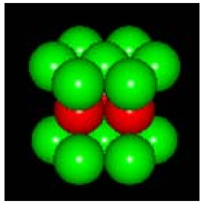
Surface centered: sc

Porosity n_0=0.48

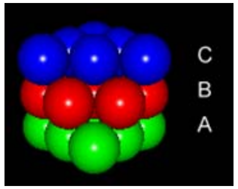


Body center cubic: bcc

Porosity n_1=0.32



Porosity n_2=0.26



Hexagonal closest packing: hcp

Cubic closest packing: ccp

Conclusions

- Clays: Micro-inhomogeneous porous materials
- Analysis of true physical & chemical behaviors in micro & macro domains
- Coupled Molecular Dynamics (MD) simulations for identifying nanoscale material properties & Homogenization Analysis (HA) for micro/macro-analysis
- Seepage, diffusion & consolidation problems
- Similitude law in micro/macro-analysis

  Bentonite is an extremely diffusion-dominant material ($Pe << 10^{-14}$).
- Submicron & molecular level of experimental verifications

  CLSM, SEM/TEM, XRD, NMR, ICP-AES/MS