Bentonite modelling at continuum level

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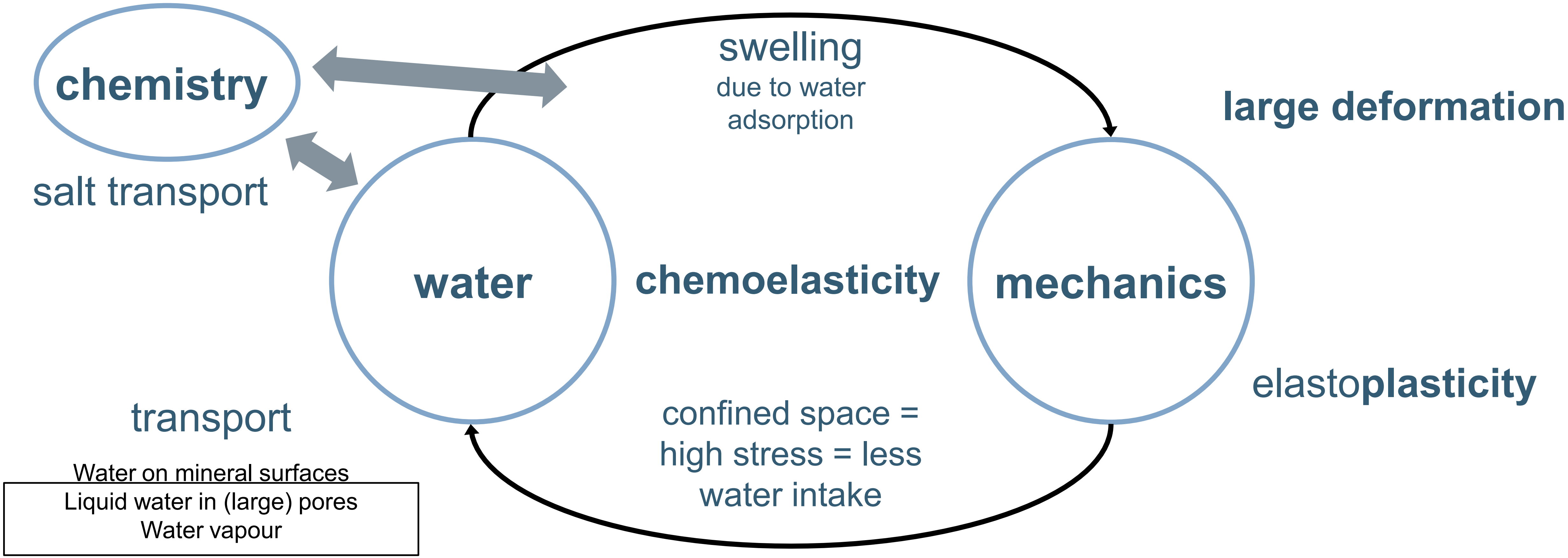
SAGE BENTONITE SEMINAR 2025

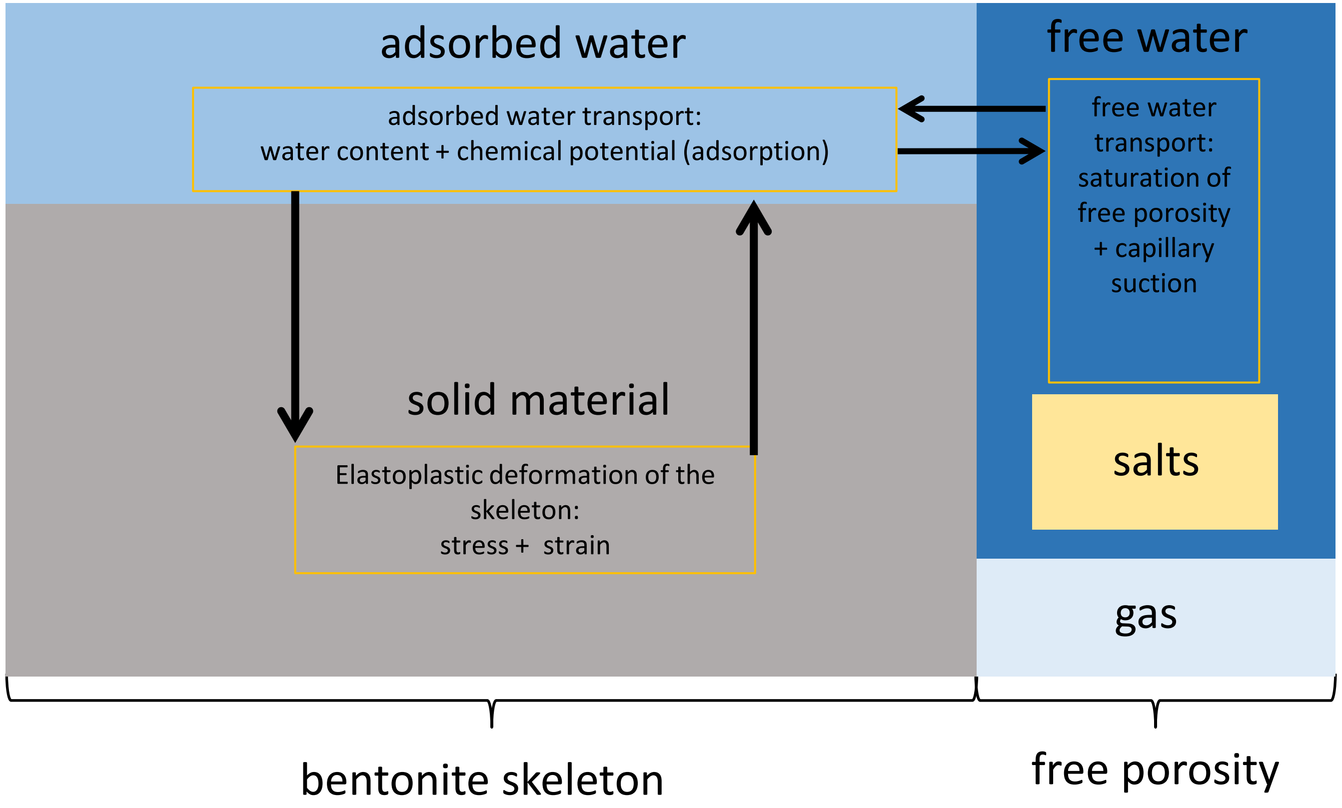
Elements needed for a bentonite model



porous material with water adsorbed to the structure

Varied multiplicative processes (VMP) model

- Large deformation model
  - Deformation in bentonite is often large
  - Elastoplasticity
  - Adsorbed water
- Multiplicative decomposition of deformation gradient
- Energetic approach to mechanical elasticity and adsorbed water transport
  - To obtain consistent couplings to the model
- Effect of chemistry
  - Model parameters
  - Boundary conditions
  - (Simple reactive transport)



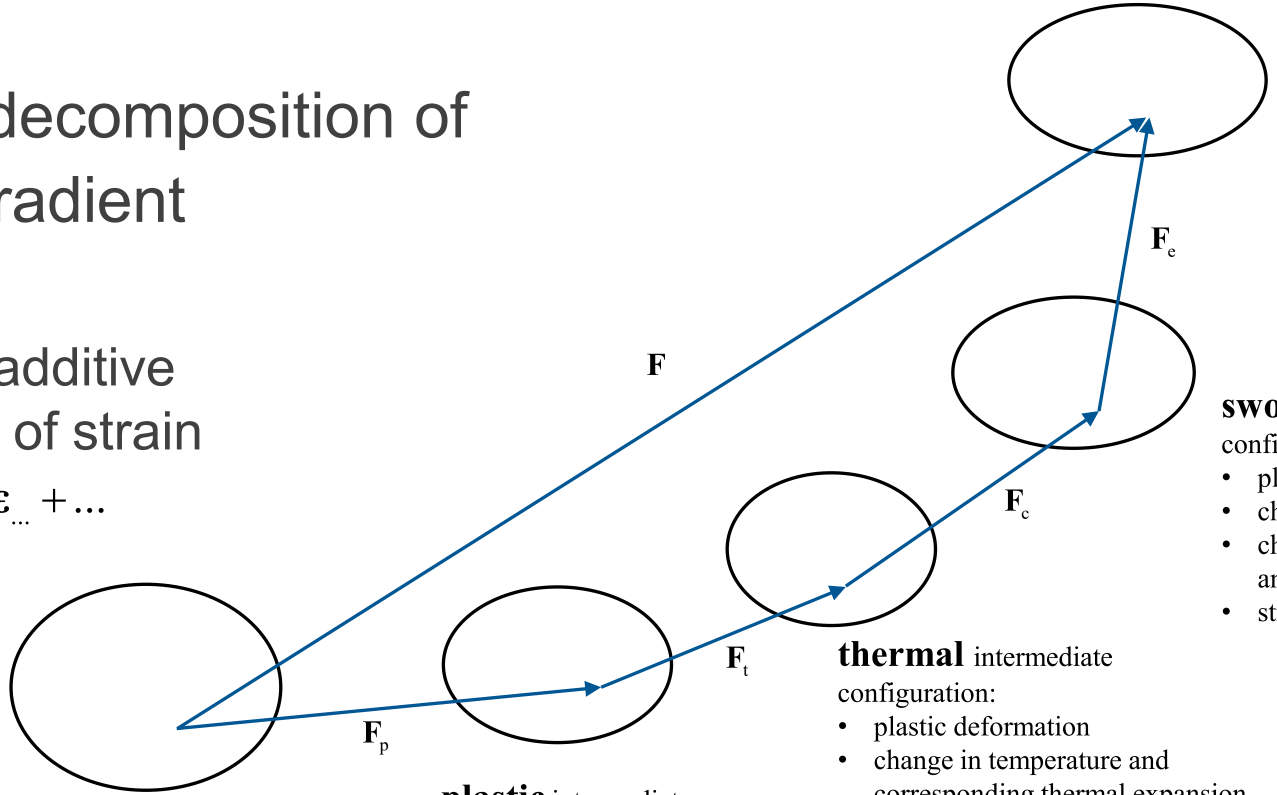
Multiplicative decomposition of deformation gradient

- Multiplicative decomposition of deformation gradient

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_c \mathbf{F}_t \mathbf{F}_p$$

  - Instead of the additive decomposition of strain

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p + \boldsymbol{\varepsilon}_{...} + \ldots$$



spatial configuration:
- plastic deformation
- change in temperature
- change in bound water content
- change in stress (corresponding to elastic deformation)

swollen intermediate configuration:
- plastic deformation
- change in temperature
- change in adsorbed water content and corresponding swelling
- stress at reference value

thermal intermediate configuration:
- plastic deformation
- change in temperature and corresponding thermal expansion
- other variables at reference values

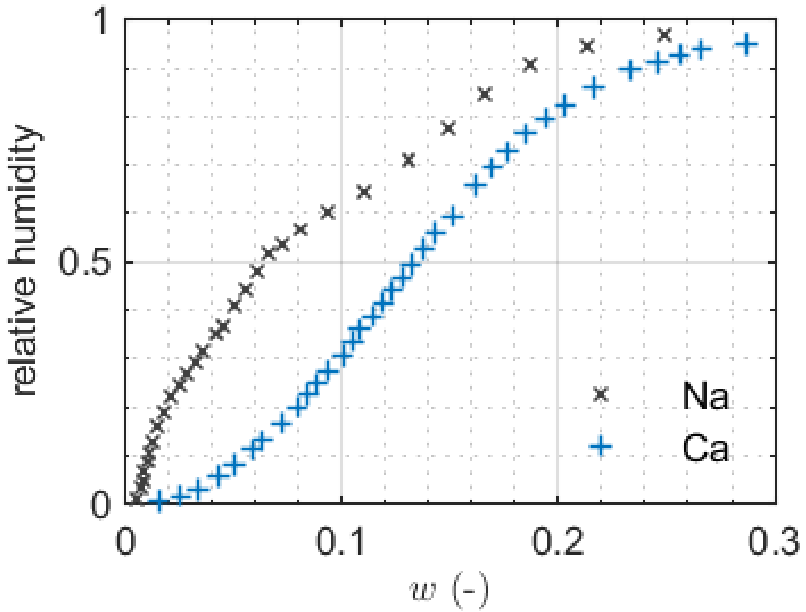
plastic intermediate configuration:
- plastic deformation
- other variables at reference values

reference configuration: all variables at reference values

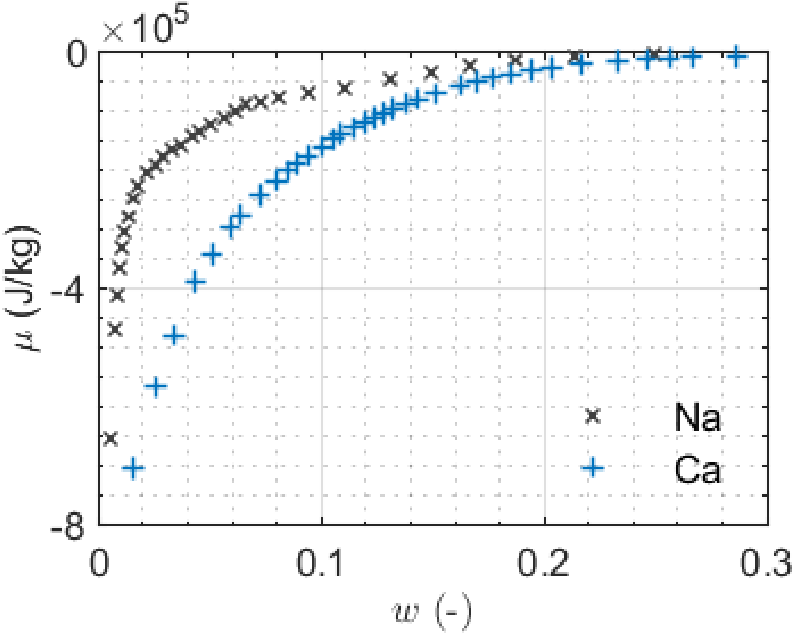
Water transport

- Adsorbed water transport
  - Driven by chemical potential gradient
  - If water adsorption isotherms are transferred ”suction” values using ideal gas law for water vapour in equilibrium with adsorbed water
    - in order of 100 MPa

$$\dot{m}_R = -\nabla \cdot \mathbf{j} + \mathrm{j} \qquad \mathbf{j} = -L\, D_{\boldsymbol{e}}\, \nabla\mu$$

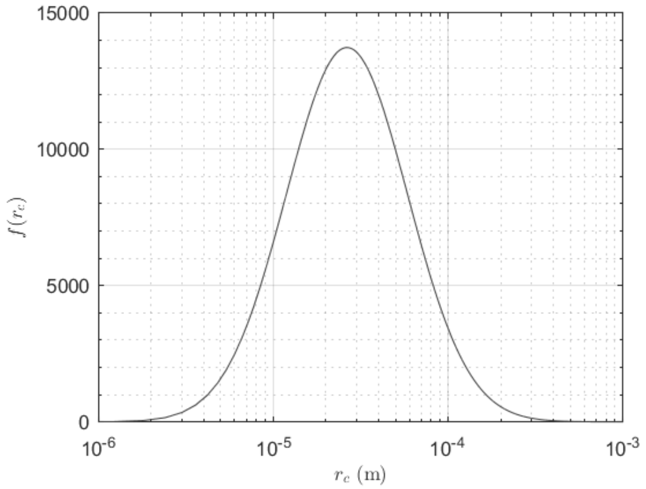


$$\mu_{chem}(w) = \frac{RT}{M_w} ln(RH)$$



Water transport

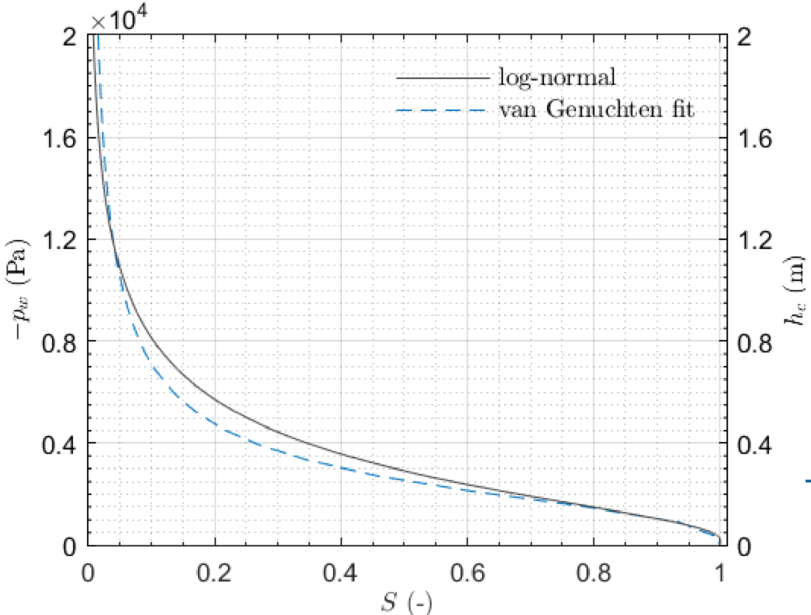
- Free (liquid) water transport
  - Driven by capillary pressure gradient
  - If pore size distribution of the gas filled porosity is transferred to suction values using capillary rise equation
    - In order of 10 kPa
    - If bentonite is dry, negligible
      - (10 kPa << 100 MPa)
- Water vapour transport
  - Driven by water vapour partial pressure gradient



$$\phi_R \rho_w \frac{\partial S}{\partial p_w} \dot{p}_w = -\,\mathrm{Div}\,\mathbf{m}_R + m_R$$

$$h = \frac{\text{constant}}{r}$$

$$\mathbf{m}_R = -\rho_w J \mathbf{C}^{-1} \frac{k_r \kappa_w}{\mu_{wv}} \nabla p_w$$



Consistent couplings

- Energetic approach for mechanical elasticity and adsorbed water transport = constitutive equations derived from free energy $\boldsymbol{\psi}$

$$\boldsymbol{\psi} = \boldsymbol{\psi}_{mech} + \boldsymbol{\psi}_{chem} + \boldsymbol{\psi}_{mixed}$$

pure mechanical

pure chemical (water adsorption)

chemomechanical

$$\text{stress} = \frac{\partial \boldsymbol{\psi}}{\partial \text{ strain}} = \frac{\partial \boldsymbol{\psi}_{mech}}{\partial \text{ strain}} + \frac{\partial \boldsymbol{\psi}_{mixed}}{\partial \text{ strain}}$$

Normal stress-strain relation

swelling

$$\mathbf{T}_n = \kappa \ln J_\phi + 2\ \mathrm{G}\ \mathrm{dev}\ \mathbf{E} + \frac{\kappa}{\rho_w}(m_R - m_{R0})\mathbf{I}$$

volumetric

shear

Chemical potential (water adsorption)

$$\mu = \frac{\partial \boldsymbol{\psi}}{\partial m_R} = \frac{\partial \boldsymbol{\psi}_{chem}}{\partial m_R} + \frac{\partial \boldsymbol{\psi}_{mixed}}{\partial m_R}$$

water mass content

from water adsorption isotherm for bentonite powder

swelling back-coupling

$$\mu = \mu_{chem}(m_R) + \frac{1}{\rho_w}\mathrm{p} \leftarrow = -\frac{1}{3}\mathrm{tr}\ \mathbf{T}$$

Adsorbed water mass flux $\quad \mathbf{j} = -L\ D_{\boldsymbol{e}}\ \nabla\mu$

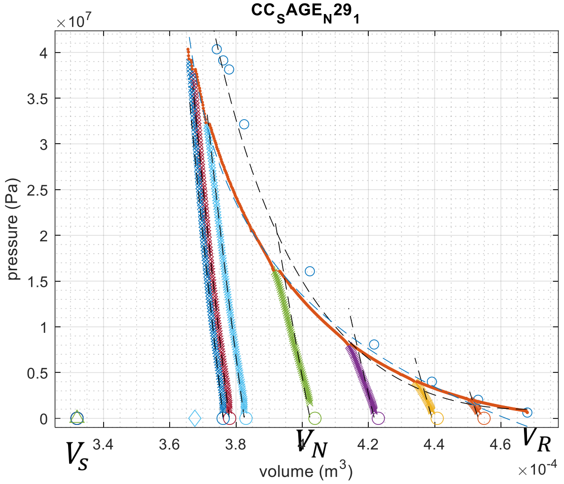
Mechanical model

- Force balance $$\mathrm{Div}\,\mathbf{T}_{\mathrm{PR}} + b_{0\mathrm{R}} = 0$$
- Yield condition $$\lambda \geq 0, \quad f_{\mathrm{y}} \leq 0 \quad \textbf{and} \quad \lambda f_{\mathrm{y}} = 0,$$
- Plastic flow rule $$-\frac{1}{2}\mathbf{F}\dot{\mathbf{C}}_{\mathrm{p}}^{-1}\mathbf{F}^{\mathrm{T}} = \lambda \frac{\partial f_{\mathrm{p}}}{\partial \tau}\mathbf{B}$$
- Yield surface $$f_{\mathrm{y}} = q^2 + M^2\,(p - p_{\mathrm{c}})\,p = 0$$

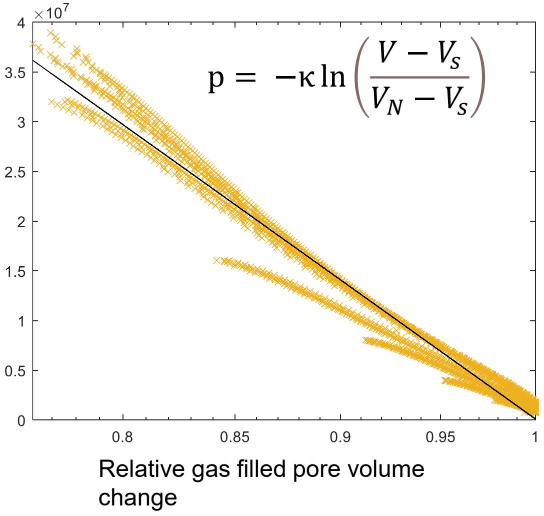
Volumetric elastoplastic constitutive models

- Wanted behaviour
  - pressure → infinity when gas filled porosity → 0
- Condition dependent
- See the other presentation for constitutive model and regression model fitting

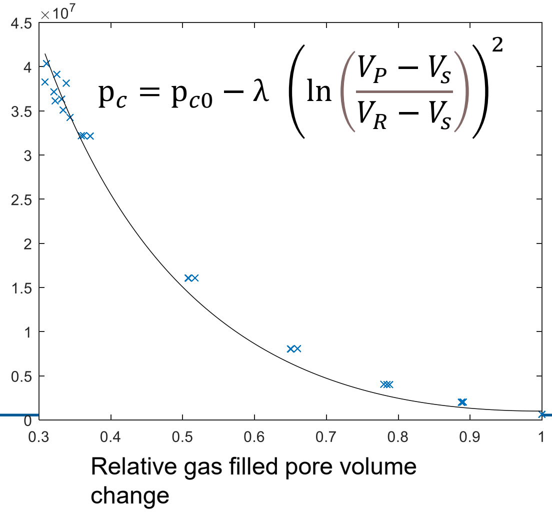
Example: one sample data and const. model fitting



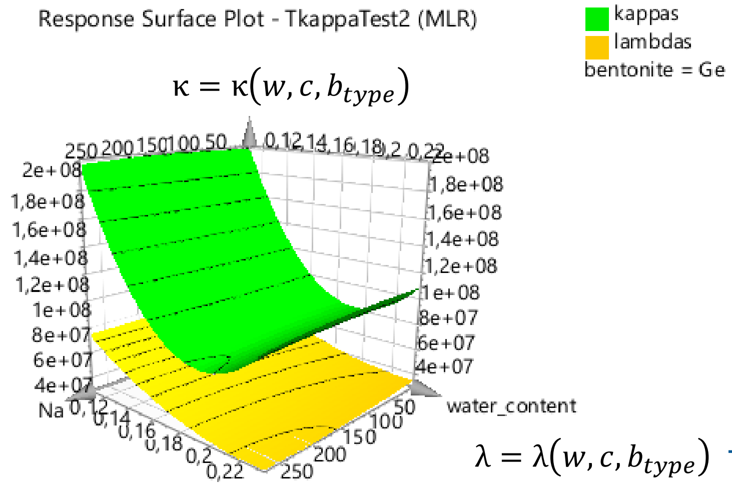
Example: three samples elastic data and const. model fitting



Example: three samples plastic data and const. model fitting



Example: regression model fitting for Georgian bentonite



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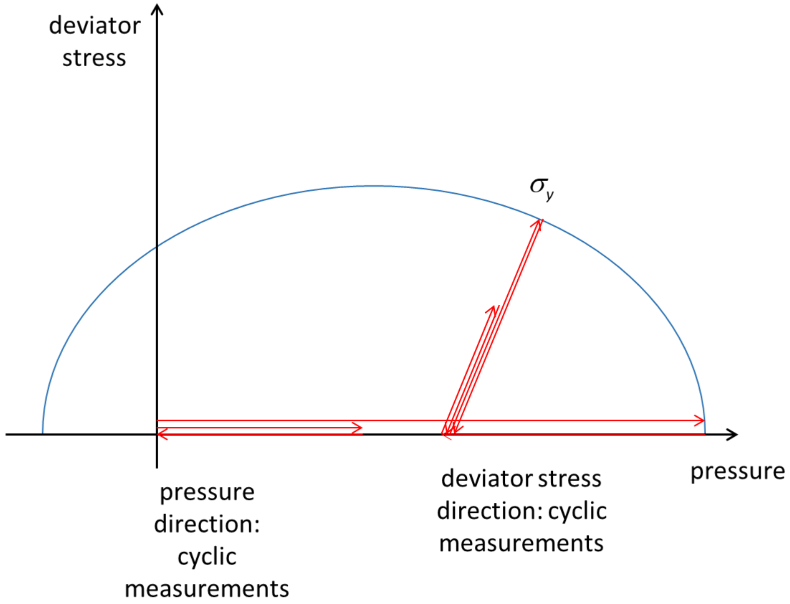
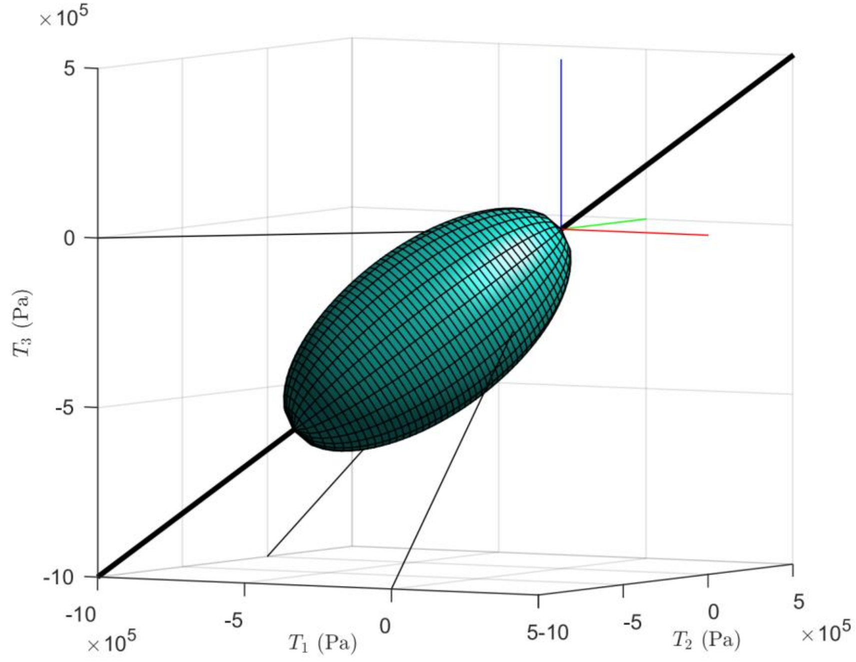
General elastoplastic constitutive models





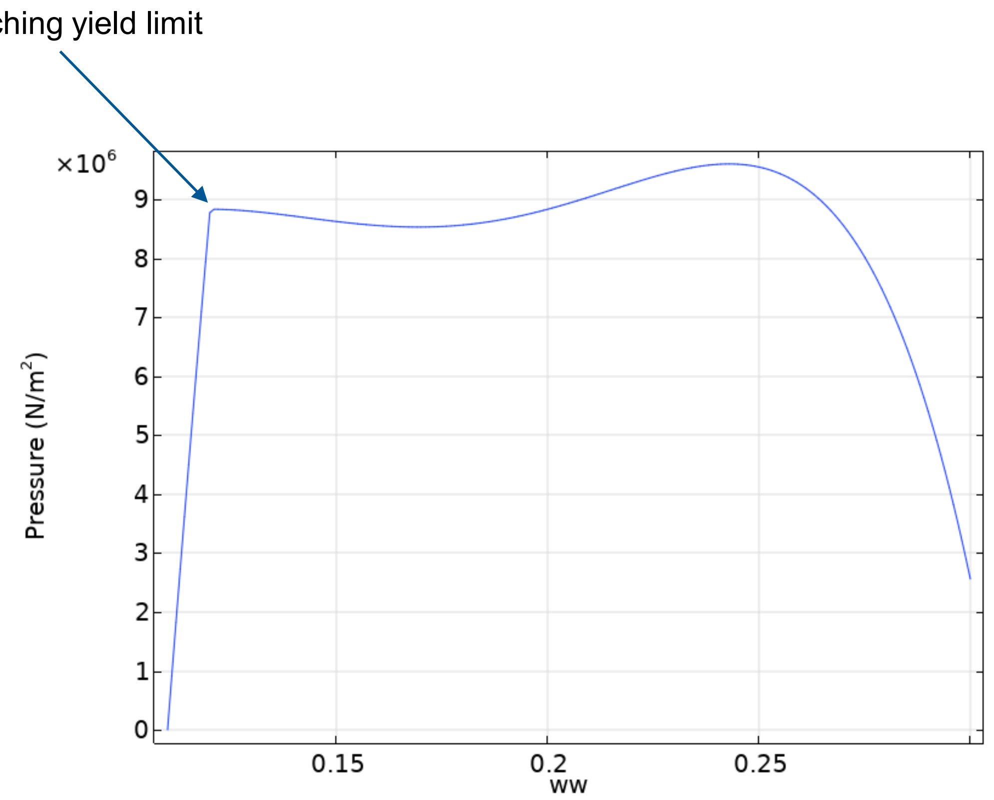
SAFER 2028

VMP model implementation

- In COMSOL Multiphysics
- Simulations started
- Preliminary volumetric elastic and plastic experimentally based surrogate models
  - Update required
- Converge is not stable
  - Likely related to the volumetric elastoplastic model (at least)
- Bugs in the implementation being fixed
- Work on-going

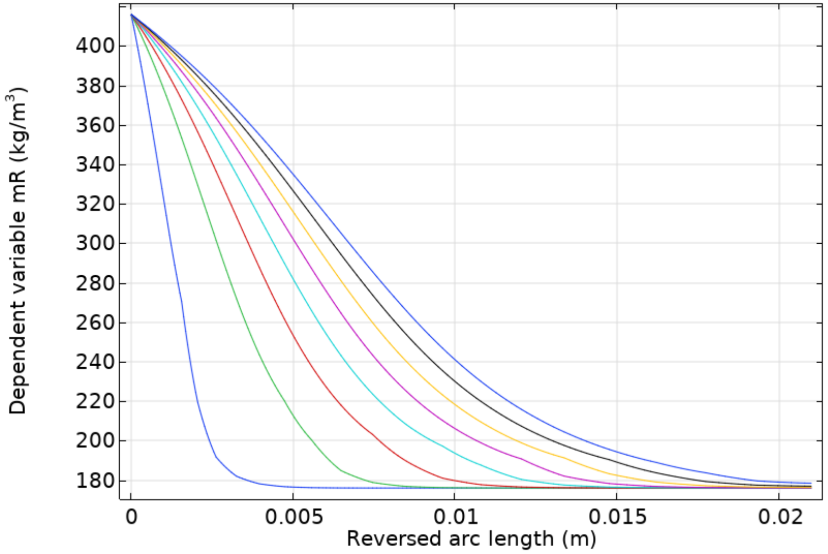
Simulation: water content increase

- Gravimetric water content (ww in figure) increase from 0.11 upwards
- SAGE volumetric mechanical data
  - Preliminary elastic and plastic experimentally based surrogate models
  - (bug found in the model implementation)
- Related to EURAD2 ANCHORS work package simulation exercises



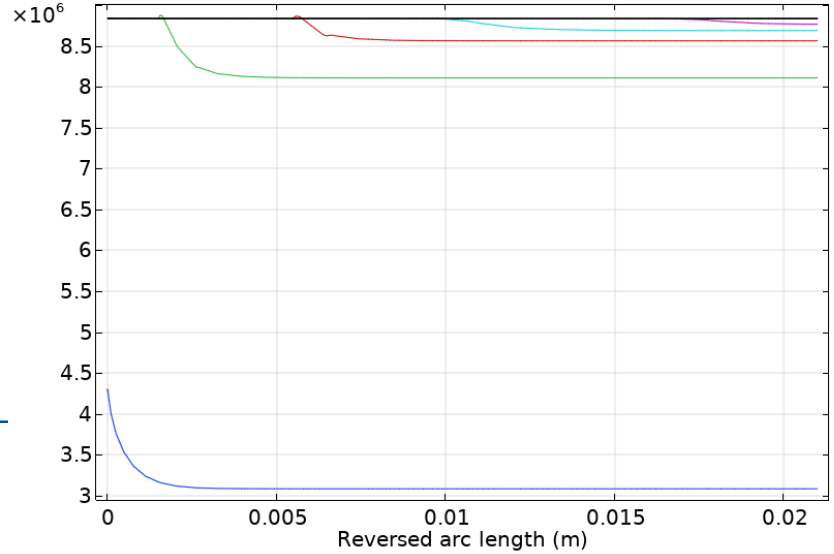
Simulation: bentonite wetting

- Water enter the sample from top (left in figures)
- Very preliminary results
- Constant yield limit

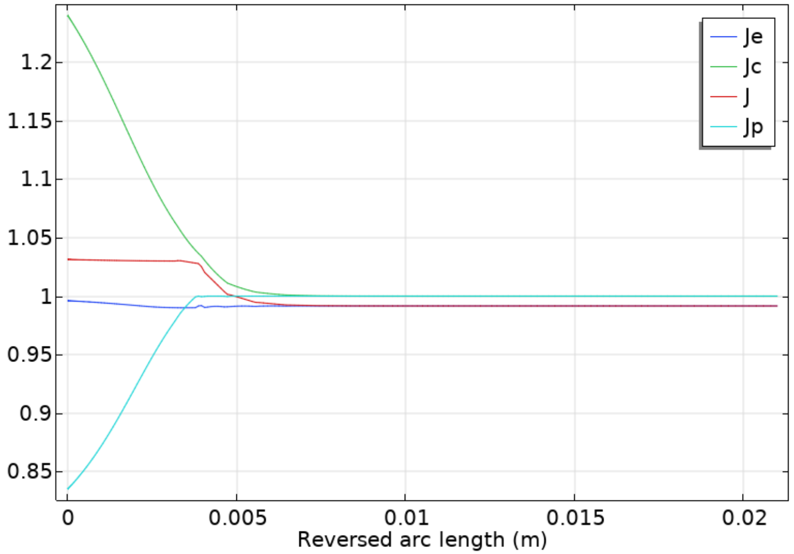


Water content profiles at various times

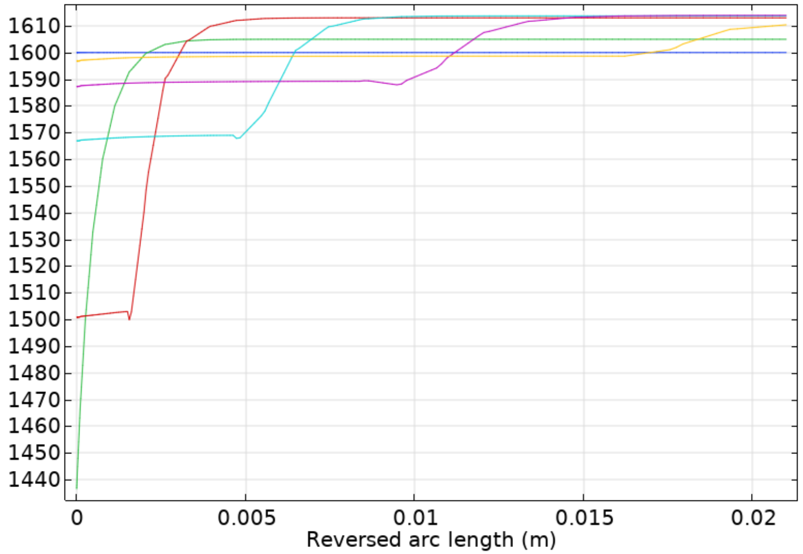
Pressure profile at various times



Relative volume change:
e – elastic, c – swelling, p – plastic, and total



Dry density profiles at various times



Summary and some realisations

- VMP model implemented in COMSOL Multiphysics
  - Large deformations
  - Swelling coupling and back-coupling
  - Adsorbed water transport driven by chemical potential gradient
  - Model formulation has evolved
- First very preliminary simulations run
  - Work continues
- Bentonite swelling stress is dictated by the volumetric yield limit
  - Plastic material model dependency on bentonite type, chemical state and conditions?

Thanks!