Modeling of the CO₂ Plume

Ramon Carbonell

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CIUDEN: Spanish government foundation to promote, among other things, Carbon Capture and Storage

MUSTANG: EU 7th FP project: “A MUltiple Space and Time scale Approach for the quaNtification of deep saline formations for CO2 storagE” (2009-2013)

Hontomin is the Tech Demonstration Plant of the Compostilla OXYCFB300 EEPR project, run by ENDESA, in collaboration with CIUDEN and FOSTER-WHEE LER

EEPR “European Energy Programme for Recovery” facilitates investments on infrastructure and technology projects in the energy sector; helps improve the security of supply of the Member States and, promotes implementation of the 20/20/20 objectives for 2020.

CSIC is the “Spanish Agency for Scientific Research”, a network of research institutes.
The Players

The Research Team:
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Main issues

- Movement of the CO₂-rich phase within the geological formations (long-term sequestration).
- Understanding of different mechanisms of trapping: structural, capillary, solute and mineral.
- CO₂ dissolution into the aqueous phase (brine) (solute trapping: ideally as bicarbonate, but also carbonic acid).
- Interaction between these solutes and minerals, and the ability of the geological formation to neutralize the solution and mineralize the CO₂.
- Coupled hydro-mechanical effects (porosity and permeability changes) caused by the evolution of fluid pressures during and after CO₂ injection.
- Management of CO₂ at surface and injection strategies.
Objectives

- Development of numerical, analytical and semi-analytical tools.

- Design and planning of characterization tests (hydro-thermo-chemical-mechanical) and CO₂ injection tests that will be undertaken at the Technological Demonstration Plant (TDP) of Hontomín.

- Interpretation of characterization tests:
  - Knowledge of chemical and structural composition, heterogeneity of the geological formations.
  - To know the porosity changes.
  - To determine the hydraulic connectivity between reservoir and caprock.
  - To know the dynamics of CO₂ migration within the reservoir.
  - Hydro-mechanical response of the system: evolution of pressures in the reservoir as CO₂ is injected; mechanical resistance of caprock; risks of leakages.
  - To know if the CO₂ will be effectively trapped.

- Modeling also can contribute to the development of CCS integration models (capture-transport-storage), and new technologies (e.g., injection strategies to improve the efficiency in the short term and the effectiveness in the long term.)
Methodology (tools)

- Thermodynamics of CO₂ (gas, liquid and supercritical states) and brine.
- Thermodynamics of multi-component gaseous mixtures (EoS, fugacity coefficients, equilibrium constants).
- Analytical solutions and non-local formulations (both in time and space), upscaling: MRMT, R-MRMT.
- Use of existing codes
  - INVERT
  - TRANSIN
  - CODE_BRIGHT
  - RETRASO
  - COGERE
  - KRINET
Key issues

• Fluid mechanics (hydraulic) issues
  – Basic description
  – Scoping calculations for: Pressure impact (magnitude and extent) and CO2 bubble
  – Hydraulic characterization. Preferential flow paths

• Geo Chemical issues (coupled to hydraulic)
  – CO2 Dissolution and fingering
  – Mineral dissolution (and precipitation?)

• Mechanical issues
  – Stability
  – Microseismic activity

• Hontomin
CO2 supercritical?

**CO₂ phase diagram**

- **Subcritical** = abrupt phase change
- **Supercritical** = smooth phase change
- **Critical point**
- **Triple point**

The diagram shows the phase transitions of CO₂ as a function of temperature and pressure. The storage conditions are indicated by the blue arrow pointing to the supercritical region.
CO2 supercritical?

- For high P, high densitylow compressibility (like a liquid)

- For low P & T, low density & high compressibility (like a gas)
Buoyancy and flow

Deep aquifer (more than 1 km)
Typically with salt water/brine

$\text{CO}_2$
Scoping calculations: Regional pressure buildup

Most of the pressure build-up is associated to the resistance of water to be displaced

\[ \Delta P = \frac{Q}{2\pi T} \ln \frac{2.25Tt}{SR^2} \]

\[ R_{\text{inf}} = \sqrt{2.25Tt / S} \]

- \( Q \) - Volumetric flow rate (m\(^3\)/s)
- \( T \) - Tranmissivity (m\(^2\)/s) = \( K_b \)
- \( b \) - Aquifer thickness (m)
- \( K \) - Hydraulic conductivity (m/s) = \( k \rho g / \mu = 10^7 k \)
- \( k \) – permeability (m\(^2\))
- \( S \) – Storage coefficient
Scoping calculations: Regional pressure buildup

Most of the pressure build-up is associated to the resistance of water to be displaced

\[ \Delta P = \frac{Q}{2\pi T} \ln \frac{2.25Tt}{SR^2} \]

\[ R = \sqrt{Tt / S} \]

\[ R = \sqrt{10Tt / S} \]

\[ R_{\text{inf}} = \sqrt{2.25Tt / S} \]
Scoping calculations (regional): the bad news
Pressure buildup and Radius of influence

Assume a 1Mt/year injection rate

If compressible and permeable formation (k=10^{-12} \text{ m}^2, Ss=10^{-5} \text{ m}^{-1})

<table>
<thead>
<tr>
<th>t (days)</th>
<th>10 days</th>
<th>30 years</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rinf (km)</td>
<td>1.39</td>
<td>46.1</td>
</tr>
<tr>
<td>\Delta P (bar) (r=100m)</td>
<td>1.69</td>
<td>3.94</td>
</tr>
</tbody>
</table>

Large region affected
Risk brine migration

If low compressibility and permeability formation (k=10^{-14} \text{ m}^2, Ss=10^{-6} \text{ m}^{-1})

<table>
<thead>
<tr>
<th>t (days)</th>
<th>10 days</th>
<th>30 years</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rinf (km)</td>
<td>0.44</td>
<td>14.6</td>
</tr>
<tr>
<td>\Delta P (bar) (r=100m)</td>
<td>95.2</td>
<td>320</td>
</tr>
</tbody>
</table>

Unbearable pressure

Observations:
1) Characterization (geologic and hydraulic) needed
2) Very likely, brine pressure control will be needed

But, do not go away yet!
Cause (and solution) of scale effects

Large scale permeability, which is derived from hydraulic tests, is controlled by large fractures.

The effective permeability of every well depends on whether or not a conducting fracture is intersected. Chances of hitting a subvertical fracture are low.

Wells act as if they were poorly built.

Solution: Long horizontal wells
Low viscosity

CO₂ viscosity is some 10-20 times smaller than water.

Water viscosity 0.001 Pa·s

Pure CO₂ viscosity (Pa·s)
Viscous fingering
Viscous fingering
Fingering increases by superposition of buoyancy and viscosity effects

Diogo
R-MRMT and MRMT-R

1. Mixing induces reaction

2. The presence of mobile and immobile zones induces mixing

3. To take into account reaction induced by mixing: R-MRMT (Reactive Multi Rate Mass Transfer)
Application: Upscaling of reactive transport processes in heterogeneous media

(A) Distribution of reaction rates and concentration of conservative component. (B) Comparison between a 2D heterogeneous model and a 1D effective model of MRMT-R.

Scale effects in a system with a binary reaction of dissolution-precipitation equilibrium.: (A) Distribution of reaction rates and concentration of conservative component. (B) Comparison between a 2D heterogeneous model and a 1D effective model of MRMT-R.
Application: Upscaling of multi-phase flow in heterogeneous media
CODE_BRIGHT: 3D simulation of CO$_2$ injection at 1 kg/s into an aquifer with a slope of 5° (injection during 6 days)

0.2 days of injection

21 days after the end of injection
CO₂ buoyancy effect causes a migration of the CO₂ bubble upwards, specially after injection stop.

Gravitational forces dominate over viscous forces.

21 days after the end of injection
CO2 rich brine fingering

(\(\text{CO}_2\) rich brine is denser and sinks in native brine)
Scoping calculations on dissolution rate
Scoping calculations on dissolution rate and onset of advection

\[ m_s \approx 35u_b \Delta \rho \omega_s \]

\[ u_b = \frac{k \Delta \rho g}{\mu} \]

\[ t' = \frac{u_b}{\phi L_s} t \]

\[ b_L = \frac{\alpha_L}{L_s} \]

\[ L_s = \frac{\theta D_m + \alpha_L u_b}{u_b} \]

\[ \mu = 5.00E-04 \text{ Pa} \cdot \text{s} \]
\[ \Delta \rho = 25 \text{ kg/m}^3 \]
\[ k = 1.00E-12 \text{ m}^2 \]
\[ u_b = 4.90E-07 \text{ m/s} \]
\[ \omega_s = 2.50E-02 \]
\[ m_s = 1.07E-05 \text{ kg/m}^2/\text{s} \]

0.34 Mt/km2/yr

\[ \alpha = 10 \text{ m} \]
\[ L_s = 10 \]
\[ \phi = 0.1 \]
\[ t_{onset} = 6.58 \text{ yrs} \]

Dissolution can be very significant after a few years (which prevents further pressure buildup)

Challenge: reduce the time for the onset of advection (increase dispersion: viscous and capillary fingering, fluctuating injection)
Chemical interactions

• CO2 saturated brine will be very aggressive (pH around 3)
• This will cause:
  – Mineral dissolution
  – Partial neutralization of acidity (further solubility of CO2)
  – Depending on mineralogy of the rock and chemistry of the brine, other minerals may precipitate (e.g., if brine is rich in sulphate and rock rich in cacite, anhidrite will precipitate)
• Mineral dissolution increases the permeability of the rock
Core photos prior to and (left) and after (center) injecting a CO2 rich solution and tomographic image (right). (Wormholes)
Pressure build up in the CO2 bubble and surrounding brine may compromise mechanical stability of the cap rock and its isolating properties.
Uplift of 5 mm/yr in In Salah (Rutqvist et al., 2010, IJ GGC)

Microseismicity due to CO₂ leakage around wells in Otsego County, Michigan Basin, USA (Bohnhoff et al., 2010, IJ GGC)
Pressure buildup

Injection pressure at the top of the aquifer for a 1000 day injection period, for two intrinsic permeabilities of the aquifer. Injection pressure drops because of the lower CO$_2$ viscosity with respect to that of brine.
Fluid overpressure for a 100 days injection period, comparing pure hydraulic (H) with coupled hydromechanical (HM) simulation in and

- (a) the aquifer at the contact between the aquifer and the caprock 400 m from the injection well
- (b) in the caprock 50 m above the aquifer and 50 m away the injection well.
Stress and pressure evolution with time at the beginning of CO$_2$ injection at the base of the caprock next to the injection well (see location in inset).
A vertical section of the caprock in the vicinity of the well, with the deviatoric stress, $q$, and critical the deviatoric stress, $q_{\text{critic}}$, after 4 days of injection. Note that $q$ exceeds $q_{\text{critic}}$ in the contact between the caprock and the aquifer, thus causing the caprock to plastify.
{(q, p')} trajectory for a 100 day injection. The initial and final states are represented by A and D, respectively. The onset of plasticity takes place during early times (B-C), but plastic behavior eventually stops.
Hydro-mechanical coupling

Evolution of deformations and CO₂ saturation

Caprock plasticize as the CO₂ migrates (for a caprock relatively weak)

Plastic region propagates in a direction of 45°

Plastic deformations stabilize after 5 days of injection
Plastic strain \((EDP)\) in the caprock (left) and liquid saturation degree, \(S\), in the aquifer (right) for different injection times. Plastic strain propagates as \(CO_2\) advances at the beginning of injection.
$M = 0.6$  \hspace{1cm} $t = 1.10703 \text{ d}$
$M=0.4$  \quad t=1.09063 \text{ d}
Summary hydromechanical coupling

- Pressure buildup bounded
- HM coupling needed
- Shear conditions worst at the beginning
- Partially monitorable by measuring pressures at cap rock.
- Work on-going
In summary

- Low density and viscosity
- High solubility
- Geochemistry
- Potential mechanical coupling
- Capillary effects
- Thermal effects
- Buoyancy
- Viscous fingering
- Gravity fingering
- Chemical fingering
- Seal Rock failure risk
- Migration of CO2 and/or brine
- and, CCS expensive

The Hontomin challenge:
¿Can we understand all this qualitatively?
¿Can we take advantage of these “problems” to reduce costs?
Key issues

**Reduce costs**
- Reduce Energy:
  - Permeability how much?, how to increase it?
- Increase storage capacity
  - How much, how to increase it?

**Reduce requirements**
- Purity of CO2?
- Increase safety
- Improve social acceptance

**Tool: Increase understanding**
Key parameters

**Permeability:** Controls

- Effective: Buildup of injection pressure
- Vertical: Rate of fingering (dissolution)
- Connection: Migration of brine
- Seal: vertical migration through seal
  (But also entry pressure)
Key parameters

**Porosity**: Controls

- Storage capacity
- Porosity increase may increase permeability
- But affect mechanical properties
Key parameters

**Reactivity:** Controls
Porosity and permeability variations
State of CO2
Key issues

**Mechanical properties:** Control
Compressibility: storage capacity
Long term safety
Social perception
Water Injection-extraction

1. Pumping (Quita)

1. Pumping tests = 0.1-10L/s
2. Pumped water needs to be stored (conditioning and storage of up to 10000 m3)
3. Monitor drawdowns at all intervals to obtain Klocal, Keff, Kvert, and S. Also monitor deformation (but expect little).
Water Injection-extraction

2. Injection ("y pon")

1. Add tracer (and biocide)
2. Inject traced water
3. Rest
4. Extract water and monitor tracer(s) breakthrough. To obtain porosity structure, reactivity.
5. Repeat varying nature of tracers (conservative and reactive) and $T$
6. Repeat varying injection volume and rest time.
CO2 push-pull (Mete-saca) test

1. Inject CO2 (and gaseous tracers). Some 100 t of CO2
2. Electrical and thermal (heating) tests
3. Extract gas and evaluate mass of CO2 and concentration of gaseous tracers
4. Electrical and thermal tests
5. Informs about trapping mechanisms (specifically contact area and capillary trapped CO2)
High pressure (and flow rate) injection test ("apretón")

- Inject a high flow rate at a very high pressure (some 100 bar at surface)
- Observe pore fluid pressure, rock deformation and possible microseisms
Hydro-mechanical coupling during “apretón”

As fluid pressure increases, the seal bends

P goes up immediately

At first, P drops
Heating test ("calentón")

- Heat up the heater along the whole borehole
- Observe temperature buildup
- Deduce thermal capacity and conductivity
- Deduce presence of CO2 (either continuous phase during injection tests, or capillary trapped during CO2 "metesaca")
CO2 injection tests

- Conventional
- Fluctuating flow rate
- Liquid CO2 injection
- Others
Disolución en la base del penacho da lugar a celdas de convección en la salmuera

La base del penacho será una fiesta (disolución de CO2, convección de salmuera, dis-precip mineral....)
Thanks for your attention