Thermo hydro mechanical coupling for underground waste storage simulations

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Outline

- Underground waste storage concepts
- Main phenomena and modelisation
- Coupling
- Numerical difficulties
- Spatial discretisation for flows and stresses
- Simulation of the excavation of a gallery
Underground waste storage concepts (1/3)
Underground waste storage concepts (2/3)

- C waste Cell

- B waste cell
Underground waste storage concepts (3/3)

- Complex geometry

- Heterogeneous materials
  - Rock at initial state or damaged rock
  - Concrete
  - Engineered barriers (sealing, cells closure)
  - Fill materials
  - Gaps
  - Steel: container liners

- Different physical behaviour
  - Mechanical, thermal, chemical, hydraulic
Main phenomena and modelisation (1/2)

Flows

✓ 2 components (air or H₂ and water) in 2 phases (liquid and gaz)
✓ Transport equations:

- **Pressures**
  \[
  p_{gz} = p_{as} + p_{vp} \\
  p_{lq} = p_{w} + p_{ad}
  \]

- **Velocities**
  \[
  \frac{M_{gz}}{\rho_{gz}} = \left(1 - C_{vp}\right) \frac{M_{as}}{\rho_{as}} + C_{vp} \frac{M_{vp}}{\rho_{vp}} \\
  \frac{M_{lq}}{\rho_{lq}} = \frac{K_{\text{int}} \cdot K_{eq}^{rel}(S_lq)}{\mu_{lq}} (-\nabla p_{lq} + \rho_{lq} g)
  \]

- **Darcy + diffusion + phase change**
  \[
  \frac{M_{vp}}{\rho_{vp}} - \frac{M_{as}}{\rho_{as}} = -F_{vp} \nabla C_{vp} \\
  M_{ad} - M_{w} = -F_{ad} \nabla \rho_{ad} \\
  \frac{dp_{vp}}{\rho_{vp}} = \frac{dp_{w}}{\rho_{w}} + \left(h_{vp}^{m} - h_{w}^{m}\right) \frac{dT}{T} \\
  \frac{\rho_{ad}}{M_{ad}^{ol}} = \frac{p_{ad}}{K_{H}}
  \]

- **Sorption curve**
  \[
  P_c = f(S_{lq}) = P_{gz} - P_{lq}
  \]
Main phenomena and modelisation (2/2)

- Mechanical behaviour
  - Plastic and brittle behaviour or the rock
  - Dilatance effect at rupture stage
  - Swelling of Engineered materials.
Numerical difficulties (1/3)

For flows

✓ Non linear terms induce hyperbolic behaviour
  • Kind of equation:
    \[ \frac{\partial u}{\partial t} - \frac{\partial^2 u^m}{\partial x^2} = 0 \]
  • Stiff fronts can appear

• Big capillary effect → No « mean » pressure
Numerical difficulties (2/3)

Example of a desaturation problem

- Initial state:

<table>
<thead>
<tr>
<th>Sat</th>
<th>Porosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.7</td>
<td>0.3</td>
</tr>
<tr>
<td>1</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Near desaturation transition zone gas pressure tends to zero
Numerical difficulties (3/3)

Instabilities due to brittle behaviour

- Pre peak damage
  \[ |\sigma_1 - \sigma_3| \leq 0.7 |\sigma_1 - \sigma_3|_{\text{peak}} \]

- Fractured rock
  \[ 0 < \gamma^p \leq \gamma_e \]

- Post peak damage
  \[ \gamma_e \leq \gamma^p \leq \gamma_{\text{ult}} \]

\[ \approx 2.2 \text{ m} \]

\[ \approx 1 \text{ m} \]
Coupling (1/2)

- Incidence of flow on mechanical behaviour
  - Standard notion of pore pressure
  - Equivalent pore pressure definition for partially saturated media
    - Taking into account of interfaces in thermodynamic formulation
      \[ \pi = S \alpha p^\alpha - \frac{2}{3} \int_{S_1} p_c(S)|S| dS \]

- Incidence material deformation on flow
  - Porosity change
  - Straight increase of permeability with damage

\[ \text{homogenization} \quad D_F \quad ? \quad D_M \]
Coupling (2/2)

- Thermal evolution -> Mechanic
  - Thermal expansion

- Thermal evolution -> flow
  - Changes in Viscosity, diffusivity coefficients

- Flow, mechanic -> thermal evolution
  - No effect
Numerical methods for flow

**Choice of principal variables**

- **Capillary pressure/gas pressure**
  - Air mass balance ill conditioned for $S=1$
    \[
    \phi \frac{\partial}{\partial t} \left( \rho_a (1-S) \right) - \nabla \left( \rho_a k_a (S) \nabla p_a \right) = 0
    \]

- **Saturation/water pressure**
  - Air mass balance becomes:
    \[
    \phi (1-S) \frac{\partial p_e}{\partial t} + \phi (g(S) - p_e) \frac{\partial S}{\partial t} - \nabla \left( p_a h(S) \nabla S \right) - \nabla \left[ p_a k_a (S) \nabla p_e \right] = 0
    \]

\[P_c(S) \approx A(1-S)^{0.6}\]
\[g(S) \approx p_c\]
\[k_a(S) \approx (1-S)^3\]
\[h(S) \approx A(1-S)^{2.6}\]

At $S=1$

We have \[\frac{\partial S}{\partial t} = 0\]
Numerical methods for flow and mechanic: spatial discretisation

- Goals
  - A stable, monotone method for flow
  - Easy to implement in a finite element code

- Method 1: pressure and displacement EF P2/P1 lumped formulation
  - OK for consolidation modelling
  - OK for desaturation test (Liakopoulos)
Numerical methods for flow and mechanic : spatial discretisation

Limitations of previous formulation

- Poor quadrature rule induces lack of accuracy in stresses evaluations
- Instabilities appear when simulating gas injection problem

CFV/DM (control finite volume/dual mesh)

Goal

- formulation VF compatible with architecture of EF software

Principle

- To use primal mesh for EF formulation of mechanical equations
- To construct a finite volume cell surrounding each node of the primal mesh
- To write mass balance on that polygonal cell
CFM/DM (control finite volume/dual mesh)

- **Model equation**
  \[ \frac{\partial m(u)}{\partial t} + \nabla \cdot F(u) = F = k(u) \nabla u \]

- **Mass balance:**
  \[ A_K \frac{m_K^{n+1} - m_K^n}{\Delta t} + \sum L T_{KL} k^{KL} (u_{KL}^{n+1} - u_{KL}^{n+1}) = 0 \]

- **Up winding**
  \[ \text{si } u_{L}^{n+1} \uparrow u_{K}^{n+1} \downarrow u_{KL}^{n+1} = u_{L}^{n+1} \]

- **Loop over elements of primal mesh**
  \[ \sum e \in T_K A_K^{e} \frac{m_K^{n+1} - m_K^n}{\Delta t} + \sum e \sum L \in e \neq K T_{KL}^{e} k^{KL} (u_{KL}^{n+1} - u_{KL}^{n+1}) = 0 \]

  \[ T_{KL}^{e} = \frac{d_{L,H}^{e}}{d_{K,L}^{e}} = -\int e \nabla \lambda_K \cdot \nabla \lambda_K \]
**CFM/DM (control finite volume/dual mesh)**

- **Theoretical predictions:**
  - Stable, convergent and monotone for Delaunay meshes

- **Example**

  - For stretching $H/L > 4/3$ no convergence is achieved

  | Gas injection | $P_g$ 10 years $H/L=1$ | $S$ 10 years $H/L=4/3$ |
**Remark about interfaces**

- Differences between material properties can induce discontinuities.
- It is better to ensure constant properties over the control cell.
Numerical modelisation of brittle rocks

- Equilibrium equation

\[ \text{Div } \sigma + f = 0 \]

- Mechanical law of behaviour

\[ \sigma = F(\varepsilon, \alpha) \]

\[ \frac{\partial \sigma}{\partial \varepsilon} \text{ is not positive} \]

- Resulting weak formulation

\[ \int_{\Omega} \sigma : \varepsilon(u^i) + \int_{\Omega} f \cdot u^i = 0 \quad \forall u^i \]

- Lack of ellipticity
  - Possible bifurcations
  - Instabilities
Regularisation method

- Main idea:
  - Introduce some term bounding gradients of strain

- Second gradient

\[ \int_{\Omega} \sigma : \varepsilon(u^i) + \int_{\Omega} D \cdot \nabla \varepsilon : \nabla \varepsilon^i + \int_{\Omega} f \cdot u^i = 0 \forall u^i \]

- Simplified second gradient: micro gradient dilation model

  - For a dilatant material we can regularise only the volumic strain

\[ \int_{\Omega} \sigma : \varepsilon(u^i) + \int_{\Omega} D \cdot \nabla \text{Tr} \varepsilon \cdot \text{Tr} \varepsilon^i + \int_{\Omega} f \cdot u^i = 0 \forall u^i \]

\[ \int_{\Omega} D \cdot \Delta u \cdot \Delta u^i \]
Mixed formulation of micro gradient dilation model

- Weak formulation

\[
\int_{\Omega} \mathbf{\sigma} : \varepsilon(u) + \int_{\Omega} D \cdot \nabla \theta \cdot \nabla \theta^i - \int_{\Omega} \lambda (\nabla . u^i - \theta^i) + \int_{\Omega} \lambda^i |\nabla . u - \theta| + \int_{\Omega} f . u^i = 0 \quad \forall \{u^i, \lambda^i\}
\]

<table>
<thead>
<tr>
<th>Approximation spaces</th>
<th>( u )</th>
<th>( \theta )</th>
<th>( \lambda )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quadrangles</td>
<td>Q2</td>
<td>Q1</td>
<td>P0</td>
</tr>
<tr>
<td>Triangles</td>
<td>P2</td>
<td>P1</td>
<td>P0</td>
</tr>
</tbody>
</table>

- Possible free energy displacements modes \( w \)

\[
\int_{\Omega} \mathbf{\sigma} w : \varepsilon w = 0 \quad \int_{e} \nabla . w = 0 \quad \forall e
\]

- Two ways

  ✓ Enhancing degree of discretisation for \( \lambda \)
  ✓ Using penalisation

\[
\int_{\Omega} \mathbf{\sigma} : \varepsilon(u) + \int_{\Omega} D \cdot \nabla \theta \cdot \nabla \theta^i - \int_{\Omega} \lambda (\nabla . u^i - \theta^i) + \int_{\Omega} \lambda^i |\nabla . u - \theta| + r \int_{\Omega} |\nabla . u^i - \theta^i| \cdot |\nabla . u - \theta| + \int_{\Omega} f . u^i = 0
\]

\( \forall \{u^i, \lambda^i\} \)
Benchmark Momas: Simulation of an Excavation under Brittle Hydro-mechanical behaviour

- Cylindrical cavity
- Excavation simulation
- Initial conditions: anisotropic state of stress (11.0MPa, -15.4MP); water pressure (4.7 Mpa)

Radius of cavity: 3 meters
Horizontal length for calculation domain: 60 meters
Vertical length for calculation domain: 60 meters

Permeability: $10^{-12} \text{ m.s}^{-1}$

Time of simulation for excavation: 17 days
Time of simulation for consolidation: 10 years
Benchmark Momas: Simulation of an Excavation under Brittle Hydro-mechanical behaviour

- Mechanical elasto-plastic formulation
- Drucker-Prager Yield Criterion
- Plastic rule: associated formulation
- Softening: decrease of cohesion / shear plastic deformation

Space of effective stresses

Triaxial stress state of Drucker-Prager law for a confinement of 2 MPa
Coupled modelling – After 10 years – Shear bandings

- Shear bands are related to softening model
- Localisation bands are influenced by the mesh
- Hydro-mechanical coupling provides no regularisation
Benchmark Momas: simulation with Micro Gradient Dilation Model

Spatial discretisation with triangle elements

Visualisation of Shear bandings on Gauss Points during the excavation phase.

- Band width is always greater than 2 elements
  - We can hope this result is independent of the spatial discretisation

Displacement / deconfinement

- Regularisation gives results for higher deconfinement ratio
- With a coarser mesh, simulation stops earlier
Conclusions

- Simulation of nuclear waste storage requires to solve non-linear coupled equations in heterogeneous media.

- Some simulations need to solve jointly difficulties relative to two phase flow and brittle mechanical behaviours.

- Control finite volume/dual mesh is a reliable method for coupling darcean flows and mechanic.

- Regularised brittle models seem to be useful in coupled (saturated) simulations.

- Simplified second gradient (Micro Gradient Dilation) model gives reasonable results.