Geochemical Model of CO2 impact at the Well-Caprock-Reservoir interfaces.
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INTERFACE CO$_2$-Mechanisms - Agenda

> Introduction
  - Objectives

> Modeling Approach
  - Considered Scenario
  - Modeling tool
  - Geometry and Gridding

> Results – Discussion
  - Illustration Parisian Basin
  - Cement Alteration Mechanisms

> Conclusions
  - Limitations and Perspectives
INTERFACE CO$_2$-Mechanisms - Objectives

> **Modeling** Geochemical interactions due to CO$_2$ injection at the Well-Reservoir-Caprock INTERFACE

- Characterization of reactions pathways
- Identification of new resulting minerals
- Chemical stability of cement-caprock interface
- Consequences in Porosity Evolution of the 3 zones
Modeling Approach - Scenario

> Injection Well cement alteration due to *acid brine only*
  > CO₂ Injection downhole ⇒ Reservoir Brine acidification

> Diffusion only of HCO₃⁻ and H⁺ (from CO₂aq), *no flow, no gas phase*
  > Cement degradation due to brine contact
  > Cement leaching due to caprock contact

> Code Used: **ToughReact**
  * (finite volumes)

> 1m*2m-scale *axisymmetric* model
  * 2753 cells
  * ΔR = ΔZ = 2 mm at the interface
  * Δt = 9 sec for kinetic convergence reasons
Illustration: Parisian Basin context

Initial state, equilibrated water at $t=0$ and at the 2 Limit Conditions border-Cells ($LC_{\infty}$)

<table>
<thead>
<tr>
<th>In-Situ Minerals</th>
<th>Formula</th>
<th>Composition (% Vol)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Dogger</td>
<td>Callovo-Oxfordian clays</td>
</tr>
<tr>
<td>Calcite</td>
<td>CaCO$_3$</td>
<td>77.5%</td>
</tr>
<tr>
<td>Dolomite</td>
<td>CaMg(CO$_3$)$_2$</td>
<td>10.2%</td>
</tr>
<tr>
<td>Illite-Mg</td>
<td>$K_{0.85}Mg_{0.25}Al_{2.35}Si_{3.4}O_{10}(OH)_2$</td>
<td>0.1%</td>
</tr>
<tr>
<td>Quartz</td>
<td>SiO$_2$</td>
<td>-</td>
</tr>
<tr>
<td>Mg-Montmorillonite-Na</td>
<td>$Na_{0.33}Mg_{0.33}Al_{4.67}Si_{3.67}O_{10}(OH)_2$</td>
<td>5.8%</td>
</tr>
<tr>
<td>Siderite</td>
<td>FeCO$_3$</td>
<td>4.1%</td>
</tr>
<tr>
<td>Kaolinite</td>
<td>$Al_{2}Si_{2}O_{5}(OH)_4$</td>
<td>2.0%</td>
</tr>
<tr>
<td>Magnesite</td>
<td>MgCO$_3$</td>
<td>0.3%</td>
</tr>
<tr>
<td>Pyrite</td>
<td>FeS$_2$</td>
<td>-</td>
</tr>
<tr>
<td>Chamosite</td>
<td>$Fe_5Al_2(AlSi_4)O_{10}(OH)_8$</td>
<td>-</td>
</tr>
<tr>
<td>Celestite</td>
<td>SrSO$_4$</td>
<td>-</td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>Class_G Cement</th>
<th>Formula</th>
<th>Composition (% Vol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CSH$_{1.6}$</td>
<td>$Ca_{1.6}SiO_{3.6}:2.58H_2O$</td>
<td>38.1%</td>
</tr>
<tr>
<td>Portlandite</td>
<td>Ca(OH)$_2$</td>
<td>26.1%</td>
</tr>
<tr>
<td>Ettringite</td>
<td>$Ca_6Al_2(SO_4)<em>3(OH)</em>{12}:26H_2O$</td>
<td>13.8%</td>
</tr>
<tr>
<td>Katoite_Si1</td>
<td>$Ca_3Al_2SiO_4(OH)_8$</td>
<td>10.5%</td>
</tr>
<tr>
<td>C3FH6</td>
<td>$Ca_3Fe_2(OH)_{12}$</td>
<td>5.5%</td>
</tr>
<tr>
<td>Hydrotalcite</td>
<td>$Mg_4Al_2O_7:10H_2O$</td>
<td>5.4%</td>
</tr>
<tr>
<td>Calcite</td>
<td>CaCO$_3$</td>
<td>0.6%</td>
</tr>
</tbody>
</table>

180 bar, 75°C, Salt = 25g/kg$_w$
Results: triple point cement alteration

- Katoite: Si$_1$Ca$_3$Al$_2$SiO$_4$·(OH)$_8$
- Amorphous Silica, hydrated SiO$_2$·0.5H$_2$O
- Ferrihydrite Fe(OH)$_3$
- CSH1.6: Ca$_{1.6}$SiO$_{3.6}$·2.58H$_2$O
- CSH1.2: Ca$_{1.2}$SiO$_{3.2}$·2.06H$_2$O
- CSH0.8: Ca$_{0.8}$SiO$_{2.8}$·1.54H$_2$O
- C3FH6: Ca$_3$Fe$_2$(OH)$_{12}$
- Calcite: CaCO$_3$
- Portlandite: Ca(OH)$_2$
- Ettringite: Ca$_6$Al$_2$(SO$_4$)$_3$(OH)$_{12}$·26H$_2$O
- Hydrotalcite: Mg$_4$Al$_2$O$_7$·10H$_2$O

- Increase due to neighbor dissolution
- Increase due to neighbor dissolution
- Increase due to neighbor dissolution
- Constant calcite increase limited by HCO$_3^-$ diffusion
- Straetlingite dissolves and precipitates into CSH gel and boehmite
- CSH-Decalcification
- Al-Gel (Boehmite) AlO(OH)
- Magnesite MgCO$_3$
- Magnesite
- Calcite
- Portlandite
- CSH_1.6
- CSH_1.2
- CSH_0.8
- Silica_am
- Ferrihydrite
Mechanisms Analysis - pH-Buffering and Volumes

> Simplified Reaction pathway:
  - H+ and HCO₃⁻ Diffusion is the limiting factor for the global cement degradation process
  - pH is buffered successively by different mineral phases
  - New created phases should occupy more Volume (%), but
  - Liberated ions also migrate outside the cement

<table>
<thead>
<tr>
<th>Element</th>
<th>pH</th>
<th>11 (initial)</th>
<th>10.7</th>
<th>10.5</th>
<th>10.4</th>
<th>10.3</th>
<th>10.2</th>
<th>9.7</th>
<th>9</th>
<th>7.7</th>
<th>5.5 (final)</th>
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<td>Ca</td>
<td>Portlandite</td>
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</tr>
<tr>
<td>Si</td>
<td>CSH1.6</td>
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<td></td>
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<tr>
<td>Fe</td>
<td>C3FH6</td>
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<tr>
<td>Al</td>
<td>Katoite_Si1</td>
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</tbody>
</table>

- Calcite (+11.71%)
- Silica_am, hydrated (+13.92%)
- Ferrihydrite (+16.19%)
- Calcite
- Straetlingite (+93.27%)
- Boehmite (+17.51%)
- Magnesite (+3.11%)
System Evolution after 3 months (Ref Case)

Porosity collapses on cap rock side due to Calcite Precipitation

Calcite precipitation at the cement-clay interface due to Ca$^{2+}$ migration

Caprock

Acidified Reservoir

Calcite CaCO$_3$

Portlandite dissolution in the interface-destabilized cement

Calcite precipitation in the interface-destabilized cement
INTERFACE CO$_2$-Mechanisms - Conclusions

> **Determination of conceptual reaction pathway**
  - Possibility to extract simplified scheme to use it in a Poro-Mechanical study (part of the Project)

> **Sensibility Analysis done on the cement tortuosity**
  - Variation of the Damkholer Number (here diffusion/kinetics)

> **Limitations of the model:**
  - Cement carbonation produces a lot of H$_2$O (not considered in the mass/volume balance)
  - Gas phase not considered (some experiments show a stronger effect of wet CO$_2$ than acidified brine)
  - No heterogeneities