Two-Phase Flow Numerical Modeling: Application to a Geological Nuclear Waste Disposal

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OUTLINE

- Industrial context: Nuclear waste storage
- A classical two-phase flow model
- An example of application: modeling of a disposal cell for an intermediate level long-lived waste (Benchmark Couplex Gaz 1 submitted by Andra)
  - Presentation of the problem
  - Numerical methods:
    - Classical FE Scheme: Discretization and results
    - Hybrid Finite Volume method: overview and first results
- A first 3D study: modeling of a modulus of High level long-lived waste (Benchmark Couplex Gaz 2 submitted by Andra)
  - Results
  - Perspectives
- Conclusions
Industrial context: Underground waste storage

- A fully coupled THMC problem on a complex geometry!
- Main reasons of two-phase flow modelling:
  - Presence of initially unsaturated media (plugs, sealing ...)
  - Ventilation of the galleries
  - Thermal drying
  - Hydrogen production due to corrosion of steel components (containers, casing)
- Hydraulic specificities:
  - High level of capillary pressure (50 Mpa) and high level of gas pressure (due to corrosion)
  - Saturation closed to one in the geological media
A classical two-phase flow model

✓ 2 components (H₂ and H₂O) in 2 phases (liquid and gas)
✓ Capillary relation \( P_c = f(S_t) = P_g - P_l \)
✓ Mass conservation for water and hydrogen:

\[
\frac{\partial}{\partial t}(m_c) + \text{Div}(F^c_l + F^c_g) = Q_c \quad c = H_2, H_2O
\]

✓ Transport equations:

- Darcy’s law for each phase

\[
F_i = -\frac{k_i(S_t)}{\mu_i}(\nabla P_i - \rho_i g)
\]

\[
F_g = -\frac{k_g(S_t)}{\mu_g}(\nabla P_g - \rho_g g)
\]

- Diffusion law linking component velocities in each mixture (Fick’s Law)

\[
\frac{F^H_2O_{g}}{\rho^H_2O_{g}} + \frac{F^H_2_{g}}{\rho^H_2_{g}} = -F_g \nabla C_g
\]

\[
\frac{F^H_2O_{l}}{\rho^H_2O_{l}} + \frac{F^H_2_{l}}{\rho^H_2_{l}} = -F_l \nabla C_l
\]

- Dissolution (Henry’s Law)

- Vaporization (equilibrium equation)
Main modelisation difficulties

✓ Injection of gas in a saturated porous media
  • Geological media initially saturated: what is the initial concentration of hydrogen or air in the liquid?
  • High level of gas pressure

✓ Presence of multiple barriers
  • Very high level of heterogeneities of the different materials
  • Initial level of saturation very dependant of the material

✓ Huge non linearities
  • Capillary and Relative permeabilities functions (influencing type of equations and front shape)

Ex. for relative permeabilities

\[
\begin{align*}
    k_{rel}^1 &= \sqrt{S_i \left(1 - \left(1 - S_i \frac{1}{m}\right)^m\right)^2} \quad \text{(Van Genuchten)} \\
    k_{rel}^l &= S_i^A S_i^{B+1/\lambda} \quad \text{(Brooks&Corey)} \\
    k_{rel}^l &= S_i^3 \quad \text{(cubic)}
\end{align*}
\]

\[
\frac{\partial (\phi \rho_i S_l)}{\partial t} + \text{Div} \left( k_{rel}^l \left( \frac{k_{rel}^l(S_l)}{\mu_l} \right)(\nabla P_l) \right) = Q
\]
Modeling of a disposal cell for an intermediate level long-lived waste:

- Anisotropic problem (in the clay $K_h \neq K_v$)
- Total hydrogen Flux for each primary package:

$Q_{H2}$

- $6.25$ mol/year
- $0.5$ mol/year

$P_i = 4.2$ Mpa

$P_i = 5.5$ Mpa

$Q = 0$ $Q = 0$

$t$ (year)

500 years 10 000 years
COUPLEX-GAZ I: caracteristic curves – Van Genuchten Mualem model

\[ S_l = \frac{1 - S_{wres}}{m} + S_{wres} \]

S(Pc)

Singualrity for \( S = 1 \):

\[ \frac{\partial S}{\partial P_c} = 0 \quad \frac{\partial k^g}{\partial S_w} = \infty \quad \frac{\partial k^w}{\partial S_w} = \infty \]

2\textsuperscript{nd} order polynomial C1
Interpolation for \( S > S_{\text{max}} \)
(ex. \( S_{\text{max}} = 0.99 \))

\[ k_{rel}^l = \sqrt{S_{we}} \left( 1 - \left( 1 - S_{we} \right)^{1/m} \right)^2 \]

\[ k_{rel}^g = \sqrt{1 - S_{we}} \left( 1 - S_{we}^{1/m} \right)^{2m} \]
COUPLEX-GAZ I : Exercice definition (2/2)

✓ Couplex’s initial conditions : high contrast of saturation and capillary pressure

<table>
<thead>
<tr>
<th></th>
<th>$S_{init}$</th>
<th>$P_{C_{init}}$</th>
<th>$K$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Filler concrete</td>
<td>0.7</td>
<td>3 Mpa</td>
<td>$10^{-18}$ m$^2$</td>
</tr>
<tr>
<td>Concrete of package</td>
<td>0.6</td>
<td>4.4 Mpa</td>
<td>$10^{-19}$ m$^2$</td>
</tr>
<tr>
<td>clearance</td>
<td>0.1</td>
<td>6 Mpa</td>
<td>$10^{-12}$ m$^2$</td>
</tr>
<tr>
<td>Primary package</td>
<td>0.2</td>
<td>0.8 Mpa</td>
<td>$10^{-15}$ m$^2$</td>
</tr>
</tbody>
</table>

• In the clay (healthy, disturbed or fractured) :

  $S = 1$

  Hydrostatic liquid pressure

✓ Actually, we consider a small gas pressure : $P_g = 1$ atm (corresponding to a initial concentration of hydrogen in liquid)
Couplex Gaz modelisation’s tool (www.code-aster.org)

- Choice of the unknowns: Pc and Pg
  - In our formulation, we write
    \[ \frac{\rho_l^H}{M_{H_2}^{ol}} = \frac{P_g^H}{K_H} \]
  - In saturated area: \(S_l = 1\)

Variable transformation:
\[ \hat{P}_g = \frac{K_H}{M_{H_2}^{ol}} \rho_l^H \quad \Rightarrow \quad Pc = \hat{P}_g - P_l \leq 0 \]

A Classical Finite Element method:

- Finite Elements with Q1 elements
- Lumping of the mass matrix:
  - Non diagonal mass matrix \(\Rightarrow\) maximum principle not verified \(\Rightarrow\) Oscillations
  - Integration points at the vertex of the elements

- Time discretization = Implicite Euler
- Newton method for non linear resolution
COUPLEX-GAZ I : Gas saturation and capillary pressure profiles – X = 103 m

- Vertical cross section

- 3 steps:
  1. Capillary equilibrium (t<200 years)
  2. Small desaturation by gas production (t<10000 years)
  3. The gas disappears gradually

- Complete saturation at 60000 years!

Two-phase flow numerical modeling : Application to a Geological Nuclear waste disposal
Maximal Gas Pressure of 6,75 Mpa at 10 000 years– The pressure remains constant in the engineered area
COUPLEX-GAZ I : Using of a Hybrid Finite Volume scheme (1/4)


On an elliptic problem

\[-\nabla \cdot (\Lambda \nabla u) = f\]

- Volumic integration:
  \[-\sum_{\sigma \in \varepsilon_K} F_{K,\sigma} = \int_K f \quad \text{with} \quad F_{K,\sigma} \approx \int_{\sigma} \Lambda \nabla u \cdot n_{K\sigma} \cdot d\sigma\]

- Flow calculation
  \[F_{K,\sigma} = m_{\sigma} \Lambda_K \left[ \left( \frac{u_{\sigma} - u_K}{d_{K\sigma}} \right) + \left( \nabla_D u \right)_K \left( n_{K\sigma} - \alpha_K \frac{x_{\sigma} - x_K}{d_{K\sigma}} \right) \right]\]

  Coercivity term
  To determine
  We remove what we added

Computation of discrete flow:

- Flow
  \[(\nabla_D u)_K = M_K \cdot \sum_{\sigma \in \varepsilon_K} m_{\sigma} \left( n_{K\sigma} - \alpha_K \frac{x_{\sigma} - x_K}{d_{K\sigma}} \right) (u_{\sigma} - u_K)\]

- Consistence
  \[M^{-1}_K = \sum_{\sigma \in \varepsilon_K} m_{\sigma} \left( n_{K\sigma} \otimes (x_{\sigma} - x_K) - \alpha_K \frac{x_{\sigma} - x_K}{d_{K\sigma}} (x_{\sigma} - x_K) \otimes (x_{\sigma} - x_K) \right)\]

- Finally
  \[F_{K,\sigma} = \sum_{\sigma'} (C_K)_{\sigma,\sigma'} (u_{\sigma'} - u_K)\]
Hybrid Finite Volume for two phase flow modeling

- Mass conservation for the two constituents
  \[
  \frac{A_k}{\Delta t} \left( m_k^p - m_k^{p-} \right) - \sum_{\sigma} \sum_{\sigma'} k_{\sigma} \left( C_{k} \right)_{\sigma,\sigma'} (u_{\sigma}^p - u_{\sigma}^p) = 0
  \]

- Flow continuity
  \[
  \sum_{\sigma} \sum_{\sigma'} \left( C_{k} \right)_{\sigma,\sigma'} (u_{\sigma}^p - u_{\sigma}^p) + \sum_{\sigma} \sum_{\sigma'} \left( C_{L} \right)_{\sigma,\sigma'} (u_{\sigma}^p - u_{\sigma}^p) = 0
  \]

- Upstream flow
  \[
  \text{if } F_{k,\sigma}^p \leq 0
  \]
  \[
  k_{\sigma}^p = k^p \left( u_{\sigma}^p \right)
  \]

  \[
  \text{else}
  \]
  \[
  k_{\sigma}^p = k^p \left( u_{\sigma}^p \right)
  \]

- Unknowns:
  - \( P, S \) at the center,
  - \( P_I \) and \( P_g \) at the interface

FE structure
COUPLEX-GAZ I : Using of a Hybrid Finite Volume scheme (3/4)

Vertical cross section

Gas Pressure (X=103m)

Not exactly the same case (no gravity and isotropic permeability), but closed results
In this test, Hybrid Finite Volume method allows us:

- A better initial saturation condition (S is an unknown instead of Pc)
- Good performance (better matrix profile):

<table>
<thead>
<tr>
<th></th>
<th>FE</th>
<th>HFV</th>
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</thead>
<tbody>
<tr>
<td>Max nb of iterations per time step</td>
<td>43</td>
<td>10</td>
</tr>
<tr>
<td>Total nb of Newton iterations</td>
<td>5230</td>
<td>5220</td>
</tr>
<tr>
<td>Average nb of iterations per time step</td>
<td>12</td>
<td>3</td>
</tr>
<tr>
<td>Total CPU Times</td>
<td>24</td>
<td>26</td>
</tr>
</tbody>
</table>

Promising method (sushis developments)...
A 3D application: Couplex 2 (1/3)

3D Modeling of a modulus of High level long-lived waste:

Length of modulus: \( L_y = 100 \text{m} \)
Width of the modulus: 30m

Gas production around each cell:

- \( Q_{H2} \) (mol/year/cell)
  - 100 mol/year/cell
  - 15 mol/year/cell

\[ Q_{H2} \text{ (mol/year/cell)} \]

\[ t \text{ (year)} \]

16 mol/year/cell

Two-phase flow numerical modeling: Application to a Geological Nuclear waste disposal
A 3D application: Couplex 2 (2/3)

- Initial conditions:
  - In the geological media:
    - $S=1$; Hydrostatic liquid pressure
  - In plugs and drifts:
    - $S=0.7$; $P_g = 1$ atm

- Material datas:
  - Mualem/Van Genuchten model

Numerical scheme: Classical FE scheme (sequential computation)

Mesh: 115,000 elements – 160,000 nodes – 287,000 equations

Performances: CPU time: 100 hours for simulation of 500,000 years
A 3D application: Couplex 2 (3/3)

Gas pressure evolution

Saturation evolution

4500 yrs

cement

bentonite

Two-phase flow numerical modeling: Application to a Geological Nuclear waste disposal
Conclusions

- Description of a coupled two-phase flow model:
  - Model of gas transfer in porous media
  - 2 phases, 2 constituents
  - Diffusion in gas and liquid mixture

- Application to industrial studies (underground waste storage modeling):
  - **Benchmark Couplex 1 (2D - intermediate level long-lived waste)**
    - Treated with a classical FE method
    - Partially treated with a promising Hybrid Finite volume method
  - **Benchmark Couplex 3 (3D - High level long-lived waste)**
    - First results obtained with a sequential FE method and a coarse mesh
    - To be continued with a parallelism strategy
    - To be continued with Hybrid Finite volume method (Sushi Method – PHD O. Angelini)