

Simulation of bentonite experiments 1A01 and 1A02 in SIFEL environment

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Numerical modelling

- material models
- balance equations
- space and time discretization
- solution of linear and nonlinear systems of equations

Water transport

Implemented new continuity equation with the influence of volumetric changes of the skeleton

$$\begin{aligned}
 & \left[\frac{\alpha - n}{K_s} S_w^2 \rho^w + \frac{n S_w}{K_w} \rho^w + \frac{\alpha - n}{K_s} S_g S_w \rho^{gw} \right] \frac{\partial p^w}{\partial t} + \\
 & + \left[\frac{\alpha - n}{K_s} S_w S_g \rho^w + \frac{\alpha - n}{K_s} S_g^2 \rho^{gw} \right] \frac{\partial p^g}{\partial t} + \\
 & + \underbrace{(\alpha S_w \rho^w + \alpha S_g \rho^{gw}) \operatorname{div} \mathbf{v}^s}_{\text{volumetric changes of the skeleton}} + \left[\rho^{gw} \beta_s (\alpha - n) S_g - \rho^w \beta_{swg} \right] \frac{\partial p^g}{\partial t} + \\
 & + \left[\frac{\alpha - n}{K_s} S_w \rho^w (p^w - p^g) + \frac{\alpha - n}{K_s} S_g \rho^{gw} (p^w - p^g) + n (\rho^w - \rho^{gw}) \right] \frac{\partial S_w}{\partial t} + \\
 & + n S_g \frac{\partial \rho^{gw}}{\partial t} + \operatorname{div} (n S_w \rho^w \mathbf{v}^{ws}) + \operatorname{div} (n S_g \rho^{gw} \mathbf{v}^{gs}) + \operatorname{div} \mathbf{J}_g^{gw} = 0, \quad (1)
 \end{aligned}$$

neglecting volumetric changes led to unrealistic evolution of suction during free swelling phase

strain-displacement relationship

$$\boldsymbol{\varepsilon} = \partial \mathbf{u}$$

constitutive equation

$$\dot{\boldsymbol{\sigma}} = \hat{\mathcal{T}}(\dot{\boldsymbol{\varepsilon}}, \dot{\mathbf{q}}) = \mathcal{T}(\dot{\mathbf{u}}, \dot{\mathbf{q}}),$$

where $\hat{\mathcal{T}}(\dot{\boldsymbol{\varepsilon}}, \dot{\mathbf{q}})$ represents hypoplasticity model proposed by D. Mašín.
equilibrium condition

$$\operatorname{div}_x \dot{\boldsymbol{\sigma}} + \dot{\mathbf{b}} = \operatorname{div}_x (\mathbf{D} \dot{\boldsymbol{\varepsilon}} + \mathbf{h} \dot{\rho}) + \dot{\mathbf{b}} = \mathbf{0}$$

boundary conditions

$$\begin{aligned} \mathbf{u} &= \bar{\mathbf{u}} \quad \text{on } \Gamma_u \\ \boldsymbol{\sigma} \mathbf{n} &= \bar{\mathbf{t}} \quad \text{on } \Gamma_t \end{aligned}$$

Numerical solution (FEM)

Babushka-Brezzi condition should be met:

- Linear approximation of transport variables

- Quadratic approximation of displacements

Linear approximation of variables at both problems led to irregular stress distribution.

Two possibilities for the solution of coupled problems

- Fully coupled approach - one large system of equations
- Staggered approach - two lesser systems of equations (possible memory savings for large problems)

Staggered approach

The term of volumetric strain rate goes to the right-hand side in FEM discretization:

$$\mathbf{K}_p \mathbf{r}_p + \mathbf{C}_p \dot{\mathbf{r}}_p = \mathbf{f}_p + \mathbf{f}_{pu}, \quad (2)$$

$$\mathbf{K}_u \dot{\mathbf{r}}_u = \dot{\mathbf{f}}_u, \quad (3)$$

$$\mathbf{f}_{pu} = - \int_{\Omega} \mathbf{N}^T (\alpha S_w) \Delta \varepsilon_V d\Omega, \quad (4)$$

where $\Delta \varepsilon_V$ is the increment of volumetric strain computed in previous time step.

Mechanics

Iterate until $t \leq t_{required}$

$$(\Delta \mathbf{f})_{i+1} = \mathbf{f}(t_{i+1}) - \mathbf{f}(t_i)$$

$$(\Delta \mathbf{r}_u)_{i+1} = \mathbf{K}^{-1}(\Delta \mathbf{f})_{i+1}$$

$$(\mathbf{r}_u)_{i+1} = (\mathbf{r}_u)_i + (\Delta \mathbf{r}_u)_{i+1}$$

$$\boldsymbol{\varepsilon}_{i+1} = \mathbf{B}(\mathbf{r}_u)_{i+1}$$

$$\dot{\boldsymbol{\sigma}}_{i+1} = \hat{\mathcal{T}}(\dot{\boldsymbol{\varepsilon}}_{i+1}, \dot{\mathbf{q}}_{i+1}) = \mathcal{T}((\dot{\mathbf{r}}_u)_{i+1}, \dot{\mathbf{q}}_{i+1})$$

$$\boldsymbol{\sigma}_{i+1} = \boldsymbol{\sigma}_i + \Delta \boldsymbol{\sigma}_{i+1} \text{ where } \Delta \boldsymbol{\sigma}_{i+1} \text{ is obtained by RKF integration scheme}$$

$$\bar{\mathbf{f}}_{i+1} = \int_{\Omega} \mathbf{B}^T \boldsymbol{\sigma}_{i+1} d\Omega$$

$$\Delta \hat{\mathbf{f}} = \mathbf{f}(t_{i+1}) - \bar{\mathbf{f}}_{i+1}$$

Iteration of residual vector $\Delta \hat{\mathbf{f}}$ with the help of Newton-Raphson method

Transport processes

$$\mathbf{C}\dot{\mathbf{r}}_p(t) + \mathbf{K}\mathbf{r}_p(t) = \mathbf{f}(t) ,$$

$$(\mathbf{r}_p)_{i+1} = (\mathbf{r}_p)_i + \Delta t \mathbf{v}_{i+\alpha} ,$$

$$\mathbf{v}_{i+\alpha} = (1 - \alpha)\mathbf{v}_i + \alpha\mathbf{v}_{i+1} ,$$

resulting system of algebraic equations

$$(\mathbf{C} + \Delta t \alpha \mathbf{K}) \mathbf{v}_{i+1} = \mathbf{f}_{i+1} - \mathbf{K} ((\mathbf{r}_p)_i + \Delta t (1 - \alpha) \mathbf{v}_i) .$$

Fully coupled approach

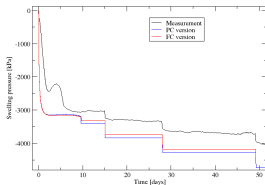
$$\begin{pmatrix} \mathbf{K}_{uu} & \mathbf{K}_{up} \\ \mathbf{0} & \mathbf{K}_{pp} \end{pmatrix} \begin{pmatrix} \mathbf{r}_u \\ \mathbf{r}_p \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{C}_{pu} & \mathbf{C}_{pp} \end{pmatrix} \begin{pmatrix} \dot{\mathbf{r}}_u \\ \dot{\mathbf{r}}_p \end{pmatrix} = \begin{pmatrix} \mathbf{f}_u \\ \mathbf{f}_p \end{pmatrix}, \quad (5)$$

where off-diagonal coupling blocks are:

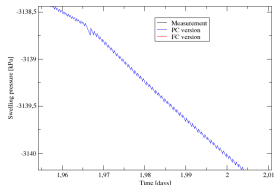
$$\mathbf{K}_{up} = - \int_{\Omega} \mathbf{B}_u^T \mathbf{m}^T (\alpha S_w) \mathbf{N}_p d\Omega, \quad \mathbf{C}_{pu} = \int_{\Omega} \mathbf{N}_p^T (\alpha S_w) \mathbf{m}^T \mathbf{B}_u d\Omega, \quad (6)$$

where $\mathbf{m} = \{1, 1, 1, 0, 0, 0\}$

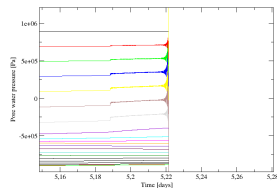
Differences between staggered and fully coupled approaches



Permeameter test simulation - course of the swelling pressure in time



Permeameter test simulation - detail of swelling pressure oscillations



TEST1A01 - detail of water pressure oscillations at the end of saturation

Technical aspects of the SIFEL implementation

Strictly separated implementation of transport and mechanical problems leads to issues connected with passing data between modules.

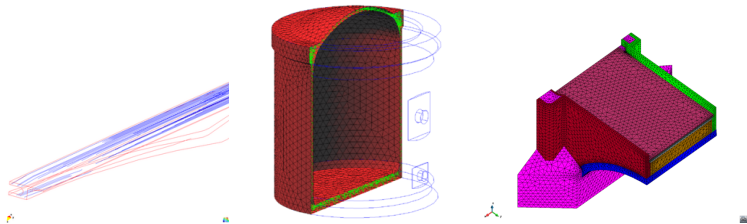
Difficulties with the passing quantities from mechanical part due to state variables lead to several approaches:

- nodal values of the given quantity is taken from the closest integration point = significant error in the case of steep gradients (old implementation, FE meshes must have the same number of elements)
- nodal values are computed exactly, state variable values are taken from the closest int. point, new value of required quantity is computed at node (new implementation, FE meshes must have the same number of elements)
- double set of integration points = exact values at required int. points in both mechanical and transport problems, (transport and mechanical FE meshes can be independent) - implementation in the progress

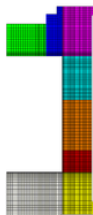
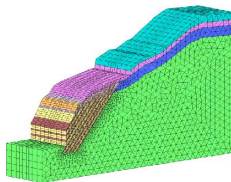
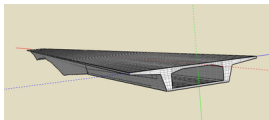
SIFEL

(mech.fsv.cvut.cz/~sifel)

- GEFEL - mathematical tools, solvers (122 000)
- MEFEL - problems of mechanics (245 000)
- TRFEL - transport processes (159 000)
- METR - coupled problems mechanics-transport processes (35 000)



- 1D, 2D, 3D problems
- static–dynamic problems
- stationary–nonstationary problems
- problems with changing geometry



Actual state

- material model for bentonites introduced by David Mašín
- coupled heat and moisture transport based on Schrefler and Gawin papers
- fully coupled and staggered approaches available
- one element benchmarks
- mock-up test simulations