Scientific Achievement
Developed RTM to assess impacts of carbonates reaction on density-driven CO₂ dissolution in brine.

Significance and Impact
The RTM results show that density increase due to carbonates dissolution causes significant enhancement in CO₂ dissolution; however no significant porosity and permeability alterations are observed.

Research Details
- The reactive transport model ignores the two phase region and considers carbonates reactions due to CO₂ dissolution in brine.
- We tested both homogeneous and heterogeneous cases with low and high mean permeability in term of Ra number.

Concentration maps of Ra = 10,000, layered heterogeneous case; (a,c,e and b,d,f) show results of with and without reactions, respectively.

Reactive Transport Modeling

Chemical reactions

\[ \text{OH}^- = \text{H}_2\text{O} - \text{H}^- \quad \text{CO}_2 (\text{aq}) = \text{HCO}_3^- + \text{H}^+ - \text{H}_2\text{O} \]

\[ \text{CaHCO}_3^+ = \text{Ca}^{+2} + \text{HCO}_3^- \quad \text{MgHCO}_3^+ = \text{Mg}^{+2} + \text{HCO}_3^- \]

\[ \text{CaCO}_3 \text{ [calcite]} = \text{H}^+ + \text{Ca}^{+2} + \text{HCO}_3^- \]

\[ \text{CaMg(CO}_3)_2 \text{ [dolomite]} = \text{Ca}^{+2} + \text{Mg}^{+2} + 2\text{HCO}_3^- - 2\text{H}^+ \]

- A sequential approach is used
- All required thermodynamics data are obtained from database file of PFLOTRAN

Data used in simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (°C)</td>
<td>60</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>100</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.20</td>
</tr>
<tr>
<td>Permeability (mD)</td>
<td>10 or 100</td>
</tr>
<tr>
<td>Diffusivity (m^2/s)</td>
<td>$4.5 \times 10^{-3}$</td>
</tr>
<tr>
<td>Viscosity (Pa.s)</td>
<td>0.001</td>
</tr>
<tr>
<td>Species</td>
<td>Initial concentration (mol/L)</td>
</tr>
<tr>
<td>CO_2(aq)</td>
<td>0.0001</td>
</tr>
<tr>
<td>H^+</td>
<td>$1.148 \times 10^{-4}$</td>
</tr>
<tr>
<td>OH^-</td>
<td>$0.8711 \times 10^{-4}$</td>
</tr>
<tr>
<td>HCO_3^-</td>
<td>0.0073</td>
</tr>
<tr>
<td>CaHCO_3^+</td>
<td>$1.789 \times 10^{-4}$</td>
</tr>
<tr>
<td>MgHCO_3^+</td>
<td>$3.878 \times 10^{-5}$</td>
</tr>
<tr>
<td>Ca^{+2}</td>
<td>0.0022</td>
</tr>
<tr>
<td>Mg^{+2}</td>
<td>$4.89 \times 10^{-4}$</td>
</tr>
</tbody>
</table>
Modeling results (1/3)

Concentration maps for homogeneous case

\[ Ra = 1000 \]

\begin{align*}
\text{With Rxn} & \quad \text{No Rxn} \\
(a) 20 \text{ years} & \quad (a) 20 \text{ years} \\
(c) 100 \text{ years} & \quad (c) 100 \text{ years} \\
(e) 900 \text{ years} & \quad (e) 900 \text{ years} \\
\end{align*}

\[ Ra = 10000 \]

\begin{align*}
\text{With Rxn} & \quad \text{No Rxn} \\
(a) 20 \text{ years} & \quad (a) 20 \text{ years} \\
(c) 100 \text{ years} & \quad (c) 100 \text{ years} \\
(e) 600 \text{ years} & \quad (f) 600 \text{ years} \\
\end{align*}

- Plumes with reactions move downward faster than without reactions.
- With a higher \( Ra (=10,000) \), plumes move faster downward and also initiated convection.
Modeling results (2/3)

Concentration maps for heterogeneous case

\[ Ra = 1000 \]

\[ Ra = 10000 \]

- Plume development hopf-bifurcation of the cells
Modeling results (3/3)

Average concentrations

to quantify saturation area of the aquifer

\[
\bar{c} = \frac{\int_{0}^{1} \int_{0}^{1} c(x, z, t) \, dx \, dz}{\int_{0}^{1} \int_{0}^{1} \, dx \, dz}
\]

Change in porosity

Average concentrations of dissolved CO₂ in the reservoir for the case of \( Ra = 10,000 \)

For \( Ra = 10,000 \), heterogeneous case

\[
k = k_0 \left( \frac{\phi}{\phi_0} \right)^3 \left( \frac{1 - \phi}{1 - \phi_0} \right)^2
\]

Permeability change is 0.06% which is also too small to instable fluid flow further