Geotechnical and Environmental Coupled Models Involving Unsaturated Soils and Rocks
CODE_BRIGHT-GHT-GiD

Part I Description

Sebastià Olivella, Jean Vaunat, Alfonso R. Dono
DECA, Escola de Camins, UPC BarcelonaTECH
Topics

• Unsaturated soils
• Multiphase flow
• Coupled problems THMC
• Laboratory investigation
• Laboratory equipment development
• Finite elements
• Material point method
• ...

• Earth dams
• Slope stability
• Tunnels
• Foundations
• Underground waste storage
• Geothermal energy
• Off shore
• CO2 sequestration
• ...

• …
The basic formulation is presented here. Variants are related to CO$_2$, solute transport, geochemistry, solubility, …

Notation example:

\[ \omega_w^w \rho_g S_g \]
### BALANCE EQUATIONS

#### MASS BALANCE OF WATER

\[
\frac{\partial}{\partial t} \left( \left( \omega_g^w \rho_g S_g + \omega_l^w \rho_l S_l \right) \phi \right) + \nabla \cdot \left( j_g^w + j_l^w \right) = f^w
\]

Unknown: \( P_l \)

#### MASS BALANCE OF AIR

\[
\frac{\partial}{\partial t} \left( \left( \omega_g^a \rho_g S_g + \omega_l^a \rho_l S_l \right) \phi \right) + \nabla \cdot \left( j_g^a + j_l^a \right) = f^a
\]

Unknown: \( P_g \)

#### INTERNAL ENERGY BALANCE FOR THE MEDIUM

\[
\frac{\partial}{\partial t} \left( \left( e_s \rho_s (1 - \phi) + e_g \rho_g S_g \phi + e_l \rho_l S_l \phi \right) \right) - \frac{\phi S_g p_g}{\rho_g} \frac{\partial \rho_g}{\partial t} + \nabla \cdot \left( i_c + i_{es} + i_{eg} + i_{el} \right) = f^E
\]

Unknown: \( T \)

#### MASS BALANCE OF SPECIES (SOLUTE TRANSPORT)

\[
\frac{\partial}{\partial t} \left( \left( \omega_g^c \rho_g S_g + \omega_l^c \rho_l S_l \right) \phi \right) + \nabla \cdot \left( j_g^c + j_l^c \right) = f^c
\]

Unknown: \( c \)

#### MOMENTUM BALANCE FOR THE MEDIUM

\[
\nabla \cdot \sigma + b = 0
\]

Unknown: \( u \)
Constitutive equations and equilibrium restrictions

\[ \rho_l = \rho_{l_0} \exp (\alpha (T-T_o)) + \alpha (T-T_o) \]

\[ \rho_g = \rho_v + \rho_a = \frac{\rho_v}{R(T+273.15)} + \frac{P_a M_a}{R(T+273.15)} \]

\[ P_v(T, P_c) = P_v(T) \times F(P_c, T) \]

\[ P_v(T) = 136075 \exp \left( \frac{-5239.7}{273+T} \right) \]

\[ F(P_c, T) = \exp \left( \frac{-P_c M_w}{R(273+T) \rho_l} \right) \]

\[ \mathbf{i}^i = -\lambda \nabla T \]

\[ \lambda = \lambda_{\text{sat}} S_e \lambda_{\text{solid}} (1-S_e) \]

\[ \lambda_{\text{sat}} = \lambda_{\text{solid}}^{(1-\phi)} \lambda_{\text{liq}}^{\phi} \]

\[ \lambda_{\text{dry}} = \lambda_{\text{solid}}^{(1-\phi)} \lambda_{\text{gas}}^{\phi} \]

\[ q_\alpha = -\frac{k k_{\alpha} \alpha}{\mu} \left( \nabla P_\alpha - \rho_\alpha g \right) \]

\[ k = k_o \frac{\phi^3}{(1-\phi)^2} \frac{(1-\phi_o)^2}{\phi_o^3} \]

\[ k_{rl} = \sqrt{S_e} \left( 1 - \left( 1 - S_e^{1/\lambda} \right)^2 \right) \]

\[ \mu_l = A \exp \left( \frac{B}{273.15 + T} \right) \]

\[ \mu_g = \frac{A \sqrt{273+T}}{1+\frac{B}{273+T}} \frac{1}{1+\frac{b_k}{P_g}} \]
Set of equations for mechanical models

\[
\frac{d\varepsilon}{dt} = \Gamma \left( \phi(F) \right) \frac{\partial G}{\partial \sigma^t}, \quad \phi(F) = \left( \frac{F}{F_o} \right)^N
\]

\[
F(J_1, J_2, J_3, s) = a J_2 - \mu^2 F_b F_s
\]

\[
F_k = \gamma \left[ -(J_1^0(s) + k_2 s + k_3)^{2-n} (J_1 + k_3 s + k_4)^{n} - k_3 s J_1^0(s) \right]
\]

\[
J_1^0(s) = \frac{3 p^c \left( \frac{J_1^0}{\lambda(0) - \kappa} \right)}{3 p^c} \quad p_o(s) = J_1^0(s) / 3
\]

\[
dJ_1^0 = \frac{1 + e}{\left( \lambda(0) - \kappa \right)} d\varepsilon^p_v \Rightarrow dp_o = \frac{1 + e}{\left( \lambda(0) - \kappa \right)} p_o d\varepsilon^p_v \Rightarrow dp_o = \frac{1 + e}{\chi(0)} d\varepsilon^p_v
\]

\[
\frac{d e_{\text{FADT}}}{d t} = \frac{l}{2 \eta_{\text{FADT}}} (\sigma' - p') I + \frac{l}{3 \eta_{\text{FADT}}} p' I \quad \frac{d e_{\text{DC}}}{d t} = \frac{l}{\eta_{\text{DC}}} \Phi(F) \frac{\partial G}{\partial \sigma^t}
\]

\[
d\sigma = D_{ijkl} \left( d\varepsilon_{kl} - \delta_{kl} \frac{ds}{K_s} - d\varepsilon^p_{kl} \right)
\]

\[
F = J^2 - \frac{M^2}{3} (p^M + p^M_o - p^M_o) \geq 0
\]

\[
n^p = \left( \cos \theta^M + \frac{1}{3 \sqrt{3}} \sin \theta^M \sin \phi^M \right) J^M - \sin \phi^M (p^M + p^M_o) \geq 0
\]

\[
d\sigma^b_{ij} = D_{ijkl}^b \left( d\varepsilon^b_{kl} - d\varepsilon^d_{kl} \right)
\]

\[
p_o = p_o \left( \frac{p_o}{p_c} \right)^{\lambda(0) - \kappa} \quad \lambda(s) = \lambda(0) \left[ 1 - r e^{-\beta s} + r \right]
\]

\[
F^{\text{SD}} = p + s - \gamma^{\text{SD}} \quad F^{\text{LC}} = J^2 - \frac{M^2}{3} (p + p_c) (p_o - p) \leq 0
\]
The system of PDE's (Partial Differential Equations) is solved numerically. The numerical approach can be viewed as divided into two parts: spatial and temporal discretizations.

**Finite elements in space:**
- Different types of elements available
- Element-wise, modified cell-wise and node-wise variables
- Secant method for non-adveective terms (a)

**Finite differences in time:**
- Storage terms: mass conservative approach (secant) (b)
- Implicit scheme (intermediate times)
- Full Newton-Raphson method to solve nonlinearities
- Only first derivatives of nonlinear functions (due to a,b)

**Solution of the linear system of equations:**
- Iterative solver, sparse storage.
After the spatial discretization of the partial differential equations, the residuals that are obtained can be written (for one finite element) as:

\[
\begin{pmatrix}
 r_u \\
 r_{P_i} \\
 r_{P_g} \\
 r_T
\end{pmatrix} = \frac{d}{dt} \begin{pmatrix}
 d_u \\
 d_{P_i} \\
 d_{P_g} \\
 d_T
\end{pmatrix} + \begin{pmatrix}
 a_u \\
 a_{P_i} \\
 a_{P_g} \\
 a_T
\end{pmatrix} + \begin{pmatrix}
 b_u \\
 b_{P_i} \\
 b_{P_g} \\
 b_T
\end{pmatrix} = \begin{pmatrix}
 0 \\
 0 \\
 0 \\
 0
\end{pmatrix}
\]

where \( r \) are the residuals, \( \frac{dd}{dt} \) are the storage or accumulation terms, \( a \) are the conductance terms, and \( b \) are the sink/source terms and boundary conditions.

After time discretization a more compact form can read as:

\[
r(X^{k+1}) = \frac{d^{k+1} - d^k}{\Delta t^k} + A(X^{k+\varepsilon})X^{k+\theta} + b(X^{k+\theta}) = 0
\]

Newton-Raphson scheme:

\[
\frac{\partial r(X^{k+1})}{\partial X^{k+1}} (X^{k+1,l+1} - X^{k+1,l}) = -R(X^{k+1,l})
\]
CODE_BRIGHT: Problem Type in GiD

Problem data

Materials

Intervals

Conditions

\[ f_i^c = (\omega_i^c)^P \bigg( P_i^P - P^P \bigg) + \beta_i \bigg( \rho_i^P \omega_i^c \bigg) - \rho_i \omega_i^c \]
CONSORTIUM CODE_BRIGHT

SKB (SWEDEN) Coordination
POSI VA (FINLAND)
ANDRA (FRANCE)
GRS (GERMANY)
Code_Bright in social networks

7th Workshop of CODE_BRIGHT on May 21st 2015.
Submission deadline (extended abstract of 4 pages): April 30th.
http://bit.ly/7th_Workshop

The Department of Geotechnical Engineering and Geosciences of the Technical University of Catalonia (UPC) is organising the seventh workshop of CODE_BRIGHT users to be held on May 21st 2015.
Call for contributions to this workshop is now open. Authors are invited to submit an extended abstract (including figures and references) of four pages not later than April 30th.
https://www.etcg.upc.edu/.../.../code_bright/workshop/
**Tutorials**

- **Beginners**
  - Detailed description of:
    - Geometry; Boundary conditions
    - Materials, Mesh; Post-process
  - Type of analysis: Linear, uncoupled
  - Examples:
    - Foundation (M problem)
    - Heat flow problem (T problem)
    - Drainage around a trench (H problem)
    - Conservative contaminant migration (H-W problem)
    - Gas Injection Problem (H problem)
    - CO2 injection in a sample and in an aquifer (H problem)

- **Advanced users**
  - Basic description of:
    - Geometry; Boundary conditions
    - Materials, Mesh; Post-process
  - Type of analysis: Non-linear, coupled
  - Examples:
    - Dam (H-M problem)
    - Mock-up test (T-H-M problem)
    - CO2 injection in an aquifer-caprock system (H-M problem)
    - Sequential Excavation method (H-M problem)
    - Consolidation of a porous medium with a vertical joint (H-M problem)
    - Hydraulic shear test with a horizontal joint (H-M problem)
    - BExM tutorial (H-M problem)
    - Atmospheric tutorial (T-H-M problem)

**WE USE THEM AT BACHELOR AND MASTER SELECTED CLASSES**
Geotechnical and Environmental Coupled Models Involving Unsaturated Soils and Rocks
CODE_BRIGHT-GiD
Part II APLICATIONS
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The spent nuclear fuel elements are disposed of in a repository located deep in the Olkiluoto bedrock. The release of radionuclides is prevented with a multi-barrier disposal system consisting of a system of engineered barriers (EBS) and host rock such that the system effectively isolates the radionuclides from the living environment.
THM applications

Erdem Toprak PhD
and related papers

Temperature

67.2
66.389
63.579
61.768
59.958
58.147
56.337
54.526
52.716
50.905

Temperature

67.2
66.389
63.579
61.768
59.958
58.147
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GiD

GiD

GiD
Buffer and backfill materials

- Friedland clay
- MX-80
- Rod pellets
- Minelco granules
- Pillow pellets
Rod Pellets

Infiltration

Oedometer Test
Interpretation of double structure by means of simple models
Windows environment – CPU time

Personal Computer Windows
Intel Visual Fortran with OpenMP

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<th>Wall clock time</th>
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Main frame computer Unix
Intel Fortran with OpenMP

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3D model
THM
(3982 x 5dof = 19910 dof)
Concluding remarks

- This case uses ≈90% of CPU time for the solver. If the solver was fully parallelizable (90%), speed up would be limited by 10.
- Only matrix times vector operations have been parallelized.

However:
Parallelized portion “p” is problem dependent

But:
It increases with problem size
Theoretical vs calculated speed up

Windows PC

- Theoretical $p = 0.9$
- Theoretical $p = 0.85$
- Calculated (KBS3V-3D)

3D model THM (3982 x 5dof = 19910 dof)

Unix MainFrame

- Theoretical $p = 0.9$
- Theoretical $p = 0.85$
- From model
Theoretical vs calculated efficiency

3D model THM (3982 x 5dof = 19910 dof)
HORIZONTAL SPENT FUEL DISPOSAL

Project by POSIVA
Contract by Saanio and Riekkola Oy

- CANISTER
- BUFFER (in Supercontainers and in Distance blocks)
- HOST ROCK
Ivan Puig post doctoral work
MODEL GEOMETRY AND COMPONENTS

- 5th canister
- Buffer block: distance blocks
- 4th canister
- Fracture crossing location
- Gap (Installation state), otherwise, Slot (Initial state)
- Supercontainer
RESULTS: HOST ROCK THICKNESS

Temperature: tunnel axis distribution

(Initial state)

±20 m host rock
(close-field only)

±100 m host rock
(close-field and far-field)
RESULTS

(Initial state)

Temperature: whole domain distribution

10 years

100 years

1000 years
RESULTS: OPEN-GAP EFFECT

Degree of Saturation
1 year (after canisters placement)
RESULTS: OPEN-GAP EFFECT

Temperature at canisters center:

- Installation
- Initial

~ 8 years slower

Temperature at 3rd canister

- Installation
- Initial

~ 8 years slower
RESULTS: OPEN-GAP EFFECT

Degree of Saturation

Installation:

~ 4 years faster

Initial:
Pullout in lab: Calibrate the numerical model!

Finite element mesh: Hexahedral elements & structured mesh (1350 elements & 1652 nodes)

Ivan Puig Damians contributions as part of PhD at UPC
Pullout in lab: Series of tests! STEEL LADDERS
Fully Pullout in lab: 2·10^-6 m/s displacement applied at the head-edge of the reinforcement... ...which generates about 20-cm axial displacement at 11 step

Total displacements with deformed mesh (factor x10)
Pullout in lab: Series of tests! POLYMERIC STRIP

- Displacement (mm)
- Pullout load, Pr (kN)
- z = 1.0 m
- z = 3.5 m
- z = 7.0 m
- 3D Model:
  - z = 7.0 m (c_i = 14 kPa)
  - z = 3.5 m (c_i = 9.4 kPa)
  - z = 1.0 m (c_i = 1 kPa)

Measured:
- z = 7.0 m
- z = 3.5 m
- z = 1.0 m

F* = 0.40
F* = 0.50
F* = 0.56
### 3D Models

**Vertical displacements with Original Mesh:** (factor $\times 1$)

**med mesh**
- Factor: $\times 1000$

**Axial stresses at reinforcing elements**

- Structured mesh & Hexahedral elements
  - Nº elements: 322008
  - Nº nodes: 335748

**Fill-panel interface material**
- Elastomeric joint material (bearing pads)
- Strip footing

**Precast concrete panels**
- Foundation (natural soil)

**Facing panels**
- Bearing material

**Reinforcement-to-facing connection detail**

**End-reinforcement detail**

**Natural Soil (retained fill)**
- Reinforced fill (heavy compaction)
- Reinforced fill (low compaction)

**Precast concrete panels**

**Structured mesh & Hexahedral elements**
- Nº elements: 322008
- Nº nodes: 335748

**Reinforced fill (heavy compaction)**

**Reinforced fill (low compaction)**

**Precast concrete panels**

**Foundation (natural soil)**

**3D Models**
A 1D gas injection test, performed on compact bentonite, is currently underway at the British Geological Survey.

The test is comprised of two stages:

- **hydration** (using distilled water)
- **gas testing** (using helium)

After gas breakthrough and a period of gas flow through the sample, the injection pump was stopped whilst the stresses and porewater pressures have been continuously monitored.
Pressure from test data

![Graph showing pressure (kPa) vs. time (d) for different arrays and injection parameters. The graph highlights phases such as Hydration, Gas pressurization, and Gas Breakthrough.](image-url)
Inflow and outflow from test data

Flow rate (m$^3$/s) at STP

-1.0E-08 -5.0E-09 0.0E+00 5.0E-09 1.0E-08 1.5E-08 2.0E-08

0 10 20 30 40 50 60 70 80 90 100 110 120 130

Time (d)

Inflow

Hydration

Outflow

Gas pressurization

Gas Breakthrough

No gas injection
Model generation: volumes and mesh

Volumes-material definition

Porous stone

Clay

F.E. mesh definition
Intrinsic permeability heterogeneous in 3 zones (weighting 1/6, 1/6, 2/3).
Porosity set to 0.40, 0.41 and 0.42 respectively for:
k₀ = 2.15, 3.90, 7.10 x 10⁻¹⁹ m² and p₀ = 37.8, 27.0, 19.4 MPa
Elastic modulus = 307 MPa and Poisson ratio = 0.44

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<th>Porosity</th>
<th>Intrinsic permeability</th>
<th>Water retention curve</th>
<th>Relative permeability</th>
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<th>b₀</th>
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<td>2.66×10⁻⁶</td>
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<tr>
<td>-</td>
<td>m²</td>
<td>MPa</td>
<td>n-power</td>
<td>m</td>
<td>m</td>
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at 50 days

(INJECTION)
Gas advection at 60 days

at 60 days
(INJECTION)
Gas advection at 70 days

**(INJECTION)**

at 70 days

Contour Fill of $q_{\text{gas\_advective}}$, $|q_{\text{gas\_advective}}|$.  

Step 70

![Graph showing gas pressure over time](image)

- **measured**
- **calculated**

Injection

Backpressure

Gas pressure (kPa)

Time (days)
Gas advection at 80 days

at 80 days
(INJECTION)

Graph showing measured and calculated gas pressure over time.
Gas advection at 90 days

at 90 days
(INJECTION)

Gas pressure (kPa)

Time (days)

measured

calculated

Injection

Backpressure

Contour Fill of \( q_{\text{gas advective}} \), \( |q_{\text{gas advective}}| \).
Flow rates and fluxes

Figure 6. Inflow evolution results: (a) Hydraulic model, (b) HM model_1, and (c) HM model_2.

Figure 7. Outflow evolution results: (a) Hydraulic model, (b) HM model_1, and (c) HM model_2.
**Pressures and stresses**

**Figure 8.** Pore pressure evolution results: (a) Hydraulic model, (b) HM model_1, and (c) HM model_2.

**Figure 9.** Injection and backpressure evolution results: (a) Hydraulic model, (b) HM model_1, and (c) HM model_2.

**Figure 10.** Stress results evolution results (hydro-mechanical models): (a) HM model_1 and (b) HM model_2.
• CI MNE and in particular GID play a key role in our research and technological development

• Thanks for your attention

• Questions?

• Other applications: CO2, Yucca M, Earth Dams, Metro Station, …
Modelling of Lechago Dam

Núria Pinyol doctoral and post doctoral contributions

A paper modelling Beliche Dam published in Geotechnique was awarded by Institution of Civil Engineers (Crampton Price)
5. Comparison with field measurements

Settlements. Base case

Inclinometer I1

Inclinometer I3

Inclinometer I6
Modelling of Lechago Dam

Central cross-section:

Geometry, materials and mesh:

Rockfill shells
Clay core
Drain material
Bedrock
Soft deltaic soil
Alluvium soil
Modelling of Lechago Dam

**Rockfill material:** A constitutive model for Rockfill (Oldecop and Alonso, 2000)

**Clay core:** Barcelona Basic Model (Alonso et al., 1990)

**Oedometric test**
(Experimental data by Oldecop and Alonso, 2001)

**Triaxial test at suction of 0.1 MPa**
Confined stress = 0.5 MPa
(Experimental data by Chávez, 2004)

**Saturated oedometric test on a compacted clay sample initially saturated at constant vertical stress (0.02 MPa)**

**Oedometric test on a compacted clay sample. Saturation at constant vertical stress (0.6 MPa)**
Modelling of Lechago Dam

Hydro-Mechanical response: Vertical displacements
Modelling of Lechago Dam

Hydro-Mechanical response: Pore water pressure
Thanks for your attention
Sequential excavation

Cut and cover stations

Thickness: from 0.30 m to 0.60 m

Shotcrete + Wiremesh

Marquês
Sequential excavation

Sequential excavation of elliptical shaft in unsaturated soil

Salgueiros Station: Metro do Porto
Sequential excavation

- Coupled behaviour of Hydro and Mechanical Phenomena
- Unsaturated conditions: Mohr-Coulomb model
- Stiffness and strength variation with depth
Sequential excavation

Results: Ground Displacements

- Stiffness variation due to the suction and strain levels
- Higher values of $K_0$ - 0.7 or even greater
- Stiffness for the structural elements
Results: Ground Displacements

- Complete different behaviour for the different point of the ellipse
- Small shafts, although having 3,30m diameter were very flexible
- Important horizontal movements
CO₂ emissions have risen dramatically over the last decades

**Affection to climate**
CO₂ Capture & Sequestration (CCS)

**INTRODUCTION**

\[ \rho_{CO_2} < \rho_w \]

\[ \mu_{CO_2} \approx 0.1 \mu_w \]

\[ z > 800 \text{ m} \]

\[ \Delta T \Rightarrow \Delta \sigma' \]

\[ \Delta P \Rightarrow \Delta \sigma' \]
CO₂ density varies significantly within the CO₂ bubble because of pressure and temperature differences.
CO2 thermally equilibrates with the formation abruptly. CO2 dissolution into the brine increases temperature.

Exothermal CO₂ dissolution

CO₂ bubble interface

Cold CO₂ injection

20 °C

57.5 °C
Mechanical stability

Isothermal injection increases horizontal stresses due to lateral confinement. Thermal contraction of the rock decreases both vertical and horizontal stresses. This increases the mobilized friction angle in the aquifer, but decreases it in the caprock.

Victor Vilarrasa (PhD at UPC supervised by Carrera and Olivella) received EGU award for contributions on CO2 sequestration
Deep geological repository for high-level nuclear waste

- THM coupling in the host rock

Yucca Mountain, Nevada, US

INTERNATIONAL BENCHMARK - DECOVALEX III
Deep geological repository for high-level nuclear waste

- Yucca Mountain, Nevada, US
  - Unsaturated fractured tuff
  - No engineered barrier
THM coupling in the host rock

- Evaporation and condensation of water (fractured rock)

- Fracture response to an increase of temperature

Shear slip

Fracture closing

FE mesh for double structure THM calculations

6508 nodes
15973 elements
5 d.o.f.

matrix

fracture
Degree of saturation at 4 year: Matrix and fracture

Different water content per unit volume of pores due to different retention properties

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