Modelling advective gas flow in compact bentonite: Lessons learnt from different numerical approaches


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Introduction
Nuclear waste has **high level of radioactivity** and a **long half-life**.

For protecting human being and ensure environmental safety. After years of international research, it is considered that "Deep Geological Disposal" is the preferred option.

To isolate it from the biosphere, nuclear waste is buried in the geology below more than 400m, and then the canister and buffer materials are used to cover and place.

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**Fig.1. Schematic cross-section (reference from Rebecca Lunn)**

**Fig.2. Design concept for the Deep Geological Disposal (figure from Gilles Corman)**
Gas may be generated due to the corrosion of metallic materials under anoxic conditions ($H_2$), the radioactive decay of waste ($Rn$) and the radiolysis of water ($H_2$).

- When gas production rate is slow, gas dissolve in porewater, and migrate by advection and diffusion.
- When gas production rate exceeds gas diffusion rate, a discrete gas phase will form, parts of porewater is displaced by gas.

**Fig. 3.** The mechanisms of gas migration in clays. (from Marschall et al.)
When gas pressure accumulates to a very high value (called gas breakthrough), gas pressure cannot withstand stress acting on the rock mass, gas might follow by pathway dilation and tensile fractures, and then escape from the bentonite.

Fig.3. The mechanisms of gas migration in clays. (from Marschall et al.)
Therefore, gas migration in the bentonite becomes a key issue for the safety assessment of the nuclear waste disposal.

However, the detail of the mechanisms of gas migration is unclear. Several international projects aim to understand have already been conducted.

An international projects called DECOVALEX-2019, the Task-A is modelling gas injection experiments to develop novel numerical techniques.
Objective

To develop novel numerical techniques about gas migration. This paper summarizes the outcomes of work in Task-A and a synthesis of the work of the participating modelling teams.
In this task, two different gas injections experiments undertaken by the British Geological Survey (BGS) were used:

(a) Test-1: a 1D gas flow test
(b) Test-2: a 3D (spherical) gas flow test

Two different gas injections

Red arrows: gas outflow emitted from the gas filters into bentonite
Green arrows: gas outflow detected by gas filters

Gas injection experiments

Pressure vessel (in order to imitate the surrounding) contains bentonite sample.
**Experimental data: Test-1**

**Fig. 4. Schematic drawings of Test-1**

**Table 1**

<table>
<thead>
<tr>
<th>Start Time (days)</th>
<th>Injection pump rate (µL/h)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>39</td>
<td>0</td>
<td>Gas pressure: 3 MPa</td>
</tr>
<tr>
<td>46.135</td>
<td>500</td>
<td>Initial gas volume: 235 ml</td>
</tr>
<tr>
<td>54.149</td>
<td>375</td>
<td>Start of injection pump</td>
</tr>
<tr>
<td>60.959</td>
<td>0</td>
<td>Reduce injection pump flow rate</td>
</tr>
<tr>
<td>71.369</td>
<td>0</td>
<td>Gas refilled (+59.95 ml, pressure maintained)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Injection pump stopped</td>
</tr>
</tbody>
</table>

Day 39 add additional helium and then gas pressure increase.

Day 63.8 gas breakthrough (because pathways open, then gas escape).

**Gas pressure decrease after breakthrough**

**Fig. 5. Experimental data from day 0 to day 120**
Experimental data: Test-2

Day 757 major gas breakthrough

Table 2
Injector schedule for the point-injection experiment.

<table>
<thead>
<tr>
<th>Start Time (days)</th>
<th>Injection pump rate (µL/h)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>720.3</td>
<td>125</td>
<td>Gas pressure: 5 MPa</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Initial gas vol.: 211 ml</td>
</tr>
<tr>
<td>768.3</td>
<td></td>
<td>Gas refilled (+91.3 ml @ 9.5 MPa)</td>
</tr>
<tr>
<td>799.2</td>
<td></td>
<td>Gas refilled (+72.6 ml @ 8.7 MPa)</td>
</tr>
<tr>
<td>807.4</td>
<td></td>
<td>Gas refilled (+61.2 ml @ 8.4 MPa)</td>
</tr>
<tr>
<td>827.0</td>
<td></td>
<td>Gas refilled (+9.3 ml @ 8.3 MPa)</td>
</tr>
<tr>
<td>831.1</td>
<td></td>
<td>Gas refilled (+47.7 ml @ 8.2 MPa)</td>
</tr>
</tbody>
</table>

Fig. 6. Schematic drawings of Test-2

Fig. 7. Experimental data from day 735 to day 835

Have three times gas breakthrough events
Methodology
Different modelling approaches have been developed through experimental data.

1) Classical two-phase flow models
2) Enhanced two-phase flow models
3) Single-phase flow models
4) Conceptual chaotic model

Table 3
Main properties of the modelling approaches that have been developed during the task (for both experiment 1 and experiment 2).

<table>
<thead>
<tr>
<th>Model</th>
<th>Funding centre</th>
<th>Model type</th>
<th>Mechanical deformation</th>
<th>Hydraulic approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. BGR/UFZ-E</td>
<td>CNSC-PD</td>
<td>continuous</td>
<td>elasticity</td>
<td>two-phase</td>
</tr>
<tr>
<td>2. CNSC-PD</td>
<td>CNSC</td>
<td>continuous</td>
<td>elastoplastic damage</td>
<td>two-phase</td>
</tr>
<tr>
<td>3. KAERI-D</td>
<td>KAERI</td>
<td>continuous</td>
<td>elastic damage model</td>
<td>two-phase</td>
</tr>
<tr>
<td>4. NCU/TPC-V</td>
<td>Taiwan Power Company</td>
<td>continuous</td>
<td>visco-elastic</td>
<td>two-phase</td>
</tr>
<tr>
<td>5. UPC/Andra-ED</td>
<td>ANDRA</td>
<td>continuous</td>
<td>elasticity with dilatancy</td>
<td>two-phase</td>
</tr>
<tr>
<td>6. LBNL-D</td>
<td>US DOE</td>
<td>discontinuous</td>
<td>elastic damage and fracture</td>
<td>two-phase</td>
</tr>
<tr>
<td>7. Quintessa/ RWM-ECap</td>
<td>RWM</td>
<td>continuous</td>
<td>elasticity</td>
<td>single-phase</td>
</tr>
</tbody>
</table>

Table 4
Main numerical features of the modelling approaches that have been developed during the task (for both stage experiment 1 and stage experiment 2). See Appendix A for more details. Note that FE stands for Finite Element, FD stands for Finite Difference and FV for finite volume.

<table>
<thead>
<tr>
<th>Model</th>
<th>Test</th>
<th>Software</th>
<th>Space discretisation method</th>
<th>Number of calibrated parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. BGR/UFZ-E</td>
<td>1,2</td>
<td>OpenGeoSys 5.8</td>
<td>FE</td>
<td>Not provided</td>
</tr>
<tr>
<td>2. CNSC-PD</td>
<td>1,2</td>
<td>COMSOL Multiphysics® 5.4</td>
<td>FE</td>
<td>25</td>
</tr>
<tr>
<td>3. KAERI-D</td>
<td>1</td>
<td>TOUGH2/ FLAC3D</td>
<td>FD</td>
<td>5</td>
</tr>
<tr>
<td>4. NCU/TPC-V</td>
<td>1,2</td>
<td>COMSOL Multiphysics®</td>
<td>THMC 7.1</td>
<td>7</td>
</tr>
<tr>
<td>5. UPC/Andra-ED</td>
<td>1,2</td>
<td>Code_bright 8.6</td>
<td>FE</td>
<td>11</td>
</tr>
<tr>
<td>6. LBNL-D</td>
<td>1,2</td>
<td>TOUGH-RBSN</td>
<td>FV</td>
<td>Not provided</td>
</tr>
<tr>
<td>7. Quintessa/ RWM-ECap</td>
<td>1,2</td>
<td>QPAC 4.2</td>
<td>FV</td>
<td>12</td>
</tr>
</tbody>
</table>
1. Classical two-phase flow models: BGR/UFZ-E

Mass conservation equation:

- **Water phase**
  \[
  \frac{\partial \phi \rho_w S_w}{\partial t} + \phi \rho_w S_w \nabla \cdot \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{q}_w = 0
  \]

- **Gas phase**
  \[
  \frac{\partial \phi \rho_g (1 - S_w)}{\partial t} + \phi (1 - S_w) \rho_g \nabla \cdot \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{q}_g = 0
  \]

Momentum balance equation:

\[
\nabla \left[ \sigma' - \alpha (P_g - S_w P_c) \mathbf{I} \right] + \rho g = 0
\]

The pressure-dependent permeability relationship:

\[
k = f(P_g) = \begin{cases} 
(1 + a P_g) k_{int} & , P_g \leq P_{crit} \\
(b(P_g - P_{crit}) + 1 + a P_{crit}) k_{int}, & \text{otherwise}
\end{cases}
\]

\[
\phi: \text{the porosity of the medium (-)}
\rho_w: \text{the density of water phase (kg/m}^3\text{)}
\rho_g: \text{the density of gas phase (kg/m}^3\text{)}
S_w: \text{the water saturation (-)}
q_w: \text{the flow velocity of water (kg/m}^2\text{·s)}
q_g: \text{the flow velocity of gas (kg/m}^2\text{·s)}
u: \text{the displacement vector (m)}
\sigma': \text{the effective stress tensor (Pa)}
\alpha: \text{the Biot coefficient (-)}
P_g: \text{the gas pressure (Pa)}
P_c: \text{the capillary pressure (Pa)}
\mathbf{I}: \text{the identity tensor}
\rho: \text{the total density (kg/m}^3\text{)}
g: \text{the gravity acceleration (m/s}^2\text{)}

p_{crit}: \text{the critical value of gas pressure (Pa)}
k_{int}: \text{the intrinsic permeability tensor (-)}
a, b: \text{the calibrated constant parameter (m}^2\text{)}
1. Classical two-phase flow models: CNSC-PD

- This hydraulic model is coupled to a non-linear poro-elastoplastic damage model that uses a modified extended Barcelona Basic Model.

- The Pall and Moshenin model is used for the intrinsic permeability:

\[ k_{ij} = \frac{D_{VS}^2 \varphi^3}{180 (1 - \varphi)^2} \]

- \( D_{VS} \): the volume-surface mean diameter (m)
- \( \varphi \): the porosity (-)
1. Classical two-phase flow models: KAERI-D

- The classical multi-phase Darcy's law is used and combined with a mass balance equation for each component.

- This classical two-phase flow model is coupled to the elastic damage model proposed by Tang et al.

- The stress-strain relationship is divided into an elastic phase and a damage phase

\begin{align*}
\text{Before gas breakthrough (elastic model)} : & \quad \sigma' = C : \varepsilon \\
\text{After gas breakthrough (damage model)} : & \quad \sigma' = (1 - D) C : \varepsilon \\
\end{align*}

\[ k_{\text{int}} = k_{\text{int,undamaged}} + k_{\text{int,damaged}} \]
1. Classical two-phase flow models: NCU/TPC-V

Mass conservation equation:

\[
\frac{\partial \rho_\alpha \phi_{S_\alpha}}{\partial t} + \nabla \cdot (\rho_\alpha V_\alpha) + \nabla \cdot (\rho_\alpha \phi_{S_\alpha} V_s) = M^\alpha, \alpha \in \{L\} \quad \sum_{\alpha=1}^{L} S_\alpha = 1
\]

\[
\frac{\partial \rho_s \phi_s}{\partial t} + \nabla \cdot (\rho_s \phi_s V_s) = 0
\]

\(\rho_\alpha\): the density of \(\alpha\)-th fluid phase (kg/m\(^3\))

\(\phi\): the volume fraction (-)

\(S_\alpha\): the normalized saturation of \(\alpha\)-th fluid phase (-)

\(V_\alpha\): the Darcy velocity of \(\alpha\)-th fluid phase (m/s)

\(V_s\): the velocity of the solid (m/s)

\(M^\alpha\): the sum of the artificial source/sink rate of all species in \(\alpha\)-th fluid phase (kg\cdot m\(^3\)\cdot s\(^{-1}\))

\(\rho_s\): the density of the solid phase (kg/m\(^3\))

\(V_s\): the velocity of the solid phase (m/s)

\(\phi_s\): the volume fraction of the solid phase with porosity \(\phi = 1 - \phi_s\) (-)
1. Classical two-phase flow models: NCU/TPC-V

Momentum balance equation:

\[-\nabla \cdot \mathbf{T} + \sum_{\alpha \in \{L\}} \nabla (S_\alpha p_\alpha) - \sum_{\alpha \in \{L\}} \rho_\alpha \phi S_\alpha + \rho_s \phi_s \mathbf{g} \nabla z = -\phi_s \rho_s \frac{d^2 \mathbf{u}}{dt^2} \approx 0\]

\(\mathbf{T}\): the Cauchy stress tensor in the continuum mechanics (Pa)
\(p_\alpha\): the pressure of the \(\alpha\)-th fluid phase (Pa)
\(\mathbf{g}\): the gravitational acceleration (m/s\(^2\))
\(z\): the potential head (m)
\(\mathbf{u}\): the displacement of the media (m)

\[k_{int} = k_{int,0} \left(\frac{1}{1 + (\phi_0 - \phi)}\right)^n\]

\(k_{int,0}\): the reference intrinsic permeability
\(k_{int}\): the intrinsic permeability
\(\phi_0\): the reference porosity
\(n\): the fractional exponent depending on the particle size and packing structure
2. Enhanced two-phase flow models: UPC/Andra-ED

UPC-Andra-ED is a heterogeneous continuous two-phase model, where the standard equations of balance of water, balance of gas and equilibrium of stresses are solved.

This approach is characterized by the coupling of these standard equations to embedded fractures, which allow the representation of preferential pathways.

\[ k_{int} = k_{matrix} + k_{fractures} \]

\[ = \frac{k_0(1-\varphi_0)^2}{\varphi_0^3} \frac{\varphi^3}{(1-\varphi)^2} + \frac{b^3}{12a} \]

- \( k_0 \): the reference permeability (m²)
- \( \varphi_0 \): the initial porosity (-)
- \( \varphi \): the porosity (-)
- \( b \): the fracture aperture (m)
- \( a \): the spacing between fractures (m)
2. Enhanced two-phase flow models: LBNL-D

- LBNL-D is a **discontinuous** two-phase flow model with mechanical deformation and fracture/damage processes.

- The Rigid-Body-Spring Network (RBSN), a lattice approach, is linked to the flow simulator (TOUGH2) in order to facilitate a discrete representation of fracture formations.

- Permeability is porosity dependent.

\[
k = \begin{cases} 
    k_0(1 - \varphi_0)^2 \frac{\varphi^3}{\varphi_0^3 (1 - \varphi)^2}, & \text{if unfractured} \\
    k_0 + \frac{b^3}{12a}, & \text{if fractured}
\end{cases}
\]

- \(k_0\): the reference permeability (m\(^2\))
- \(\varphi_0\): the initial porosity (-)
- \(\varphi\): the porosity (-)
- \(b\): the fracture aperture (m)
- \(a\): the element width (m)
3. Single-phase flow models: Quintessa

- In this model, gas transport through the system is modelled using Richards’ equation.

\[
\frac{\partial}{\partial t} (\theta_g \rho_g) = -\nabla \cdot (\rho_g q_g)
\]

\(q_g\) is the Darcy flux vector (m/s), where

\[
q_g = -\frac{k_g}{\mu_g} \left( \nabla P_g + \rho_g g \nabla z \right)
\]

- The gas permeability and gas porosity are made up of capillary(cap) and micro-scale deformation(creep) components:

\[
k_g = k_{cap} + k_{creep}
\]

\[
\theta_g = \theta_{cap} + \theta_{creep}
\]

\[
r = \begin{cases} 
  r_0 + \gamma (\sigma_c (P_g, \sigma_{total}) - \sigma_{c0}), & \sigma_c > \sigma_{c0} \\
  r_0, & otherwise
\end{cases}
\]

- \(\theta_g\): the volume fraction of the gas (-)
- \(\rho_g\): the density of gas (kg/m³)
- \(q_g\): the Darcy flux vector (m/s)
- \(k_g\): the intrinsic permeability for gas (m²)
- \(\mu_g\): the gas viscosity (Pa·s)
- \(P_g\): the gas pressure (Pa)
- \(\rho_g\): the gas density (kg·m⁻³)
- \(g\): the acceleration due to gravity (m·s⁻²)
- \(z\): the elevation (m)
- \(r_0\): the reference capillary radius (m)
- \(\gamma\): the capillary compressibility (mPa⁻¹)
- \(\sigma_c\): the excess stress for capillary opening (Pa)
- \(\sigma_{total}\): the total stress of the system
- \(\sigma_{c0}\): the reference pressure for capillary opening (Pa)
Results & Discussion
Experimental data

- Experimental data can be summarized by four key components:
  
  (i) quiescence phase
  
  (ii) gas breakthrough
  
  (iii) peak value
  
  (iv) a negative decay

Fig. 8. The radial stress of Test-1

Fig. 9. The radial stress of Test-2
Test-1 results

Fig. 10. Experimental versus numerical radial stresses with different teams
There are three times gas breakthrough events from the experimental data. But most models only predict a single breakthrough event. Hence, comparing the numerical predictions with the experimental results fairly is difficult since it is not obvious which of the experimental breakthroughs are best for the comparison.
Different codes and different test geometries have been used by the teams which makes it difficult to compare results directly across the teams.

Model comparison is extremely difficult due to significant differences in the number of parameters that need to be calibrated in each model.

These differences lead to models with very different degrees of freedom, and thus their fair comparison is a very complex task. This paper just want to summarize and show the outcomes of different models.
Conclusions
Seven different numerical models have been developed to simulate both Test-1 (1D gas flow) and Test-2 (spherical 3D gas flow). However, none of the models describe the full complexity of the physical processes observed in these experiments.

Only two models considered heterogeneous distributions of material properties. However, it needs to be further explored and analyzed since it might provide one possible route to represent localization of flow.

The models need to be up-scaling, since only experiments under controlled laboratory conditions were modelled, models that are tractable at repository scales are needed.
Thank you for your attention.