Developments in a Coupled Thermal-Hydraulic-Chemical-Geomechanical Model for Soil and Concrete

S.C. Seetharam* and D. Jacques
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*suresh.seetharam@sckcen.be
Outline

- Potential applications
- Objective
- Governing equations
- COMSOL-MATLAB
- Sample Benchmarks
- Conclusions and perspectives
Potential applications

- Significant experimental and numerical research on coupled THCM behaviour for soil and concrete applications.

Current interest

- Nuclear waste repository
- Ground freezing
- Petroleum
- Geotechnical in general

Deep disposal
Near-Surface disposal
Potential applications...

THCM: In situ Processes in deep disposal repository in Boom Clay

CHM: Impact of bitumen waste on Boom clay

THM: Design phase - Half scale test - Supercontainer

H, CM, CH: Near surface disposal concept based on concrete as predominant material

http://science.sckcen.be/en/Institutes_groups/EHS
### Well known process interaction matrix for Porous media applications

<table>
<thead>
<tr>
<th></th>
<th>Temperature</th>
<th>Hydraulic</th>
<th>Chemical</th>
<th>Mechanical</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>Conduction</td>
<td>Convection</td>
<td>Dufour effect</td>
<td>Volumetric deformation</td>
</tr>
<tr>
<td></td>
<td>(Fourier’s Law)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hydraulic</td>
<td>Thermal osmosis</td>
<td>Pressure flow</td>
<td>Chemical osmosis</td>
<td>Volumetric deformation</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(Darcy’s law)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chemical</td>
<td>Soret effect</td>
<td>Advection</td>
<td>Diffusion</td>
<td>Volumetric deformation</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(Fick’s Law)+Reactions</td>
<td></td>
</tr>
<tr>
<td>Mechanical</td>
<td>Thermal expansion</td>
<td>Swelling/Shrinkage</td>
<td>Swelling/Shrinkage</td>
<td>Stress/Strain Equilibrium</td>
</tr>
</tbody>
</table>
Objective

Develop a generic fully coupled THCM model within COMSOL-MATLAB environment

MATLAB Environment

THCM Model (COMSOL)

Geochemical Model
Source term for the "C component" (e.g. PHREEQC)
Governing equations

**Energy conservation**

\[
\begin{align*}
\frac{\partial}{\partial t} \left[ (1-n)C_p \rho_s \right] + \frac{n}{C_p} \left[ S_p \rho_s \right] + \frac{n}{C_p} \left[ S_p \rho_s \right] = (T - T_f) + \ln S_s \rho_s
\end{align*}
\]

**Mass conservation – pore water pressure**

\[
\begin{align*}
\frac{\partial \rho_w}{\partial t} + \frac{\partial \rho_s}{\partial x} &= -\nabla \cdot \left[ \rho_w \psi_w + \nabla \psi_w + \nabla z \right]
\end{align*}
\]

**Stress equilibrium**

\[
\nabla \left[ (C : (\varepsilon - \varepsilon_{th} - \varepsilon_{le})) - \chi P_s I - P I \right] + b = 0
\]

**Mass conservation – pore gas pressure**

\[
\begin{align*}
\frac{\partial \rho_{da}}{\partial t} &= -\nabla \left[ \rho_{da} \psi_{da} \right]
\end{align*}
\]

**Charge conservation**

\[
\begin{align*}
\frac{\partial \theta c_i}{\partial t} &= \nabla \cdot \left( \rho \nabla \psi_c \right) + \frac{F \theta}{\varepsilon} \sum c_i z_i = 0
\end{align*}
\]
Inbuilt solute interface (introduce cross coupling terms using source term)

Dilute species model used because it offers numerical stability schemes – this means the formulation requires further adaptation to include porosity.

3 governing equations (TH)

PDE form (based on equations in slide 7)

Geomechanical (M)

Inbuilt solid mechanics interface (introduce cross coupling terms (e.g. pore water pressure) and geomechanical constitutive laws applicable for soil and concrete)

Implemented soil models (useful for describing Boom clay behaviour) using COMSOL’s generic plasticity feature:

- Mohr-Coulomb
- Drucker-Prager
- Etc…

Multi-component (as many governing equations as the number of chemicals, $C_i$)
Benchmark 1

Infiltration under isothermal conditions (Hydro-mechanical coupling)

\[
\frac{\partial \rho \theta}{\partial t} = -\nabla \cdot \rho \left( -K \left[ \nabla \psi_m + \nabla z \right] \right)
\]

\[
\nabla \left( (C : \varepsilon) - \chi P_f I - P_s I \right) + b = 0
\]
Infiltration under isothermal conditions...

Test equipment (CIEMAT, Spain) and model idealisation for the infiltration experiment under isothermal conditions

Porosity: COMSOL (left) and Chen et al. (right) – scale not same
Benchmark 2

THM response of the in-situ ATLAS III Experiment

\[ \frac{\partial}{\partial t} \left[ \left(1-n\right)C_{\rho}\rho + n\left(C_{\rho}S_{\rho}(T)\right) \right] (T-T_r) = \nabla \cdot (-\lambda \nabla T) + \left(C_{\rho} y_n \rho \right)(T-T_r) \]

\[ \frac{\partial \rho_i(T)}{\partial t} \theta_i = -\nabla \cdot \rho_i \left(-K_i(T) \nabla \psi_i \right) \]

\[ \nabla \cdot \left( C \left( \varepsilon - \varepsilon_{th} - \varepsilon_{w} \right) \right) - P \mathbf{1} = 0 \]
Conceptual model and data

Boom clay

Pore pressure fixed = 4.5 MPa

Key features:
- Fully coupled THM
- Axisymmetric
- Fully saturated
- Viscosity and density as a function of temperature
- Thermo-Elasto-plastic (Drucker Prager) model
- Two materials = steel + boom clay
- COMSOL computation time = 0.5 hours

\[
f = J + \frac{2\sqrt{3}\sin\varphi}{3 - \sin\varphi} (p - c \cdot \cotg\varphi)
\]

\[
g = J + \frac{2\sqrt{3}\sin\psi}{3 - \sin\psi} (p - c \cdot \cotg\psi)
\]

Chen and Li, 2009
Temperature and pore water pressure evolution
Radial displacement, mean effective stress and plastic strain

Note: Plastic region is insignificant and hence not shown (limited to few elements in the domain.)
Benchmark 3

Chemo-osmotic flow

\[ \frac{\partial \rho \theta_l}{\partial t} = -\nabla \cdot (\rho (-K_l [\nabla \psi_m + \nabla \psi_o])) \]

\[ \frac{\partial (\theta c_i)}{\partial t} = -\nabla \cdot (D \nabla c_i + c_i v_i) \]
Keijzer’s experiment

<table>
<thead>
<tr>
<th></th>
<th>Porous stone</th>
<th>Clay</th>
<th>Porous stone</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_i$</td>
<td>$0.1 \text{ mol/l}$</td>
<td>$0.1 \text{ mol/l}$</td>
<td>$0.01 \text{ mol/l}$</td>
</tr>
<tr>
<td>$P_f$</td>
<td>$0 \text{ Pa}$</td>
<td>$0 \text{ Pa}$</td>
<td>$0 \text{ Pa}$</td>
</tr>
</tbody>
</table>

Pressure evolution at the interface between the left porous stone and the clay

Transient pressure profile

Clay zone

- $dC_i/dn = 0$
- $dP_f/dn = 0$
- $P_f = 0$

![Graph showing pore water pressure evolution over time](image-url)

- COMSOL
- Measured (Bader and Kooi, 2005)
Benchmark 3

Reactive transport (COMSOL-MATLAB)

\[ \frac{\partial (\theta c)}{\partial t} = -\nabla \cdot (D \nabla c + c \nabla \theta) - R \]

Phreeqc coupling via MATLAB – use sequential non-iterative approach (other approaches also tried, no difference for the specific problems chosen)
Ion exchange, Mineral dissolution verifications

\[ \text{CaCl}_2 \rightarrow \text{Na-K-NO}_3^{2-} + \text{Exchanger} \]

Advection-diffusion

Comparison made with open source code HP1, developed at SCK-CEN

Initial portlandite = 4 mM

Low pH boundary

Ca \approx 20 \text{ mM}, \quad \text{pH} \approx 12.5

Diffusion only

Ca \approx 20 \text{ mM}, \quad \text{pH} \approx 12.5

Portlandite dissolution

Note: More complex chemistry successfully demonstrated in a forthcoming journal publication

Conclusions and perspectives

- Model implementation and benchmark results highly encouraging.

- Further work ongoing in terms of chemo-mechanical coupling, plus more and more verifications/validations.

- Computational constraints especially iterating between COMSOL-MATLAB. Perhaps COMSOL can consider this in future versions.

- COMSOL: easy to implement and serves as a powerful research tool.
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Studiecentrum voor Kernenergie
Centre d’Etude de l’Energie Nucléaire
Belgian Nuclear Research Centre

Stichting van Openbaar Nut
Fondation d’Utilité Publique
Foundation of Public Utility

Registered Office: Avenue Herrmann-Debrouxlaan 40 – BE-1160 BRUSSELS
Operational Office: Boeretang 200 – BE-2400 MOL